Quantum Criticality, Magnetic Frustration, and Unconventional Superconductivity in Heavy Fermion Metals

by

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A Thesis Submitted in Partial Fulfillment of the Requirements for the Degree

Doctor of Philosophy

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Houston, Texas
April 10th, 2014
Abstract

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Rare earth and actinide metal compounds have emerged as quintessential systems to experimentally and theoretically explore zero temperature quantum phase transitions. These so called heavy fermion metals provide a platform to systematically study physics on the edge of our understanding, where conventional approaches fail to describe the experimental observations. In this thesis, we are concerned with the theoretical description of the different types of quantum phases and phase transitions that are possible within heavy fermion metals.

We first focus on understanding the unconventional quantum critical scaling properties observed in heavy fermion metals. Guided by the extended dynamical mean field theory (EDMFT) of the Kondo lattice, we study the physics of Kondo destruction in simplified quantum impurity models. Using the continuous time quantum Monte Carlo (CT-QMC), we show Kondo destroyed quantum critical points (QCPs) give rise to local correlation functions that obey frequency and magnetic field over temperature scaling, and have a linear in temperature relaxation rate. Our results are consistent with the experiments on the quantum critical heavy fermion metals YbRh$_2$Si$_2$, CeCu$_{6-x}$Au$_x$, and $\beta$-YbAlB$_4$. 
Motivated by experiments on CeRhIn$_5$ and related heavy fermion systems, we then focus on the superconducting properties of the Kondo destroyed QCPs. We introduce and solve an effective model that has both Kondo destruction and pairing correlations, using a combination of CT-QMC and the numerical renormalization group (NRG) methods. We then solve the cluster EDMFT equations across the QCP for two and three dimensional magnetic fluctuations, using the CT-QMC as the cluster solver. In the two dimensional case, we find that the Kondo screening is driven critical at the antiferromagnetic QCP. In each case studied, we find that the pairing susceptibility is strongly enhanced in the vicinity of the QCP. Our results point to the exciting possibility of an unconventional superconducting pairing mechanism, which results from Kondo screening being driven critical on the border of antiferromagnetic order.

We then proceed to study the effect of magnetic frustration on heavy fermion metals by considering the Shastry Sutherland Kondo lattice model. We solve the model within a large $N$ mean field approach. Our results are particularly pertinent to the frustrated heavy fermion metals Yb$_2$Pt$_2$Pb and YbAl$_3$C$_3$, of which both realize VBS ground states despite being metallic. Our results represent a significant step forward in constructing a global phase diagram of heavy fermion metals.
This work is dedicated to the Pixley and Coburn families for giving me the opportunity to follow my dreams.
I would first like to thank my PhD adviser Qimiao Si, who has been guiding me along this exciting research path. Despite me being a young graduate student stumbling my way through research, Qimiao has always treated me as an equal. His kind, patient, and insightful approach to mentoring has taught me how to become an independent theoretical physicist, allowing me to develop the technical tools I need and giving me the freedom to explore some of my own ideas and collaborations. In addition, Qimiao has given me the opportunity to present my research at various conferences and collaborate with scientists all over the world. Not only has Qimiao been an excellent adviser but has also become a mentor and a friend, his guidance and intuition has proven invaluable throughout my graduate career and for this I am truly thankful.

I would like to thank my collaborators who have come through Rice University Mártın Kormos, Adilet Imambekov, Rong Yu, Pallab Goswami, and Ang Cai, as well as Kevin Ingersent and Lili Deng at the University of Florida. I would also like to thank Stefan Kirchner for all of his guidance and mentorship, for the many trips to Dresden, Germany, and collaborations at the Max Planck Institute for the Physics of Complex Systems. Each trip to Dresden, Germany, was as life changing as the last, these experiences have helped me become the man I am today. I would like to thank Andriy Nevidomskyy for his collaborations and many discussions, which always help remind me how much I enjoy doing physics. I would also like to thank Matthew Foster for serving on my PhD committee, as well as for everything he has taught me inside and outside of the classroom. I would also like to thank Emil Nica, Jianda Wu, Zhentao Wang, Yang-Zhi Chou, Hong-Yi Xie, and Wenxin Ding for numerous discussions and for making my time in the condensed matter theory group at Rice University very enjoyable. Lastly, I would also like to thank Gustavo Scuseria for being on my PhD committee and helping me improve the quality and readership of this thesis.

I would like to thank my close friends I have had the luck of getting to know in Houston, Texas. My time here wouldn’t have been the same without J. J. Thomson, Lindsey Anderson, Brian DeSalvo, Eva Dyer, Sara Haber, Marcel LaFlamme, Karen Rosenthal, Josh Rueckheim, Aditya Shashi, and Alex and Eli Witus. Having the opportunity to be close friends and go through the training to be a theoretical physicist with
Aditya Shashi has been invaluable to me, I look forward to his insights and friendship for a long time to come. From establishing “The Institute” many years back to its utter destruction, which then lead to the birth of the “Bakery” (like a phoenix rising out of the ashes), Brian DeSalvo has been an excellent friend, housemate, confidant, and all around stand up guy. I would like to thank my friends from long ago that continue to have an impact on my life T. C. Calhoun, Sam and Britton Douglass, Ian Evarts, Jack Kellames, and Zack Walter. I would also like to thank my college friends Josiah Failing, Glenn Grey, Chris Meyer, Dan Nagy, Leo Ronin, Alex Wang, Cameron Wong, and Arla Yost for their continuing support. Lastly, I would like to thank all of my close friends far and wide for helping me get back up after I get knocked down because we all fall down sometimes.

I would never have made it to where I am today without the continual love, guidance, and support of my family. Not only have my parents always pushed me to follow my passions they have helped me however they can. My mother Janice Pixley has always helped nurture my creative spark, while helping me develop a deep love for learning. She has always helped me believe in myself no matter the odds. My father John Pixley helped expose me to the beauty of science at a young age. He has taught me the true meaning of hard work and what it means to be a respectable man. I would like to thank my brother Aaron Pixley for helping me discover a love for academics and for his help in following this passion even though it takes one very far from the beaten path. My brother has taught me the true meaning of courage, his influence and friendship have been and will continue to be invaluable throughout my life.

In the past three years of my life I have been lucky enough to get to know and fall in love with Sara Haber. Sara is incredibly supportive in all of my different endeavors, she is always ready to help me think through any issue, or even help me make nice figures (such as figures 1.1 and 1.2 in this thesis). Sara’s loving, carefree, beautiful, and genuine spirit help remind me of what happiness should be like, what I am looking for in life, and the man I am trying to become. She is my best friend, my better half, and I love her for this. For these reasons and many more I would like to thank Sara for helping me along this journey and for continuing to make it so much more wonderful.
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5.13 Summary of the pairs of bath exponents $(r, s)$ studied in this work. Results for $r = 0$ describe a metallic conduction band, while those for $r > 0$ correspond to pseudogapped problems. Squares, triangles, and circles respectively correspond to quantum criticality of the F, B, and M types, as described in the text. Filled symbols summarize NRG results for the BFK model while open symbols represent CT-QMC results for the BFA model. Solid lines show the conjectured boundaries $s = 1 - 2r$ and $x_B(s) = s = x_F(r)$ between the different types of criticality.

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6.1 Division of the lattice into $N/N_c$ clusters, of size $N_c = L_c^2$. The vector $\mathbf{r}$ labels each cluster, while sites within the cluster are labelled by $\mathbf{R}$. Interactions are divided into within the cluster $J_c$ and between clusters $\delta J$, (which is also done for the hopping elements $t_c$ and $\delta t$.) We have omitted the channel index $\alpha$ for clarity.

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7.1 Schematic representation of the two-impurity Bose-Fermi Anderson models considered in this work. The impurity spins interact via a direct exchange coupling $I$ (or $I_z$ for Ising exchange), and the difference of their $z$ components couples with strength $g$ to a dissipative sub-Ohmic bosonic bath having dispersion $\omega_q$. For very large impurity separation, each impurity effectively hybridizes with strength $V$ with its own conduction band of dispersion $\epsilon_k$. 
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7.4 Schematic RG flow on the $g-I_z$ plane for the two-impurity Bose-Fermi Anderson model with Ising interimpurity exchange $H_{12}$. Trajectories with arrows represent the flows of the couplings ($g$ and $I_z$) with the decrease of energy. There are two stable fixed points, indicated by filled circles, which govern the Kondo-screened (Kondo) phase and the local-moment (LM) phase. The Kondo fixed point is at $(g, I_z) = (0, 0)$, while the LM fixed point is at $(g, I_z) = (\infty, 0)$. On the phase boundary, the RG flow is from the Kosterlitz-Thouless (KT) fixed point toward the Kondo-destruction (KD) fixed point. The KT and KD fixed points are both unstable and are shown by open circles. The direction of the RG flow on the phase boundary reflects the discussion in the text, i.e., all the points for nonzero $g$ on the phase boundary have the same critical behavior as the KD QCP on the $g$ axis.

7.5 (a) Binder cumulant $U^s_4(\beta, I_z, g)$ vs $g$ for an Ising $H_{12}$ with $I_z = 1.25D$, $s = 0.8$, and at the labeled temperatures. Error bars come from a jackknife analysis of CT-QMC data. The intersection of curves gives the critical bosonic coupling $g_c/D = 0.465(5)$. (b) A scaling collapse of the same data near $g_c$ according to Eq. (7.4) yields a correlation-length exponent $\nu(s = 0.8)^{-1} = 0.45(8)$. (c) Flow of a low-energy NRG eigenstate vs iteration number $N$ for a Heisenberg $H_{12}$ with $I = 0.2D$, $s = 0.6$, and six values of $\Delta g \equiv 10^6(g - g_c)$, where $K_0g_c = 1.08742545(1)$. (d) Low-energy crossover scale from the NRG, fitted to $T^* \propto |g - g_c|^\nu$ yielding $\nu(s = 0.6)^{-1} = 0.40(2)$.
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7.7 (a) Static singlet pairing susceptibility $\chi_d(T, I_z, g)$ vs $I_z$ for an Ising $H_{12}$ with $s = 0.8$ along the line $g = 0.372I_z$, which crosses the Kondo-LM phase boundary at $I_z^c = 1.25D$. Note that $\chi_d$ saturates for temperatures $T \leq D/250$. (b) Static singlet pairing susceptibility $\chi_d(T = 0, I, g)$ vs $I$ for a Heisenberg $H_{12}$ with $s = 0.6$ along the line $g = 2.54I$, which crosses the Kondo-LM phase boundary at $I_c = 0.40D$. In both (a) and (b), $\chi_d$ is peaked just on the Kondo side of the phase boundary and remains elevated at the QCP over its value for $g = I_z = I = 0$.

8.1 Tiling of the two dimensional Brillouin zone with the two site cluster (a), where the ferromagnetic fluctuations are confined to the zone center [the blue region (+)] and the antiferromagnetic region at the zone corners [the red region (-)]. The magnetic density of states in two dimensions (b) and three dimensions (c) corresponding to the tiling used.
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8.3 Static lattice spin susceptibility at the ordering wave vector $\chi_{\text{AF}}$ and antiferromagnetic order parameter $M_{\text{AF}}$ as a function of the RKKY interaction $I$, for temperatures $T/T_K^0 = 0.0167$ (left plot) and $T/T_K^0 = 0.0111$ (right plot). We see $\chi_{\text{AF}}$ diverging on approach to the thermal phase transition and $M_{\text{AF}}$ jumping at the transition temperature $T_N$, to a finite value, displaying a first order thermal phase transition.

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8.5 Finite temperature phase diagram of the periodic Anderson model solved within a C-EDMFT approach. We find the HFL and the AF phases are separated by a non fermi liquid quantum critical regime. The boundary $E_{\text{loc}}^*$ is a cross over at finite temperature, where as $T_N$ is a finite temperature classical transition. At zero temperature, the two phase boundaries merge at the quantum critical point, and $E_{\text{loc}}^*(T = 0)$ becomes a true transition.
8.6 Local pairing susceptibility in the singlet (left plot) and triplet (right plot) channels. We find the singlet channel is enhanced on approach to and at the QCP, where as the triplet channel is monotonically suppressed.

8.7 Pairing susceptibility across the QCP for two dimensional magnetic fluctuations, showing a large pairing enhancement at the LCP.

8.8 Magnetic order parameter $M_{AF}$ as a function of $I$ for a variety of temperatures (left plot) and the static local spin susceptibility in the ordering channel as a function of $I$, for $3-d$ magnetic fluctuations. We have plotted $\chi_{loc}$ on the same scale as the $2-d$ case, to show the much weaker temperature dependence across the the transition.

8.9 Static local pair susceptibility in the singlet channel across the SDW transition (left plot). Lattice pair susceptibility in the singlet extended s-wave pairing channel (right plot). We find the lattice pair susceptibility is strongly enhanced across the SDW transition, consistent with the notion of quantum critical SDW fluctuations providing the “glue” for cooper pairs [45].

8.10 Momentum dependence of the static spin susceptibility $\chi_{lat}(q, i\omega_n = 0)$ at a temperature $T = 0.0167 T_K^0$ in the full Brillouin zone $-\pi \leq q_x \leq \pi$, and $-\pi \leq q_y \leq \pi$ in the HFL phase (top plot), in the NFL phase (middle plot), and in the AF phase (bottom plot).
9.1 (a) Proposed global phase diagram of heavy fermion metals. Here, \( \text{AF}_S \) and \( \text{AF}_L \) refer to antiferromagnetic states without or with static Kondo screening. \( P_L \) is the paramagnetic heavy Fermi liquid, and \( P_S \) refers to a paramagnetic phase without static Kondo screening. Adapted from ref. [84, 85]. The dashed trajectory is the main focus of this work. 

(b) Shastry-Sutherland lattice, denoting the Heisenberg exchange couplings \( J_1 \) on all the horizontal and vertical bonds, and \( J_2 \) along the diagonals. The unit cell is the dashed square, containing four sites \( A, B, C, D \). 

(c) The bond singlet parameters.

9.2 Large-\( N \) phase diagram as a function of frustration \((J_2/J_1)\) and Kondo coupling \((J_K/t_1)\), for a metallic filling \( n_c = 0.5 \). The phases are described in the main text. The solid lines represent first-order transitions, and the dashed lines surrounding the grey area locate the boundaries of the intermediate phases that exhibit partial Kondo screening (PKS).
9.3 (a) The bond and Kondo singlet parameters at a fixed ratio $J_2/J_1 = 2.0$ as a function of $J_K$, displaying a first order transition from the SSL-VBS to the HFL phase. We have rescaled the parameters so that they are dimensionless and show the three independent quantities for the solution that breaks no lattice translational symmetry. Band structure along high symmetry directions in the reduced Brillouin zone in the SSL-VBS phase with $J_K = 0$ and $J_2/J_1 = 2.0$ (b) and in the HFL phase with $J_K = 2.1t_1$ and $J_2/J_1 = 2.0$ (c). The thick blue lines are the gapped spinon dispersion in the SSL-VBS phase, whereas the other bands are those of the conduction electrons on the SSL. In (c) the bands in the vicinity of the Fermi energy ($\epsilon_F = 0$) have small velocity, displaying the renormalized heavy mass in the HFL phase.

9.4 Phase diagram of the Shastry-Sutherland Kondo lattice incorporating magnetic order for a metallic filling $n_c = 0.5$. Thin (thick) lines represent first order (continuous) transitions.

A.1 $\chi_{0}^{-1}(\tau)$ for $\alpha = \{0.2, 0.4, 0.6, 0.8\}$ at $\beta = 1500\Lambda$. 
A.2 The schematic RG flow diagrams for the pseudogap BFK model projected onto the plane spanned by the impurity-boson coupling $g$ and the spin-flip exchange scattering $J_\perp$, valid for bath exponents $(r, s)$ such that the quantum criticality is of the (a) B or M, and (b) F types. We have not shown in these diagrams a third axis describing the longitudinal exchange coupling $J_z$. The dashed line marks the boundary between the Kondo and localized phases. Arrows show the direction of RG flow of the effective couplings between fixed points represented by circles: free moment (FM, at $J_z = 0$), Kondo (K, at $J_z = \infty$), localized (L, a line of fixed points spanning $0 \leq J_z \leq \infty$), fermionic critical (FC, at $J_z = J_\perp$), and Bose-Fermi critical (BFC, at $J_z = \infty$ in region B but at finite $J_z > J_\perp$ in region M). Very similar RG flow diagrams can be constructed for the pseudogap BFA model.

C.1 Full large-N phase diagram of the SS Kondo lattice, for $t_2 = t_1$ and $n_c = 0.5$. The phases are described in the text.

C.2 Phase diagram of the SS Kondo lattice incorporating magnetic order using $x = 0.75$, while keeping $t_2 = t_1$ (a) and for $x = 0.70$ with $t_2 = 0$. In both cases, the conduction electron filling, $n_c = 0.5$, is unchanged from before. The thin (thick) lines represent first order (continuous) transitions.
C.3 (a) Fermi surface corresponding to the band structure in Fig. 3(b) of the main text, in the VBS phase. Here, $J_2/J_1 = 2$, $J_K/t_1 = 2.1$. Since the spinon bands are gapped, this corresponds to the band structure of the conduction electron dispersion alone, defined on the SSL with $t_1/t_2 = 1$ and $n_c = 0.5$; (b) Fermi surface corresponding to the band structure in Fig. 3(c) of the main text, in the HFL phase. The bare parameters are the same as in (a). Note that the Fermi volume does not change from (a) to (b), due to the even number of spins per unit cell as described in the main text.

C.4 (a) Band structure in the VBS phase when the diagonal hopping vanishes, $t_2/t_1 = 0$, and for $J_2/J_1 = 1.6$, $J_K/t_1 = 0$ and $n_c = 0.5$. The parameter $t_1 = 1.0$ sets the unit of energy. The blue lines are the gapped spinon bands. The Fermi energy is at $\epsilon_k/t_1 = 0$; (b) The corresponding Fermi surface.

C.5 (a) Band structure in the HFL phase, for parameters as in Fig. C.4. The fermi energy is also at $\epsilon_k/t_1 = 0$; (b) The corresponding Fermi surface.

C.6 The phase diagram of the Heisenberg model in the slave-fermion approach. The parameter $x$ and the phases are described in the main text.
A.1 As defined in chapter 5, $g_u$ is the value of the bosonic coupling $g$ that yields the highest temperature of entry into the quantum-critical regime. In the fourth column, “F”, “B”, and “M” refer to three different types of universality classes Fermionic, Bosonic, and Mixed, as defined and discussed in chapter 5. Exponents $x$, $\beta$, and $\nu$ are as defined in Eqs. (5.15), (5.18), and (5.16), respectively, while $1/\nu_B(s)$ is the reciprocal of the order-parameter exponent at a pure-bosonic QCP with the same $s$, as calculated in the metallic ($r = 0$) BFK model. All values of $1/\nu_B$ and those values of $1/\nu$ followed by an asterisk were obtained from the corresponding value of $\beta$ using hyperscaling [Eq. (5.21)] under the assumption that $x = s$. Any exponent followed by “§” has been set to that for the pure-fermionic pseudogap Kondo model (see the line labeled “no bosons” for each value of $r$) since $g_u = 0$ indicates that the bosonic bath plays no part in the criticality. A number in parentheses represents the uncertainty in the last digit, equal to 1 where omitted.
The field of condensed matter physics is incredibly rich and aims to understand a broad range of questions related to the different properties that phases of matter can have. The results of condensed matter physics have led to fundamental and far reaching implications, both in a variety of fields of physics and technological advances of mankind. The subfield of strongly correlated electron systems seeks to understand quantum condensed matter systems, where interactions between the constituent particles are so large that they fundamentally change the state of matter and lead to novel phases and phase transitions. One famous example in electronic systems is the Mott transition \[1\]; here, upon increasing the strength of the electron-electron repulsion, the system can change from a metal into an electronic insulator. In a number of cases, the unusual properties that result from strong correlations can be quite useful and have led to a number of real world applications including magnetically levitated trains, magnetic resonance imaging \[2\], and spintronic devices \[3\]. As a result of quantum mechanics, there are a variety of systems with novel types of phases beyond just solid, liquid, and gas, such as itinerant magnets, superfluidity, superconductivity, quantum Hall states, valence bond solids, and quantum spin liquids; the list only continues to grow.
There are a number of fascinating open questions in the field of strongly correlated electron systems, which result from the combination of a large number of particles in a solid (on the order of $10^{23}$ [4]) and strong inter particle interactions. Due to strong correlations, it is not possible to describe the system as one effective particle (or quasiparticle) moving in an average background (or mean field) created by the rest [5]. In addition, the lack of a small parameter makes perturbation theory [6] inapplicable. As a result the concept of quasiparticles, which are so salient in Landau’s Fermi liquid theory, can break down and new theoretical approaches are necessary. This becomes quite evident in band structure calculations using density functional theory [7], which are very successful at describing experiments on weakly correlated systems but completely fail when the electron correlations are too large [8]. For all of these reasons developing a unifying theoretical framework to describe and understand strongly correlated systems remains a pressing problem.

One of the most active areas of research in strongly correlated phenomenon is the nature of high temperature superconductivity, which remains an open and hotly debated question today [11, 12]. In copper oxide (or cuprate) materials, the parent state is a quantum antiferromagnetic Mott insulator and is highly correlated. Upon doping the material, magnetic order is suppressed and yields to high temperature superconductivity [13], with a transition temperature as high as 138$K$ [14]. Recently, the iron pnictide superconductors have also been discovered, with a high temperature superconducting phase on the border of magnetism [15, 16, 17]. Additionally, superconductivity in the strongly correlated heavy fermion materials [18] and organic superconductors [19] have also been found to emerge after suppressing magnetism. In these last two cases even though the transition temperature is low, it may still be regarded as “high temperature” when the energy scale is rescaled to that of a normal metal\(^1\) [21]. In each case, shown schematically in figure 1.1, it has been found that

\(^1\)More precisely, the ratio of $T_c/T_F$ is much larger then conventional superconductors, where $T_c$
Figure 1.1: Schematic finite temperature ($T$) phase diagram as a function of an external tuning parameter ($\delta$), applicable to various strongly correlated electron systems on the border of an antiferromagnetism (AF) and displaying superconductivity (SC). There is an intermediate non-Fermi liquid (NFL) phase, above an intervening superconducting dome. In such a context the superconductivity tends to be unconventional. The NFL and superconducting dome separate the magnetically ordered phase from the metallic Fermi liquid phase (FL), and $T^*$ is a cross over energy scale to the FL regime. In the absence of superconductivity (no black dome), the quantum critical point has been observed in a number of experiments [9] as the Néel temperature $T_N$ is driven to zero, and has been seen to give rise to a NFL region. In the presence of superconductivity, it becomes difficult to experimentally determine if a quantum critical point lies beneath the dome. Nonetheless, a quantum critical point (QCP) would be a natural explanation for the NFL region above the superconducting dome (hence the use of QCP?) [10].

suppressing magnetism by applying pressure, a magnetic field, or doping can give rise to superconductivity. The main open question common to all of these experiments is: what is the pairing mechanism, i.e. what generates the attractive electron-electron interaction that leads to the formation of Cooper pairs [22] and superconductivity?

These experiments have made it evidently clear that superconductivity and quantum magnetism are intimately related. The consistent proximity of superconductivity is the superconducting transition temperature and $T_F$ is the Fermi temperature [20].
ity and magnetism in the phase diagrams of a wide class of systems implicates some fundamental principle connecting the two phases. Moreover, being able to provide a unified understanding to the schematic phase diagram of figure 1.1, that so commonly occurs in a wide variety of strongly correlated electron systems, is one of the most fundamental problems in strongly correlated electron systems. The theme captured in the schematic phase diagram common to all of these strongly correlated systems, irregardless of their microscopic details, is competing phases. Whereby applying an external tuning parameter one ordered state competes and gives way to another, such as AF to SC or NFL in figure 1.1.

In order to understand the existence of each phase, it becomes necessary to understand the different types of transitions that are possible to take the system into and out of each phase. Therefore, in an attempt to understand strongly correlated phenomenon, we are naturally led to the study of phase transitions (see section 1.1 for a review). In the absence of any zero point motion, classical phase transitions are driven by changes in temperature. As a result of strong interactions and quantum mechanics, the theory of phase transitions takes on an entirely new light. In this case phase transitions can in principle take place at zero temperature due to competing interactions alone. These are known as quantum phase transitions [23], where in the case of a second order transition the quantum critical point (QCP) separates the ordered and disorder phase at zero temperature. In practice, while it is not possible to reach absolute zero temperature quantum phase transitions dramatically effect physical properties at a finite but low temperature [24], as seen in a variety of experiments.

Over the past two decades, heavy fermion systems (discussed in detail in chapter 2) have emerged as prototypical systems to experimentally study quantum phase transitions. Away from the critical point, heavy fermion metals can (for the most
part) be described within Fermi liquid theory [9], albeit with a large effective mass. Fermi liquid theory assumes that the ground state of an interacting gas of electrons is adiabatically connected to the non-interacting case by “slowly” turning on the electron-electron interaction [6]. As a result, the excitations (or quasiparticles) of the Fermi liquid have a one to one correspondence with the excitations of the non-interacting electron gas, and the original dynamical properties of the electron gas are renormalized, such as the mass \( m \). Therefore, thermodynamic relations for an electron gas still hold (such as the specific heat for low temperatures \( C_V \approx \gamma_C T \), where \( \gamma_C \propto m \)) although, with the original parameters replaced by the renormalized ones [6] (i.e. \( m \rightarrow m_{\text{eff}} \)). Fermi liquid theory has proven to be incredibly successful at describing most metals. Indeed, heavy fermions have been a prime example of a Fermi liquid, thanks to the large effective mass that makes the Fermi liquid features even more pronounced and easier to observe experimentally [9, 25]. Similar to what we have discussed previously, for the case of certain antiferromagnetic heavy fermion metals application of an external tuning parameter can suppress (or induce) magnetic order. In systems that don’t become superconducting this will then expose a quantum critical point [9]. Surprisingly, in the vicinity of the quantum phase transition the electronic properties can develop non-Fermi liquid behavior, such as a specific heat coefficient \( \gamma_C \propto -\ln(T/T_0) \) that is logarithmically divergent for low temperatures, or a linear in temperature resistivity [9]. In this regard, both superconductivity and non-Fermi liquid behavior appear on the border of magnetism (see figure 1.1).

It is an intriguing question to ask in general, what leads to the breakdown of Fermi liquid theory? It turns out, apart from heavy fermions, non-Fermi liquid behavior has been observed in a large variety of strongly correlated electron systems such as the copper oxide [13] and iron pnictide [15] high temperature superconductors. In one dimension, Fermi liquid theory completely breaks down for the interacting electron
gas; fortunately, in this case the system is correctly described by the Luttinger liquid theory \[26\]. However besides one dimension, there is no unifying theory behind the existence or description of non-Fermi liquid behavior, and each problem has to be studied on a case by case basis. In certain systems the experimental results cannot be described within conventional theories, and as a result have naturally lead to fundamental questions of principle.

In a large number of cases non-Fermi liquid behavior has been observed on the border of magnetism in the vicinity of a quantum critical point \[27\], or above the superconducting dome \[11\]. As shown schematically in figure 1.1, in the absence of superconductivity the NFL regime is anchored by the quantum critical point \[9\]. Whereas in the presence of superconductivity, the NFL regime can extend over a significant temperature region above the dome \[11\]. It is actually quite natural for the strongly interacting quantum critical fluctuations \[23\] to couple to the electron sea, which is enough to disrupt and destroy a Fermi liquid. In this sense quantum criticality can provide a natural setting to study non-Fermi liquid behavior in detail. Moreover, a quantum critical point hiding beneath the superconducting dome is a plausible explanation for the NFL region above it \[10\].

The failure of Fermi liquid theory, or more broadly the failure of a single particle description, has lead to the development of a variety of new theoretical techniques. In one dimensional strongly correlated systems, there are a number of exact results and sophisticated quantum field theory approaches that have proven to be very successful \[26\]. However, when going beyond one dimension most of these techniques no longer apply and new techniques are necessary. As a result numerical techniques such as quantum Monte Carlo \[28\] have played a large role. Unfortunately in electronic systems, the interchange of two particles can lead to negative probabilities\(^1\) or the

\(^1\)This happens as a result of two particles exchanging location, with the antisymmetric wave function generating a minus sign.
fermionic sign problem [29] and consequently the Monte Carlo approaches can fail. A different approach all together is the dynamical mean field theory (DMFT) [5] (and its extensions [30] discussed in detail in section 2.4). Guided by classical mean field theory which is exact in infinite dimensions [31], the DMFT describes the infinite dimensional limit of a strongly correlated problem. As a result, the DMFT maps a correlated lattice problem to a single quantum impurity embedded in a self consistent electronic bath (or a dynamic field), where the strong correlations of the lattice model are captured dynamically in the impurity problem. Another technique (referred to as large $N$) enlarges a particular symmetry group [32, 33], with the number of generators given by some power of $N$, and then uses $1/N$ as a small parameter to construct mean field theories around a strongly correlated ground state [34]. In addition to changing symmetries, the concept of “slave” particles has been particularly successful [34]. Whereby the original particles are represented using slave particles that are subject to a constraint, in order to reproduce the properties of the original degrees of freedom. In this body of work, we use DMFT based approaches as well as sophisticated large $N$ mean field theories to gain an understanding of strongly correlated electron systems.

In the following thesis we address a variety of different types of quantum phases and phase transitions that come into play in the physics of heavy fermions. In chapters 3, 4, and 5 we develop and use a method to probe the finite temperature dynamical scaling regime of a quantum critical point. In chapters 6, 7 and 8 we show that the suppression of magnetism with a concomitant electronic delocalization transition gives rise to an enhanced pairing susceptibility, which represents a new unconventional pairing mechanism mediated by local quantum critical fluctuations. Lastly, by studying the interplay of magnetic frustration and itinerancy in chapter 9, we provide the first direct calculation of a global phase diagram of heavy fermion metals. While
our results are particularly pertinent to experiments on heavy fermion systems, they also have significant implications for quantum phase transitions, unconventional superconductivity, and the theory of strongly correlated electron systems as a whole. We use heavy fermion metals as a prototypical setting to explore both non-Fermi liquid behavior and quantum phase transitions in general. In doing so, we develop a framework to understand and interpret unconventional experimental results, as well as predict the behavior of a variety of different experiments that remain to be done.

As has become clear by considering a wide class of strongly correlated electron systems, we need to use an understanding of phase transitions [4, 31] to make progress. In the remainder of the introduction, we first review classical phase transitions and their extension to zero temperature for the case of itinerant magnets. We then discuss unconventional superconductivity and go on to introduce the broad questions we are attempting to understand in this work. In the following chapter we review the theoretical description of heavy fermions and then we are able to redefine and describe the main questions we seek to answer in this thesis.

1.1 Landau Theory of Phase Transitions

Various systems undergo phase transitions from one state of matter to another due to changes in their environment, such as temperature, pressure, or volume. Phase transitions are ubiquitous in the natural sciences ranging from the melting of ice into water, the thermal suppression of magnetism, and the formation of matter itself in the early stages of the universe. The theory of phase transitions is rooted in the concept of broken symmetry, where an underlying symmetry of the Hamiltonian is spontaneously broken [31]. This leads to the definition of an order parameter $O$, which is finite on the ordered side (signaling the broken symmetry state) and vanishes on the disordered side. For continuous phase transitions at a temperature
\(T\), the order parameter vanishes continuously on approach to the critical temperature \(T_c\). Examples of order parameters and their corresponding broken symmetry are the magnetization (broken \(\mathbb{Z}_2\) [Ising spins], \(O(3)\) [Heisenberg spins]), or the superfluid density [broken \(U(1)\)].

The Landau theory of phase transitions approximates the free energy by an expansion in terms of fluctuations of the order parameter, which is consistent with the symmetries of the original problem. For a magnet in \(d\)-dimensions\(^1\), at a temperature \(T\), and a magnetization \(M(x)\), this leads to the Landau Free energy functional [31]

\[
\mathcal{F}_L = \int_0^L dx \left( \frac{r_0}{2} M(x)^2 + a(\nabla M(x))^2 + \frac{u}{4} M(x)^4 \right), \tag{1.1}
\]

in a volume \(V = L^d\), where \(r_0\) measures the distance to the critical point, \(a\) reflects the cost of spatial fluctuations, and \(u > 0\) is the strength of magnetic interactions. The partition function is then given by [31]

\[
Z = \int D[M(x)] e^{-\beta \mathcal{F}_L[M(x)]}, \tag{1.2}
\]

where \(D[M(x)] \equiv \prod_{i=1}^N dM(x_i)\) is the functional integral measure, we have defined the inverse temperature \(1/\beta = k_B T\), where \(k_B\) is Boltzmann’s constant [4]. In the absence of interactions \(u = 0\), the partition function can be determined exactly; this is referred to as the Gaussian model. Incorporating a finite \(u\) at the mean field level assumes a uniform order parameter (independent of \(x\)), minimizing the free energy \(\partial \mathcal{F}_L/\partial M = 0\), yields an order parameter \(M = \sqrt{-r_0/u}\). This shows clearly, \(r_0 < 0\) on the ordered side \((M_\uparrow 0)\), \(r_0 > 0\) on the disordered side \((M = 0)\), and \(r_0 = 0\) at the

\(^1\)A standard model applicable to study classical magnetism is the Ising model [4, 31], defined as \(H = \sum_{i,j} J_{ij} S_i^z S_j^z\), where \(J_{ij}\) is only finite for nearest neighbor sites and \(S_i^z = \pm 1\). Even though Landau theory is applicable to various models, for the following discussion we have in the back of our mind the Ising model as the microscopic Hamiltonian that gave rise to the Landau functional [4, 31] in equation (1.1).
critical point. Therefore, \( r_0 \) measures the distance to the critical point. Expanding \( r_0 \) in the vicinity of the critical point we have \( r_0 \propto t \equiv T/T_c - 1 \), which leads to the critical exponent associated with the magnetic order parameter

\[
M \propto (-t)^\beta,
\]

where, at the mean field level \( \beta = 1/2 \). It is also possible to define critical exponents for other thermodynamic variables as power laws in \( t \) such as the specific heat (\( \alpha \)), the susceptibility (\( \gamma \)), the response to an external field (\( \delta \)), the correlation length (\( \nu \)), and the anomalous dimension\(^1 \) (\( \eta \)) [31]. Based on scaling alone, the critical exponents can be related to each other as well as to the dimension \( d \) of the problem,

\[
d\nu = 2 - \alpha,
\]

\[
\gamma = \nu(2 - \eta),
\]

\[
\alpha = 2 - 2\beta - \gamma.
\]

Since there are three equations and five exponents, only 2 are independent. Equation (1.4) relates the critical exponents to the dimension of the problem and is known as a “hyper scaling” relation. The critical exponents are universal and are independent of the microscopic details of the model, each universality class has its own corresponding critical exponents [31]. Interestingly, the scaling hypothesis is only valid below the upper critical dimension as we shall now discuss.

The introduction of the renormalization group (RG) [35] to critical phenomenon makes it possible to calculate critical exponents to much higher accuracy then possible at the mean field level. The concept of the RG has led to the notion of running

\(^1\text{In this case, it is not a power law in } t, \text{ but is actually the real space decay of correlation functions} [31] G(r) \sim r^{-d+2-\eta}.\)
coupling constants, that is whether or not a particular coupling increases (is relevant) or decreases (is irrelevant) as the energy scale in the problem is lowered. Using the scaling dimensions of $M$ and $r_0$, we can determine the scaling dimension of the interaction $u$, and conclude whether or not the interaction $u$ is relevant in an “RG sense”. Such an analysis leads to $[u] = 4 - d$ (without incorporating any perturbative effects). Therefore, for dimensions $d > 4$ the interaction is irrelevant and the critical exponents are determined by the Gaussian model alone whereas for $d < 4$ the interaction is relevant and the renormalization group treatment is necessary to accurately calculate critical exponents. This then defines the upper critical dimension, $d_u = 4$ where the interaction is marginal (i.e. doesn’t change under a change of energy scale) and gives rise to logarithmic corrections to critical exponents. It is straightforward to show that the critical exponents associated with the Gaussian model are equivalent with the mean field solution apart from the specific heat exponent $\alpha$ in dimensions $d < 4$, where the Gaussian approximation yields $\alpha = 2 - d/2$ [31]. However, for dimensions $d > 4$, the critical exponents obtained within mean field theory are all independent of dimension, and therefore violate the hyper scaling relation (1.4). Exactly at the upper critical dimension $d = 4$, logarithmic corrections to the critical exponents spoil hyper scaling [31]. To conclude, we reach the important conclusion that for problems with a dimension $d > 4$ the Gaussian theory is exact and hyper scaling is violated for $d \geq 4$.

### 1.2 Spin Density Wave Quantum Critical Point

As we have previously discussed, at very low temperatures significant quantum effects can alter the nature of matter in unexpected yet distinct ways. In the seminal theoretical work of Hertz [36], which was later revisited and refined by Millis [37], Landau’s theory of phase transitions was generalized to zero temperature and intro-
duced the concept of quantum phase transitions. Starting from the Hubbard model

\[ H_{\text{Hub}} = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \]  

(1.7)

(where \(c_{i\sigma}\) destroys an electron at site \(i\) with spin \(\sigma\) and \(n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}\)), Hertz constructed the quantum analog of the Landau Functional [equation (1.1)]. This is done most naturally within a Grassman path integral representation [38]. Writing the Hubbard interaction in terms of the \(z\) component of the spin operator \(S_z^i = \sum_{\alpha,\beta} c_{i\alpha}^\dagger (\sigma^z_{\alpha\beta} / 2) c_{i\beta}\) yields \(n_{i\uparrow} n_{i\downarrow} = -2(S^z_i)^2 + 1/2(n_{i\uparrow} + n_{i\downarrow})\). Following Hertz [36, 37], the spin-spin interaction is then decoupled using a Hubbard-Stratonovich field \(\phi\), and the fermions are integrated out [38]. In the assumption of long wave length low energy fluctuations of the order parameter \(\phi(x, \tau)\), which is now a function of space \(x\) and imaginary time \(\tau\) (which lies in the range \(0 \leq \tau \leq \hbar \beta\)), the action (or quantum Landau functional) becomes

\[ F_L = \sum_{n=-\infty}^{\infty} \int_0^\Lambda d^d q \left( \frac{r_0}{2} + bq^2 + \gamma_0 \frac{|\omega_n|}{q^a} \right) |\phi(q, \omega_n)|^2 + \frac{u}{4} \int dxd\tau \phi(x, \tau)^4. \]  

(1.8)

We have written the Gaussian part of the action in terms of the momentum \(q\) and the bosonic Matsubara frequency \(\omega_n = 2\pi n/\beta\). The damping \(\gamma_0\) is a result of the particle hole bubble contribution from Fermi surface excitations and we have introduced the exponent \(a\), which is different for ferromagnetic and antiferromagnetic instabilities [36, 37]. For the case of an antiferromagnetic (ferromagnetic) instability \(a = 0(1)\), in the following we will focus on the antiferromagnetic instability which we refer to as the spin density wave (SDW) transition. In applying the RG to the above action, reducing the overall energy scale to \(\Lambda' = \Lambda e^{-l}\) (for \(l \ll 1\)) we find that under a rescaling \(q' = e^l q\) and \(\omega_n' = e^l \omega_n\) the terms in the Gaussian part of the action \(q^2\) and \(|\omega_n|\) scale differently. Following Hertz [36], we introduce the dynamic exponent \(z\) so
that $q$ and $\omega_n$ scale the same, namely

$$
q' = e^l q, \quad \omega'_n = e^{zl} \omega_n.
$$

(1.9)

Similar to the classical case, to determine the scaling dimension of $u$ we rescale the entire action to obtain $[u] = 4 - (d + z)$. Therefore, we can regard the quantum Landau functional as a classical one but in elevated dimensions

$$
d_{\text{eff}} = d + z.
$$

(1.10)

We are now able to conclude, quantum critical points (in the form discussed here) act like classical phase transitions in $d_{\text{eff}}$ dimensions and therefore belong to the same universality class as the classical case. We can now apply the reasoning of classical Landau theory to conclude the critical theory for $d + z > 4$ should be describable by the Gaussian theory alone ($u = 0$).

Even though the quantum critical point only exists at zero temperature, its effects are felt at finite temperatures in a region known as the quantum critical regime. The quantum critical regime resembles a fan anchored at the quantum critical point, separating the ordered and disorder phases (see figure 1.2). In the quantum critical regime the appearance of hyper scaling at the QCP implies [39, 40] correlation functions obey $\omega/T$ scaling (after $\omega_n$ has been analytically continued to real frequencies), whereas this scaling form is violated above the upper critical dimension due to the presence of a dangerously irrelevant variable. It has become clear two energy regimes need to be distinguished [40], the quantum coherent ($\hbar \omega \gg k_B T$) and relaxational ($\hbar \omega \ll k_B T$) regimes. The coherent regime describes collision free phase coherent transport while the relaxational regime describes collision dominated incoherent transport [40]. Lastly, based on the discussion in the introduction and
Figure 1.2: Schematic finite temperature \((T)\) phase diagram vs. external control parameter \((\delta)\) of quantum critical points. The shaded colored region in the vicinity of the solid black line (labeled “classical critical”) the system can be described by classical Landau theory. In between the ordered and disordered phases is the quantum critical regime, where effects of the QCP are felt for a range of temperatures. For itinerant QCPs, the quantum critical regime can also correspond to the NFL regime shown in figure 1.1.

summarized in figure 1.1, it is quite natural to expect quantum critical properties will have a dramatic effect on superconductivity.

1.3 Unconventional Superconductivity

In the conventional theory of superconductivity developed by Bardeen, Cooper, and Schrieffer (BCS) [22], electron-phonon interactions give rise to an effective attractive interaction between electrons in the vicinity of the Fermi surface (i.e. within a band-width of the Debye frequency around the Fermi energy). This then gives rise to a superconducting ground state, with a complex order parameter and a Landau theory similar to equation (1.1) can be constructed. Additionally, within an RG approach, it was shown by Shankar [41] that electrons in three dimensions are unstable towards
a superconducting ground state for an infinitesimal attractive interaction. Therefore, independent of how the attractive interaction is generated, once it has been, the Fermi liquid is unstable to a superconducting ground state.

Unconventional superconductivity refers to a broad class of systems that exhibit pairing mechanisms that are not phonon mediated. There are now a variety of known experimental examples that exhibit unconventional pairing, such as $^3$He [42], the copper oxide high temperature superconductors [43], and heavy fermion metals [9]. As discussed previously, the unifying question common to understanding new pairing mechanisms across a number of systems is what is providing the attractive interaction? In each case we have discussed, the superconducting phase is in close proximity to a magnetic quantum critical point, and it is therefore very natural to think that quantum critical fluctuations may be somehow responsible for generating the attractive interaction. In this regard it is very useful to note, it has been shown quantum critical points are accompanied by an accumulation of entropy as signaled by a diverging Grüneisen ratio [44, 18]. Due to the large build up of entropy in the vicinity of the QCP, which implies a wide availability of accessible quantum states, new phases such as superconductivity tend to nucleate and form. In the context of the SDW quantum critical point, the work of Scalipino et. al. [45] have shown quantum critical SDW fluctuations can mediate the attractive electron-electron interaction and give rise to a pairing instability. For the SDW quantum critical point, only portions of the Fermi surface that are connected by the ordering wave vector become critical or “hot” [46, 47, 48]. Therefore the pair mediating critical fluctuations are only coming from the hot spots of the Fermi surface. The concept of quantum critical fluctuations mediating superconductivity will be a central focus of chapters 6, 7, and 8. However, in this thesis we will be concerned with a quantum critical point that has a corresponding jump in the Fermi surface [18, 49] and as a result the entire Fermi surface
becomes hot [50]. This represents an entirely new pairing mechanism unexplored until now. Lastly, we will be concerned with a strongly correlated problem and will need to depart from the weak coupling, SDW approach.

1.4 Summary

At this point it is useful to pause and reflect on the consequences of what we have reviewed so far. First, we have considered the concept of critical exponents and universality. We have presented the work of Hertz [36] and Millis [37], which shows itinerant magnetic quantum critical phenomena can be described by a classical theory in elevated dimensions. If the SDW theory is “the theory” for itinerant quantum phase transitions, then the quantum critical behavior of itinerant magnetic systems appears to be more or less understood. However, as experiments on heavy fermion metals have shown, this is very far from the truth and the problem of quantum critical phenomenon is quite rich with a number of fundamental questions that remain to be answered.

As we will discuss in detail in the following chapter, experiments on heavy fermion metals have clearly established the existence of quantum critical points and therefore serve as ideal settings to study quantum criticality [18]. These experiments and their consequences (which we will review in detail in the following chapter), have led to the notion of beyond Landau quantum critical points. The notion raises a number of profound questions, such as:

1. How could the zero temperature generalization of Landau theory fail?

2. What is the correct universality class associated with the transition?

3. How does quantum criticality affect superconductivity?
4. Are there new intermediate non-Fermi liquid phases?

5. What are the role of quantum fluctuations, (since they can’t be as benign as predicted by the SDW theory)?

These questions serve as the main focus of this thesis. In the following chapter we clarify the meaning of each question as it has been posed through experiments on heavy fermion metals.
Rare earth and intermetallic compounds are composed of atoms which have a combination of $d$ and $f$ orbitals. The $d$ orbitals tend to be more itinerant and give rise to conduction electrons, while the $f$ orbitals are tightly bound due to the large orbital angular momentum and give rise to local magnetic moments \[25\]. For the case of alloys made of Ce or Yb, the $f$ shell has either one electron or one hole, respectively, and therefore they effectively represent spin-1/2 local moments immersed in a Fermi liquid. The hybridization between the local moments and the itinerant electrons give rise to a very large effective mass for the charge carriers, sometimes on the order of 1000 times the mass of a normal electron \[25\]. As a result these compounds are commonly referred to as heavy fermions. The large effective mass appears in a number of thermodynamic quantities, such as the slope of the specific heat at low temperatures $C_V \sim \gamma C T$, since for a Fermi liquid $\gamma_C \propto m_{\text{eff}}$.

The large effective mass has dramatic consequences on a variety of physical properties. Firstly, the Fermi energy \[E_F = (\hbar k_F)^2/(2m_{\text{eff}})\] is significantly smaller then in a conventional metal and therefore the ground state can be readily tuned \[9\] using a variety of external probes such as pressure, magnetic field, and chemical doping. In addition, the large effective mass gives rise to a greatly reduced Fermi velocity
$v_F = \frac{\hbar k_F}{m_{\text{eff}}}$, which has dramatic implications for superconductivity. In the conventional BCS theory [22] the Fermi velocity is several orders of magnitude greater than the sound velocity associated with phonon excitations. As a result, the electron-phonon interaction is retarded, which is actually essential to providing the attractive interaction. In the case of heavy fermions, the Fermi velocity is the same order of magnitude as the sound velocity and as a result the electron-phonon interaction can not provide the attractive electron-electron interaction needed to form Cooper pairs. This was pointed out immediately with the first discovery of unconventional superconductivity in the heavy fermion compound CeCu$_2$Si$_2$ by Steglich et al [21].

### 2.1 Impurity Models

Before discussing the effective models used to describe heavy fermion systems, we will first consider a single magnetic impurity (representative of a single $f$-orbital) immersed in a bath of electrons (representative of a $d$-orbital band). Such a model is physically interesting in its own right and is representative of a conventional metal with a dilute concentration of magnetic impurities, such as iron impurities in a piece of copper. The Anderson impurity model [51, 25] describes a single $f$-orbital in a sea of conduction electrons, and is defined as

$$H_{\text{AIM}} = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\sigma} \epsilon_f n_{f\sigma} + Un_{f\uparrow}n_{f\downarrow} + \sum_{k,\sigma} \left( V_k c_{k\sigma}^\dagger f_{\sigma} + V_k^* f_{\sigma}^\dagger c_{k\sigma} \right). \quad (2.1)$$

Where $c_{k\sigma}$ destroys an electron of momentum $k$ and spin $\sigma$ with a dispersion $\epsilon_k$, $f_{\sigma}$ destroys an electron in an $f$ orbital with spin $\sigma$, in an energy level $\epsilon_f$, with an onsite electron-electron repulsion $U$, and we have defined $n_{f\sigma} = f_{\sigma}^\dagger f_{\sigma}$. We have introduced the hybridization $V_k$ between the conduction electrons and the local moment, which is related to the matrix element between the two orbitals [51]. In the vicinity of the
Fermi energy, with a momentum independent hybridization $V_k = V$, the strength of the inter band hopping process is described by the hybridization function [25], which is defined as $\Gamma_0 = \pi \rho_0 |V|^2$ where we have introduced the density of states of the conduction electrons at the Fermi energy $\rho_0 = \rho(\epsilon_F)$. In the limit $\Gamma_0/|U + \epsilon_f|, \Gamma_0/|\epsilon_f| \ll 1$, the Anderson impurity model can be mapped [52] to the Kondo model

$$H_{KM} = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + W \sum_\sigma c_{0\sigma}^\dagger c_{0\sigma} + J_K s^c \cdot \mathbf{S}. \quad (2.2)$$

We have defined the conduction electron destruction operator at the impurity site $c_{0\sigma} = \sum_k c_{k\sigma}$ and have only considered momentum in the vicinity of the Fermi surface. This leads to momentum independent $W$ and $J_K$, where $W$ is a potential scattering term and $J_K$ is the Kondo coupling between the spin density of the conduction electrons at the impurity site $s^c = \sum_{\alpha, \beta} c_{0\alpha}^\dagger (\sigma_{\alpha\beta}/2) c_{0\beta}$ and the spin−1/2 magnetic impurity $\mathbf{S}$. In the limit of a particle hole symmetric Anderson impurity $U = -2\epsilon_f$, the potential scattering term vanishes, $W = 0$ [25].

Despite the seeming simplicity of the Kondo and Anderson Hamiltonians, the physics of each model is quite rich and it requires renormalization group methods in order to understand the low temperature behavior [35, 53, 25]. This became clear after Kondo [54] applied third order perturbation theory in $J_K > 0$ (antiferromagnetic) to calculate the resistivity, and found [54]

$$\rho(T) \approx \rho_0 + aT^2 - b \log(k_B T/D), \quad (2.3)$$

for a bandwidth $D$. In addition to the contributions from nonmagnetic impurity scattering ($\rho_0$) and the conduction electrons ($aT^2$), Kondo’s result finds an additional contribution.

---

1. The mapping applies the Schrieffer-Wolff transformation [52] and then projects out unoccupied and double occupied states in the limit of large $U$ and $|\epsilon_f|$.
2. See appendix A for the details of the momentum dependence.
logarithmic term, which gives rise to a resistivity minimum and a logarithmically divergent resistivity in the limit of low temperature. The existence of the resistance minimum in metals with a dilute concentration of magnetic impurities had been known for some time [25] and Kondo’s result [54] provided the first satisfactory theoretical explanation. However, at the same time Kondo’s result posed the question: what happens in the limit of low temperature?

Using a variety of theoretical approaches [25], where renormalization group arguments [53, 35] played a central role, it was shown the unusual low temperature behavior results from the magnetic impurity becoming quenched (or screened) by the conduction electrons. The perturbative RG treatment of Anderson et. al. [53], found an RG equation for the Kondo coupling to leading order

\[ \frac{dJ_K}{d\log(D)} = -2\rho_0 J_K^2 \]  

(2.4)

that increases (decreases) as the energy scale of the problem or the bandwidth \( D \), is lowered for \( J_K > 0 \) \((J_K < 0)\), and gives rise to the RG flow shown in figure 2.1. Integrating the RG equation from an initial bandwidth \( D \) and Kondo coupling \( J_K \) to a final bandwidth \( \tilde{D} \) and Kondo coupling \( \tilde{J}_K \) we find the characteristic energy scale [25]

\[ D \exp \left( -\frac{1}{2\rho_0 J_K} \right) = \tilde{D} \exp \left( -\frac{1}{2\rho_0 \tilde{J}_K} \right) \approx k_B T_K. \]  

(2.5)

The above equation defines the Kondo temperature \( T_K \), and the use of \( \approx \) is because the result came from a perturbative in \( J_K \) RG treatment. In addition, the Kondo temperature acts as a scale invariant [25] for temperatures below \( T_K \) a positive \( J_K \) starts to flow to strong coupling along a scaling trajectory completely characterized by \( T_K \), as shown in figure 2.1. Unfortunately, after \( J_K \) flows to strong coupling the perturbative RG solution is no longer applicable. Going beyond the perturbative
Figure 2.1: Schematic RG flow diagram of the Kondo model [53] in terms of the dimensionless Kondo coupling $j \equiv \rho_0 J_K$, split into transverse $j_\perp$ and longitudinal $j_z$ components. There is a Kosterlitz-Thouless quantum phase transition when $j_z$ is tuned from ferro- to antiferro-magnetic, and $j > 0$ flows to strong coupling.

RG, the numerical renormalization group (NRG) of Wilson [35] determined the full solution of the problem. Wilson showed quite conclusively, the ground state of the Kondo model for an antiferromagnetic $J_K$, is a completely screened magnetic impurity in the the limit of zero temperature, whereas a ferromagnetic $J_K$ gives rise to an asymptotically free magnetic impurity. This results in an impurity contribution to the spin susceptibility [25], $\chi_{\text{imp}}(T, J_K) = \chi(T, J_K) - \chi(T, J_K = 0)$ that goes to a finite value as $T \to 0$ for $J_K > 0$ ($\chi_{\text{imp}} \sim b/T_K$), whereas the $J_K < 0$ case, acts like a free moment with a Curie Weiss susceptibility ($\chi_{\text{imp}} \sim c/T$) in the limit of low $T$.

When the concentration of impurities is no longer dilute, as a result of hybridization the conduction electrons can mediate a Ruderman-Kittel-Kasuya-Yosida (RKKY) spin-spin interaction\(^1\) \[^{55, 56, 57}\] between the impurities $I_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$. In terms of the Kondo coupling [58], the RKKY interaction $I$ scales as $I \propto \rho_0 J_K^2$. When the concentration of impurities becomes dense enough to accommodate roughly one impurity per lattice site, as is relevant for the description of heavy fermion metals, it is then necessary to consider a lattice of magnetic impurities. This then prompted

\[^1\text{The RKKY interaction } I_{ij} = I(r_i - r_j) \text{ is a decaying oscillating function in space, depending on the distance between ions it can be either ferro- or antiferro-magnetic [55, 56, 57].}\]
Figure 2.2: Doniach Phase diagram comparing the Kondo and RKKY energy scales for a typical bandwidth $D$. For a weak $J_K$ on the left of the black dashed line, the RKKY interaction dominates $T_{RKKY} = \rho_0 J_K^2$ and should order magnetically. Whereas for large $J_K$, the Kondo temperature $T_K$ becomes the dominant energy scale and the ground state should be a heavy Fermi liquid.

Doniach [59] to compare the effective RKKY and Kondo interaction scales. Since $J_K$ flows to strong coupling, the relevant Kondo energy scale is the Kondo temperature $T_K$ [in equation (2.5)]. As shown in figure 2.2, for a typical bandwidth $D$, in the limit $J_K/D \ll 1$ the RKKY interaction dominates ($I/T_K \gg 1$) and the ground state should be magnetically ordered, whereas for $J_K/D \gg 1$, the Kondo interaction dominates ($I/T_K \ll 1$) and the ground state should be a heavy Fermi liquid. Therefore, Doniach concluded there should be an itinerant magnetic phase transition in Kondo lattice systems [59]. In order to understand the quantum critical properties beyond a qualitative level, we move away from a single impurity and discuss the Kondo lattice and periodic Anderson models in the following section.
2.2 Heavy Quasiparticles

The appropriate model to describe a lattice of local moments, interacting with a sea of electrons is known as the Kondo lattice Hamiltonian, defined as

\[ H_{KL} = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + J_K \sum_i s_i^c \cdot S_i + \sum_{i,j} I_{ij} S_i \cdot S_j, \] (2.6)

where the conduction electron spin is defined as \( s_i^c = \sum_{\alpha,\beta} c_{i\alpha}^\dagger (\sigma_{\alpha\beta}/2) c_{i\beta} \), which is Kondo coupled to the lattice of local moments with a strength \( J_K \), and we have explicitly included an RKKY spin-spin interaction \( I_{ij} \). For the case of mixed valence, where the \( f \) electron filling is not close to unity, charge excitations must be included which leads to the periodic Anderson lattice Hamiltonian

\[ H_{AL} = \sum_{\langle i,j \rangle,\sigma} t_{ij}(c_{i\sigma}^\dagger c_{j\sigma} + h.c) + \sum_i (\epsilon_f n_{fi} + U n_{fi\uparrow} n_{fi\downarrow}) + \sum_{i,\sigma} (V c_{i\sigma}^\dagger f_{i\sigma} + h.c.) + \sum_{\langle i,j \rangle} I_{ij} S_{fi} \cdot S_{fj}. \] (2.7)

Now the conduction electrons are hybridized to a lattice of impurities with strength \( V \). The Hamiltonians in equations (2.6) and (2.7) serve as the fundamental models to describe heavy fermion physics and their solution as well as the quantum critical properties associated with each is a central focus of the following thesis. In the limit of one impurity, equations (2.6) and (2.7) reduce to the Kondo and Anderson impurity models respectively.

For the following discussion we restrict ourselves to the Kondo lattice case and consider the model in the limit of a large Kondo coupling \( J_K/I_{ij} \gg 1 \). In this case, we can neglect the spin-spin interaction in the following discussion. Using a fermionic representation of the local moments \( S_i = \sum_{\alpha,\beta} f_{i\alpha}^\dagger (\sigma_{\alpha\beta}/2) f_{i\beta} \), with the constraint \( \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} = 1 \), we can determine the mean field theory of the Kondo
Figure 2.3: The Kondo mean field parameter $b_0$ (after being rescaled by $2/J_K$ to be dimensionless) as a function of the Kondo coupling $J_K/t$ for a fixed conduction electron filling $n_c = 0.25$ on a square lattice, with a dispersion $\epsilon_k = -2t[\cos(k_x) + \cos(k_y)] - \mu$. For $b_0 = 0$ the local moments are decoupled from the conduction band, whereas for a finite $b_0$, the two bands are hybridized and the model is in the HFL phase.

lattice Hamiltonian following Read and Newns [60, 61]. This mean field construction is exact in the limit of large $N$, where the symmetry group $SU(2)$ is generalized to $SU(N)$. At the physical $N = 2$ level, this leads to the mean field Hamiltonian

$$H_{KL}^{MF} = \sum_{k,\sigma} \left( \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \mu_f f_{k\sigma}^\dagger f_{k\sigma} - b_0 (f_{k\sigma}^\dagger c_{k\sigma} + h.c.) \right),$$  \hspace{1cm} (2.8)$$

where the dispersion $\epsilon_k$ is the Fourier transform of $t_{ij}$, the chemical potential $\mu_f$ enforces the constraint on average $\sum_\alpha \langle f_{i\alpha}^\dagger f_{i\alpha} \rangle = 1$, and the hybridization is self consistently determined $b_0 = (J_K/2) \sum_\sigma \langle f_{i\sigma}^\dagger c_{i\sigma} \rangle$. The mean field theory allows for a simple qualitative picture of the heavy Fermi liquid phase, a finite value of $b_0$ acts like the hybridization of the local moments and the conduction electrons, i.e. the local moments are Kondo screened. Whereas for $b_0 = 0$, the local moments are essentially decoupled from the conduction band as shown in figure 2.3. Note we haven chosen a gauge such that the phase of $b_0$ is absorbed into the constraint field [61]. Diagonalizing
the mean field Hamiltonian we arrive at the heavy quasiparticle Hamiltonian \( H_{KL}^{MF} = \sum_{k,\sigma,\lambda=\pm} E_{k\lambda} \alpha_{k\sigma \lambda}^{\dagger} \alpha_{k\sigma \lambda} \) where the dispersion is given by

\[
E_{k\pm} = \frac{1}{2}(\epsilon_k + \mu_f) \pm \frac{1}{2}\sqrt{(\epsilon_k - \mu_f)^2 + 4b_0^2}.
\] (2.9)

The dispersions \( E_{k+} \) and \( E_{k-} \) correspond to the light and heavy bands respectively, as shown in figure 2.4 for a square lattice. Lastly, the heavy quasiparticles are related to the original degrees of freedom by

\[
c_{k\sigma} = u_k \alpha_{k\sigma +} + v_k \alpha_{k\sigma -},
\] (2.10)

\[
f_{k\sigma} = v_k \alpha_{k\sigma +} - u_k \alpha_{k\sigma -},
\] (2.11)

and the coherence factors are given by \( u_k = b_0 v_k/(\epsilon_k - E_{k+}) \) and \( u_k^2 + v_k^2 = 1 \). Within the mean field solution the effective mass scales with the Kondo temperature as \( m^* \propto 1/T_K \) [58], since \( T_K \) is generally quite small \( m^* \) is enhanced accordingly. If we now count the number of electrons that contribute to the Fermi volume, using Luttinger’s theorem [62] we find \( V_{FS} \propto 1 + n_c \), whereas in the absence of Kondo screening (\( b_0 = 0 \)) we have \( V_{FS} \propto n_c \), where \( 0 < n_c < 1 \). This allows us to distinguish between a “large” and “small” Fermi surface, such a distinction is useful in determining the relevant phases. We note that we are assuming there are an odd number of spins per unit cell, otherwise the Fermi volume doesn’t change (since \( 2 + n_c \) fills a lower band completely, then the partially filled band is just \( n_c \)).

### 2.3 Spin Density Wave Transition

Assuming the chemical potential lies within the heavy band \( (\bar{\epsilon}_k \equiv E_{k-}) \), while only keeping the low energy degrees of freedom in the vicinity of the Fermi surface, we
Figure 2.4: Band structure in the heavy Fermi liquid phase \((J_K/t = 5.0)\), along the high symmetry direction \(k_x = k_y\) for a square lattice with a nearest neighbor tight binding \(t\). The light band \(E_{k^+}\) is shown in blue, and the heavy band \(E_{k^-}\) in red (in units of \(t\)). The Fermi energy is displayed as the \(k_x\) axis, which intersects the heavy band at a point of very small curvature and as a result gives rise to a very large effective mass [20].

can drop the light band \((E_{k^+})\) and consider a one band model. Since, we know the quasiparticles do interact beyond the mean field level (and this phase is a Fermi liquid, which can have weak density density interactions), we can add a phenomenological Hubbard interaction \(\tilde{U}\), which leads to the Hubbard Hamiltonian for the heavy quasiparticles (dropping the subscript “\(-\)”) \[ \tilde{H}_{\text{Hub}} = \sum_{\mathbf{k},\sigma} \tilde{\epsilon}_{\mathbf{k}} \alpha_{\mathbf{k}\sigma}^{\dagger} \alpha_{\mathbf{k}\sigma} + \tilde{U} \sum_{i} \alpha_{i\uparrow}^{\dagger} \alpha_{i\uparrow} \alpha_{i\downarrow}^{\dagger} \alpha_{i\downarrow}. \] \[ (2.12) \]

Now under the assumption that the heavy quasiparticles remain intact across the quantum phase transition, we can directly apply the theory of Hertz and Millis [36, 37] described in the previous section. This allows us to conclude the heavy quasiparticles can undergo a quantum phase transition into a SDW phase, and for spatial dimensions two and greater hyper scaling (or \(\omega/T\) scaling) is violated. The Gaussian theory determines the critical exponents exactly for three spatial dimensions (with logarithmic
corrections to the Gaussian result at \( d = 2 \).

A key assumption of the previous analysis is that the heavy quasiparticles remain undisturbed and are not destroyed at the quantum critical point. As we shall see, this assumption is only valid provided the quantum fluctuations are not too strong, and in certain cases the heavy quasiparticles can be destroyed at the quantum critical point [63]. Since the heavy quasiparticles are a consequence of Kondo screening, breaking apart the quasiparticle implies the Kondo effect is suppressed at the antiferromagnetic quantum critical point [63].

If we now consider the opposite limit \( I_{ij}/J_K \gg 1 \), as Yamamoto and Si [64] have shown the antiferromagnetic phase is stable with respect to a small but finite \( J_K \), where the lattice of local moments are essentially decoupled from the conduction band. In this case, the local moments are localized and the corresponding Fermi surface is small. We are now in a position to distinguish between three phases: the heavy Fermi liquid (HFL) phase is paramagnetic with a large Fermi surface, the SDW phase has a finite magnetic order parameter and a large Fermi surface, and lastly the antiferromagnetic phase (AF) has a finite magnetic order parameter with a small Fermi surface, see figure 2.5. In the following section we discuss passing directly from the AF to the HFL phase.

2.4 **Kondo Destruction, Experiment, and Theory**

We have briefly mentioned how a class of antiferromagnetic quantum critical points in heavy fermion metals defy a description within the standard Landau paradigm. We now review the striking experimental results which have lead to this conclusion. After reviewing the experimental results, we review the theory of local quantum criticality, and then discuss and reformulate some of the questions presented at the end of section 1.2.
2.4.1 CeCu$_{6-x}$Au$_x$

First, we consider the inelastic neutron scattering results of CeCu$_{6-x}$Ag$_x$ (ref. [65]). The doping $x$ serves as the tuning parameter, where the critical doping is $x = 0.1$ [65]. Extensive inelastic neutron scattering results have revealed the magnetic excitations are quasi two dimensional. At the critical doping, in stark contrast to the spin density wave prediction, inelastic neutron scattering results have revealed the dynamic spin susceptibility obeys $\omega/T$ scaling with a fractional exponent $\alpha < 1$ at the ordering wave vector $Q_{AF}$ [65], namely $\chi(Q_{AF},\omega,T) \sim 1/[T^\alpha f(\omega/T)]$. In addition, the $\omega/T$ scaling holds at and far away from the antiferromagnetic wave vector, as a result the momentum dependence does not appear to acquire an anomalous dimension [65]. Lastly, the exponent $\alpha$ appears in $H/T$ scaling of the magnetization [65]. Both $\omega/T$ scaling and the common exponent in $H/T$ scaling are consistent with hyper scaling, and an interacting quantum critical point below its upper critical dimension.

2.4.2 YbRh$_2$Si$_2$

We now consider some of the experimental results on YbRh$_2$Si$_2$, where in this case the magnetic field acts as the tuning parameter [66]. The phase diagram of YbRh$_2$Si$_2$ has now been accurately determined [18], interestingly the schematic phase diagram in figures 1.2 and 1.1 in the absence of the supercondcuting dome, resembles that of YbRh$_2$Si$_2$. The antiferromagnetic phase is separated from the heavy Fermi liquid phase by a quantum critical point. In either phase, the resistivity has the Fermi liquid form $\rho \sim T^2$, whereas in the quantum critical regime the resistivity becomes linear in temperature $\rho \sim T$. For a Fermi liquid, the Hall coefficient $R_H$, is related to the charge carrier density $n$, by $R_H \propto 1/n$ [20]. Therefore, since either side of the phase diagram is a Fermi liquid, we can directly relate $R_H$ to the charge carrier density and through Luttinger’s theorem [62] to the size of the Fermi surface. For the case
of a SDW transition, the Hall coefficient is expected to evolve smoothly across the QCP [63]. Interestingly, Hall effect measurements on YbRh$_2$Si$_2$ extrapolated to zero temperature have revealed a jump in $R_H$ at the critical field [67]. This then implies a sharp jump in the Fermi surface consistent with the destruction of the Kondo effect at an antiferromagnetic QCP. Such a QCP realizes the direct transition from the AF to the HFL phase. Lastly, the full width at half maximum of $R_H$ defines an additional energy scale $T^*$ that is linear in temperature [68]. As argued in ref. [68] $T^*$ is related to the vanishing Kondo energy scale and in turn the single particle relaxation rate $\Gamma_G$. Therefore, $\Gamma_G \sim T$, is consistent with a single particle Green’s function at the Fermi wave vector that obeys $\omega/T$ scaling, $G(k_F, \omega, T) \sim 1/[T^\alpha g(\omega/T)]$.

### 2.4.3 CeRhIn$_5$

We now come to the experimental results of CeRhIn$_5$. In this compound applying pressure and a magnetic field can tune the system through a number of interesting phases [69], one of which having both antiferromagnetic order and superconductivity [70]. For magnetic fields that are large enough to suppress superconductivity, de Haas-van Alphen (dHvA) experiments [20] have probed the Fermi surface across the quantum critical point in the normal state [71]. These experiments have revealed a jump in the Fermi surface across the antiferromagnetic QCP [71]. In addition the effective mass diverges on approach to the QCP from both sides of the phase diagram (we note that the effective mass also diverges for both YbRh$_2$Si$_2$ [18] and CeCu$_{6-x}$Au$_x$ [18]). As briefly discussed in the previous section $T_K \propto 1/m^*$, therefore a diverging effective mass is consistent with the Kondo energy scale going to zero. Therefore, the experiments on CeRhIn$_5$ are consistent with a Kondo breakdown quantum critical point in the normal state, and it is very interesting to consider how this QCP may effect superconductivity.
2.4.4 Local Quantum Criticality

The theory of local quantum criticality (LQC) of Si et. al. [72, 73] has been particularly successful in understanding the \( \omega/T \) scaling of the spin susceptibility in \( \text{CeCu}_{6-x}\text{Au}_x \). In addition, LQC has provided a platform and effective models\(^1\) to predict the additional energy scale \( T^* \) in \( \text{YbRh}_2\text{Si}_2 \), and the jump in the Fermi surface of \( \text{YbRh}_2\text{Si}_2 \) and \( \text{CeRhIn}_5 \). In the theory of LQC, the extended dynamical mean field theory (EDMFT) [30, 74, 75] is used to map the Kondo lattice in equation (2.6) to the Bose Fermi Kondo model with self consistent bosonic and fermionic baths. The Bose Fermi Kondo model (BFKM) is defined as

\[
H_{\text{BFKM}} = \sum_{\mathbf{k}, \sigma} E_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} + J_K s_0^c \cdot S + \sum_{\mathbf{q}} \omega_\mathbf{q} \phi_\mathbf{q}^\dagger \cdot \phi_\mathbf{q} + g S \cdot \sum_{\mathbf{q}} (\phi_\mathbf{q}^\dagger + \phi_{-\mathbf{q}}) \quad (2.13)
\]

where \( \phi = (\phi^x, \phi^y, \phi^z) \) is a vector bosonic bath, and the dispersions \( E_\mathbf{k} \) and \( \omega_\mathbf{q} \) are determined self consistently. The local impurity model is related to the lattice model through the self consistency conditions imposed on the single particle Greens function \( G_{ij}(\tau) = \langle T_\tau c_i(\tau) c_{j}^\dagger(\tau) \rangle \) and spin susceptibility \( \chi_{ij}(\tau) = \langle T_\tau S_i(\tau) \cdot S_j \rangle \). The self consistency condition is most naturally expressed in momentum and Matsubara frequencies,

\[
G_{\text{loc}, \sigma}(i\omega_n) = \sum_{\mathbf{k}} G_{\sigma}(\mathbf{k}, i\omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n - \epsilon_\mathbf{k} - \Sigma(i\omega_n)}
\]

\[
\chi_{\text{loc}}(i\nu_n) = \sum_{\mathbf{q}} \chi(\mathbf{q}, i\nu_n) = \sum_{\mathbf{q}} \frac{1}{I_\mathbf{q} + M(i\nu_n)} \quad (2.14)
\]

where \( G_{\text{loc}} \) and \( \chi_{\text{loc}} \) are correlation functions calculated within the impurity model in equation (2.13), and \( \omega_n \) (\( \nu_n \)) denote fermionic (bosonic) Matsubara frequencies. The EDMFT approximates the lattice self energies as momentum independent. In terms of

\(^1\)To be discussed in detail in chapters 3, 4, 5, 7 and 8
the impurity model the single particle self energy is \[ \Sigma(i\omega_n) = G_{0,\sigma}^{-1}(i\omega_n) - 1/G_{\text{loc},\sigma}(i\omega_n) \]
and the spin self energy \[ M(i\nu_n) = \chi_0^{-1}(i\nu_n) + 1/\chi_{\text{loc}}(i\nu_n) \], where the Weiss fields \( G_{0,\sigma}^{-1} \)
and \( \chi_0^{-1} \) are self consistently determined, and are related to the greens functions of the fermionic and bosonic baths [73]

\[
G_{0,\sigma}(i\omega_n) = \sum_k \frac{1}{i\omega_n - E_k}, \quad (2.15)
\]

\[
\chi_0^{-1}(i\nu_n) = \sum_q \frac{2g^2\omega_q}{\omega_q^2 - \nu_n^2}, \quad (2.16)
\]

Solving the EDMFT equations assuming a two dimensional magnetic density of states (similar to the case of CeCu\(_{6-x}\)Au\(_x\)), yields a magnetic quantum phase transition that is accompanied by a critical breakdown of the Kondo effect [72, 73] (for Ising anisotropy [76, 77, 78, 79, 80]). This is manifested through the local spin susceptibility diverging when the lattice spin susceptibility diverges. This can be seen from equation (2.14), which implies \( \chi_{\text{loc}}(i\nu_n) \propto \log |1 + 2I\chi(Q_{AF}, i\nu_n)| \) where \( \chi(Q_{AF}, i\nu_n) \) is the lattice spin susceptibility at the ordering wave vector \( Q_{AF} \). This solution then gives rise to an anamalous frequency dependence and \( \omega/T \) scaling in the lattice spin susceptibility [72, 73]. In contrast, assuming a three dimensional magnetic density of states leads to a spin density wave quantum critical point where \( \chi(Q_{AF}, i\nu_n = 0) \) diverges but \( \chi_{\text{loc}}(i\nu_n = 0) \) does not. We will revisit this in detail in chapters 6 and 8, when we extend the EDMT approach to a dynamical quantum cluster theory.

The theory of LQC in essence, embeds the physics of critical Kondo destruction of the impurity model into the lattice via the EDMFT self consistent equations. We can then regard the effective impurity models as “toy models” that can be studied in their own right (neglecting self consistency), where the physics and universality classes associated with a Kondo destroyed QCP can be studied in a controlled and systematic fashion. To be precise, by a Kondo destroyed QCP we mean a second order zero
temperature phase transition between a phase where the impurity spin is completely screened by the conduction band (Kondo screened) and a phase where the spin is essentially decoupled from the conduction band (Kondo destroyed). Therefore, this does not include the Kosterlitz-Thouless [81] phase transition in the standard Kondo model as the Kondo coupling is changed from ferro- to antiferro-magnetic [53].

2.4.5 Summary

Taking the experimental results from CeCu$_{6-x}$Au$_x$, YbRh$_2$Si$_2$, and CeRhIn$_5$ all into account allows us to clarify the original questions posed at the end of section 1.2. In the following, we aim to answer and redefine these questions: The failure of the Landau description is rooted in assuming the heavy quasiparticles remain intact across the QCP [63] and therefore neglect the critical modes associated with the destruction of the Kondo effect [a resolution of question 1]. The theory of local quantum criticality has provided a framework to describe the critical breakdown of the Kondo effect. In order to understand the universality class’s associated with Kondo breakdown QCPs, in chapters 3, 4, and 5 we study toy models that possess second order phase transitions where the Kondo effect is destroyed at the QCP [restatement of question 2].

In chapter 3 we develop the framework to determine the finite temperature dynamical scaling form of local correlation functions in the vicinity of the Kondo breakdown QCP. Such a scaling form is relevant to understand the unconventional dynamical scaling properties of CeCu$_{6-x}$Au$_x$ and YbRh$_2$Si$_2$. We then use this approach in chapters 4 and 5. If instead we consider the periodic Anderson model at mixed valence, a natural question to ask is: what is the role of charge fluctuations on the Kondo destroyed QCP, can such a transition occur away from the integer valence limit? We discuss the role of charge excitations in chapter 4, and show local charge excitations can also be driven critical at the Kondo destroyed QCP. In chapter 5 we go on to
explore the different types of universality classes associated with Kondo destroyed quantum critical points in single impurity models.

The experiments on CeRhIn$_5$ naturally led to the question, what is the effect of Kondo destroyed quantum critical points on superconductivity [restatement of question 3]? We address this in chapter 6 by first extending the theory of local quantum criticality to include finite size corrections and show how to calculate superconducting properties of the normal state. In chapter 7, we explore an effective toy model that comes out of the cluster extension of chapter 6, and has both Kondo destruction and local pairing correlations. In chapter 8 we study the periodic Anderson model within a C-EDMFT approach and show the model posses a LQC and a non-Fermi liquid regime [see question 4]. Also in chapter 8 we study the normal state superconducting properties of LQC in chapter 8, and show this QCP gives rise to a significantly enhanced lattice pairing susceptibility, indicating a new pairing mechanism pertinent to heavy fermion metals. In the following section we reexamine questions 4 and 5 in the context of heavy fermions.

2.5 Quantum Fluctuations

It is well known that quantum fluctuations are strongest in one dimension and diminish as the dimension is increased [26, 34]. A main conclusion in the EDMFT solution of the Kondo lattice is the distinction between two and three dimensional magnetic fluctuations. This result can be rephrased as, the magnetic fluctuations in the three dimensional case are not strong enough to suppress Kondo screening at the QCP. Quantum fluctuations can naturally be tuned in the Heisenberg part of the Kondo lattice model by introducing geometrical magnetic frustration [82], varying the size of the local moment $S$, or applying a transverse magnetic field (in the case of Ising anisotropic spin-spin interactions) [83]. Experiments are now coming to bear on
the issue. A growing number of heavy fermion compounds have recently been found with effective spin $S = 1/2$ local moments that reside on geometrically frustrated lattices. For example the compounds Yb$_2$Pt$_2$Pb, CePd$_{1-x}$Ni$_x$Al, and YbAl$_3$C$_3$ have local moments that reside on the Shastry-Sutherland, Kagome, and triangular lattices respectively.

Such considerations have prompted Si [84, 85] and Coleman and Nevidomskyy [86], to propose a “global” phase diagram of heavy fermions, where the ratio of the Kondo temperature to the RKKY interaction $T_K/I$ lies on the horizontal axis and quantum fluctuations along the vertical axis. It is quite natural how new phases can emerge when incorporating quantum fluctuations [see questions 4 and 5]. Having established the existence of the HFL, the SDW, and the AF phases we show the schematic phase diagram in figure 2.5. The consideration of quantum fluctuations introduces a new phase labeled $P_S$, where the quantum fluctuations are so strong their is no magnetic order and no Kondo screening. In such a phase, for the case of a large amount
of geometrical frustration, the local moments may be in a gapped quantum spin liquid [82] or valence bond solid ground state. We revisit this in detail in chapter 9, where we consider the Shastry-Sutherland Kondo lattice and discuss the implications for the global phase diagram of heavy fermion metals.
In the previous chapter, section 2.4, we have examined the unconventional scaling properties of heavy fermion metals. In this chapter we aim to understand the origin of $\omega/T$ scaling in the spin susceptibility and the linear in temperature single particle relaxation rate obtained in experiments on CeCu$_{6-x}$Au$_x$, and YbRh$_2$Si$_2$, respectively. Motivated by the EDMFT mapping to a single impurity model (section 2.4), we study the Kondo destroyed quantum critical point in the particle hole symmetric pseudogap Anderson model (defined below). In particular, using the insights gained from a calculation in a dynamic large $N$ limit, we are then able use the continuous time quantum Monte Carlo [87] to determine the finite temperature dynamic scaling form of correlation functions in imaginary time that give rise to $\omega/T$ scaling, and determine the relaxation rates of both spin and single particle excitations [88].
3.1 Introduction

The dynamical scaling and relaxational properties of CeCu$_{6-x}$Au$_x$ and YbRh$_2$Si$_2$, provide important clues to the nature of the heavy-fermion QCP. Yet, theoretically, such real-frequency behavior is difficult to study. At finite temperatures, two regimes need to be distinguished: the quantum coherent ($\hbar \omega > k_B T$) and quantum relaxational ($\hbar \omega < k_B T$) regimes [40]. Calculation methods (such as Monte Carlo) typically work in the imaginary time domain, and the non-zero Matsubara frequencies ($\omega_n$) are necessarily in the $|\omega_n|/T > 1$ regime. Extracting the behavior at real frequencies requires an analytical continuation, which is in general a numerically ill-conditioned procedure. The numerical renormalization group (NRG) operates on the real frequency axis, but it is not reliable for the quantum relaxational regime at nonzero temperatures.

In this chapter, we address the dynamical and relaxational properties of the particle-hole symmetric pseudogap Anderson model in both frequency regimes. Our motivations to study this model are multi-fold. The pseudogap Anderson model is the simplest impurity problem that contains the physics of critical Kondo destruction. Due to the pseudogap density of states, the lack of available states near the Fermi energy makes it difficult for the conduction electrons to screen the spin, and varying the Kondo coupling yields a QCP [89, 90, 91, 92, 93, 94, 95], which separates a Kondo-screened Fermi-liquid phase from a Kondo-destroyed local-moment phase. However, a proper understanding of the dynamical scaling at finite temperatures and the associated relaxational behavior is not yet available even in this simplest model. (See below for comparison of our results with prior studies [91, 94, 95].) Furthermore, the pseudogap Anderson/Kondo model is relevant to a number of realistic physical settings. It has been invoked in the context of non magnetic impurities in cuprate superconductors [92]. It has also been shown that a judicious tuning of a double quantum-dot system can produce a pseudogap in the effective density of states [96].
In disordered metals, a novel phase has been attributed to the occurrence of local pseudogaps near the Fermi energy at local moment sites [97]. Finally, the pseudogap Kondo model is the appropriate model to describe point defects in graphene [98].

3.2 Methods

We study the model using a continuous-time quantum Monte Carlo approach (CT-QMC) [87]. We determine the full scaling functions at real frequencies and finite temperatures for both the dynamical spin susceptibility and single-electron Green’s function. We do so, by taking advantage of insights gained from exact calculations at real frequencies and finite temperatures in a dynamical large-N limit of the model. The results in the large-N limit motivate us to analyze the imaginary-time correlators in the physical $N = 2$ model in a way that uncovers the form of a boundary conformally-invariant fixed point. The latter, in turn, can readily be analytically-continued to real frequency at finite temperatures. We establish that both the dynamical spin susceptibility and single-electron Green’s function display an $\omega/T$-scaling and contain a linear-in-$T$ relaxation rate. Having determined the finite temperature imaginary time scaling form is incredibly useful, as we will continue to use this insight in chapters 4 and 5, to interpret our results in imaginary time without performing any ill conditioned analytic continuation. As a by-product, we are able to test the CT-QMC approach, which is based on a high-temperature expansion, near a QCP; whether this method can reach low-enough temperatures with enough accuracy to resolve quantum critical features has, to our knowledge, not been addressed before.
3.3 Pseudogap Kondo model in a dynamical large-N limit

To set the stage for the CT-QMC study, we start with the SU(N) × SU(M) Kondo model \[99\] in the presence of a pseudogap in the limit of large N and M. In the remainder of the thesis, we work in units with \(\hbar = k_B = 1\). The Hamiltonian is

\[
H_{\text{PKM}} = \left(\frac{J_K}{N}\right) \sum_\alpha S \cdot s_\alpha + \sum_{p,\alpha,\sigma} E_p \, c_{p\alpha\sigma}^\dagger c_{p\alpha\sigma}.
\] (3.1)

Here, the spin and channel indices are \(\sigma = 1, \ldots, N\) and \(\alpha = 1, \ldots, M\). The conduction electron density of states takes the form:

\[
\rho(\omega) = \sum_p \delta(E_p - \omega) = \rho_0 |\omega/D|^r \Theta(D - |\omega|),
\] (3.2)

with \(2D\) being the bandwidth. That this limit has a non-trivial QCP can be seen through the particular form of the perturbative (in \(r\)) RG equation \[89\]. In the limit of large N and M, the RG beta function becomes

\[
\beta(j) = -j(r - j + \kappa j^2),
\] (3.3)

with \(j = J_K/D\) \[100\]. This establishes that the QCP survives the large-N limit and can be accessed perturbatively. To order \(r\), the large-N beta function is identical to its N= 2 counterpart \[89, 91\] suggesting that the universal critical scaling properties of the \(N = 2\) QCP are preserved by taking the large-N limit. In this limit, the local degrees of freedom are expressed in terms of pseudo-fermions \(f_\sigma\) and a bosonic decoupling field \(B_\alpha\), where \(S_{\sigma,\sigma'} = f_\sigma^\dagger f_{\sigma'} - \delta_{\sigma,\sigma'}Q/N\), and \(Q\) is related to the chosen
irreducible representation of SU(N) \[99, 101\]. The large-\(N\) equations are

\[
\begin{align*}
\Sigma_B(\tau) &= -G_0(\tau)G_f(-\tau); \quad \Sigma_f(\tau) = \kappa G_0(\tau)G_B(\tau); \\
G_B^{-1}(i\nu_n) &= 1/J_K - \Sigma_B(i\nu_n); \\
G_f^{-1}(i\omega_n) &= i\omega_n - \lambda - \Sigma_f(i\omega_n);
\end{align*}
\]

(3.4)

together with a constraint \(G_f(\tau \to 0^-) = Q/N\) \[99\]. Here, \(\kappa = M/N\), \(\lambda\) is a Lagrangian multiplier enforcing the constraint and \(G_0 = -\langle T_\tau c_{\sigma\alpha}(\tau) c_{\sigma\alpha}^\dagger(0) \rangle_0\) is the non-interacting Green’s function \[92\].

Solving the large-\(N\) equations in real frequencies for arbitrary \(\omega\) and \(T\) \[100\], the full scaling functions in both, the quantum coherent (\(\omega > T\)) and relaxational (\(T > \omega\)) regimes are obtained. At the critical coupling \(J_c(r)\), we find that all the correlators display an \(\omega/T\)-scaling. This is demonstrated in Fig. 3.1(a) for the local single-particle Green’s function \([i.e., the T-matrix, G(\omega, T), associated with G(\tau) = G_f(\tau)G_B(\tau)]\), and in Fig. 3.1(b) the local spin susceptibility \(\chi(\omega, T)\), which corresponds to \(\chi(\tau) = -G_f(\tau)G_f(-\tau)\).

Before moving on to our results in imaginary time, we find it very useful to briefly review the finite temperature scaling forms appropriate to the standard (metallic) Kondo model. It is well known that a quantum impurity model with a bulk component that is conformally invariant can be described by a boundary conformal field theory \[102, 103\]. In any such theory, a conformal mapping can be used to obtain correlators at temperatures \(T > 0\) from their \(T = 0\) counterparts. In particular, the zero-temperature two-point correlator of a primary conformal field \(\Psi\) with scaling dimension \(\lambda\) exhibits a power-law decay \(\langle \Psi(\tau, T = 0) \Psi(0, T = 0) \rangle \sim \tau^{-2\lambda}\). This gives...
rise, via a conformal mapping, to the scaling form \[104, 105\]

\[\langle \Psi(\tau, T) \Psi(0, T) \rangle \sim \left( \frac{\pi T}{\sin(\pi \tau T)} \right)^{2\lambda}. \tag{3.5}\]

The Fourier transform of Eq. (3.5) can be performed analytically and yields a function of \(\omega_n/T\) that can be analytically continued to real frequencies provided that \(2\lambda < 1\). For \(2\lambda \geq 1\), the Fourier-transform integral does not converge, necessitating introduction of a finite cutoff scale that spoils \(\omega/T\) scaling. Therefore, demonstration that a system obeys Eq. (3.5) with \(2\lambda < 1\) is sufficient to show the presence of \(\omega/T\) scaling, a characteristic feature of interacting QCPs.

A key insight from the large-\(N\) result is that the scaling functions contain more information beyond \(\omega/T\) scaling \textit{per se}. They have the particular form discussed above [equation (3.5)], that is associated with a boundary conformally-invariant fixed point, depending on \(\tau\) as a power law in \(\pi T/\sin(\pi \tau T)\) [104]. To see this, we obtain the imaginary-time dependence from the real-frequency results via

\[\Phi(\tau) = -\eta \int_{-\infty}^{\infty} d\omega \frac{\exp(-\tau \omega)}{\exp(-\beta \omega) - \eta} \text{Im}(\Phi(\omega + i0^+)), \tag{3.6}\]

for \(0 < \tau \leq \beta\). Here, \(\eta = \pm\) for bosonic/fermionic \(\Phi\). Fig. 3.1 shows the (c) Green’s function \(G(\tau, T)\) and (d) susceptibility \(\chi(\tau, T)\) versus the combination \(\pi T/\sin(\pi \tau T)\). Both collapse on a single scaling curve in terms of \(\pi T/\sin(\pi \tau T)\) for all (low-enough) \(T\). A power-law behavior for \(\tau \to 1/(2T)\) is seen over about 7 decades, and the exponents are compatible with those for the frequency dependence.
Figure 3.1: Scaling functions for the imaginary part of (a) Green’s function $G(\omega, T)$ and (b) susceptibility $\chi(\omega, T)$ for $r = 0.3$ and $\kappa = 0.5$ at the critical $J_c \approx 1.54$ (with $T_K^0 \approx 0.3D$ for $r = 0$). Both functions display $\omega/T$-scaling with scaling functions $\Phi$ obeying $\Phi(\omega/T \to 0) \to c$ or $0$ for $G$ or $\chi$, where $c$ is a nonzero constant. (c),(d) the scaling functions in imaginary time are compatible with a boundary conformal field theory, showing power law dependence on $\pi T/\sin(\pi \tau T)$.

3.4 Pseudogap Anderson model at $N = 2$

Guided by the large-N results, we turn to the scaling functions for $G(\tau, T)$ and $\chi(\tau, T)$ of the particle-hole symmetric pseudogap Anderson model at $N = 2$; the low-energy properties of this model are identical to its pseudogap Kondo counterpart. To this end, we bring to bear the recently developed hybridization-expansion Monte Carlo method [106, 107] on a quantum critical model. This CT-QMC approach involves a stochastic sampling of a perturbation expansion in the host-impurity hybridization or
a weak coupling expansion [108, 107, 106, 109]. The results are free of any finite-size effects [110].

The Anderson impurity model is defined by \( \hat{H} = \hat{H}_0 + \sum_{\sigma} \hat{H}^{(\sigma)}_1 \) where

\[
\begin{align*}
\hat{H}_0 &= \hat{H}_c + \hat{H}_{\text{loc}} = \sum_{k,\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} (\epsilon_d + \frac{1}{2} U \hat{n}_{d,-\sigma}) \hat{n}_{d\sigma} \\
\hat{H}^{(\sigma)}_1 &= \sum_k (V_{d_k} \hat{d}_\sigma^\dagger c_{k\sigma} + \text{H.c.})
\end{align*}
\]

(3.7)

with \( \hat{n}_{k\sigma} = c_{k\sigma}^\dagger c_{k\sigma} \), \( \hat{n}_{d\sigma} = \hat{d}_\sigma^\dagger \hat{d}_\sigma \), \( \epsilon_k \) being the host dispersion, \( V_{d_k} \) the hybridization, and \( \epsilon_d \) the impurity level energy. We consider the particle-hole symmetric case where \( \epsilon_d = -\frac{1}{2} U \), with \( U \) being the onsite Coulomb repulsion. The host-impurity coupling is specified by the imaginary part of the hybridization function \( \Gamma(\omega) = \pi \sum_k |V_{d_k}|^2 \delta(\omega - \epsilon_k) \). As in Eq. (3.2), we choose \( \Gamma(\omega) = \Gamma_0 |\frac{\omega}{D}|^r \Theta(D - |\omega|) \). The critical point exists only for \( 0 < r < \frac{1}{2} \) [90].

Central to the CT-QMC approach adopted here is the expansion of the partition function \( Z = \text{Tr}\{\hat{T}_\tau e^{-\beta \hat{H}_0} \prod_\sigma \exp[- \int_0^\beta d\tau \hat{H}^{(\sigma)}_1(\tau)]\} \) in the hybridization term [106]. For further details, see appendix B, where we describe the details for a more general model. We measure the single particle Green’s function \( \mathcal{G}_\sigma(\tau) = \langle T_\tau d_\sigma(\tau) d_\sigma^\dagger(0) \rangle \), the local spin susceptibility \( \chi(\tau) = \langle T_\tau S_z(\tau) S_z(0) \rangle \) and powers of the local magnetization \( \langle M_z^n \rangle = \langle (\frac{1}{\beta} \int_0^\beta d\tau S_z(\tau))^n \rangle \) where \( S_z(\tau) = \frac{1}{2}[\hat{n}_\uparrow(\tau) - \hat{n}_\downarrow(\tau)] \). The static susceptibility is obtained from \( \chi(\omega = 0) = (g\mu_B)^2 \int_0^\beta d\tau \chi(\tau) \). In qualitative agreement with results obtained for a metallic host \( r = 0 \) [111], we find that the computation time (to achieve a fixed number of measurements) for \( r > 0 \) scales as the square of the mean perturbation order. Thermalization can be traced by \( \langle n_d \rangle \) which obeys \( \langle n_d \rangle = 1 \) in the particle-hole symmetric model. We also performed a binning analysis and obtained the integrated autocorrelation time which increases with decreasing temperature but turned out to be small (compared to the number of measurements) at all tempera-
By varying $U$ we can tune the model through a QCP. Correspondingly, Fig. 3.2(a) shows that the large-$\beta$ limit of $\chi(\tau = \beta/2, \beta)$ vanishes for small $U$ (Kondo-screened phase) and is equal to the Curie constant for large $U$ (Kondo-destroyed local-moment phase). To accurately determine $U_c(r)$ we apply finite temperature scaling to the Binder cumulant [112],

$$B(U, T) = \frac{\langle M_z^4 \rangle}{\langle M_z^2 \rangle^2}. \quad (3.8)$$

In analogy with classical Monte Carlo simulations $1/T = \beta$ plays the role of the system size and $U$ the classical temperature, therefore we can extrapolate our results to zero temperature to determine the location of the QCP. We find swap moves between...
up and down spin segments [113] are necessary to accurately measure the Binder cumulant; for the results in Fig. 3.2(b) we performed a swap move every 100 measurements. The nature of the intersection of the data in Fig. 3.2(b) implies the phase transition is continuous, from the location of the intersection we obtain the critical value of $U$. For $r = 0.4$ we obtain $U_c/D = 0.085 \pm 0.002$. In the quantum critical regime the static local susceptibility displays an anomalous $r$-dependent exponent; we find

$$\chi(T, U_c, r = 0.4) \sim T^{-x},$$

with $x = 0.68(3)$ in good agreement with NRG results [91].

Now, we are in a position to discuss the finite-temperature dynamical scaling properties of $G(\tau, T)$ and $\chi(\tau, T)$. Guided by the large-$N$ results, we plot them as functions of $(\pi T)/\sin(\pi \tau T)$ in Fig. 3.3. Excellent scaling collapse is observed over about two decades, for all temperatures in the scaling regime. We reach an important conclusion:

$$\chi_{\text{crit}}(\tau, T) = \Phi \left( \frac{\pi \tau T}{\sin(\pi \tau T)} \right)^{T \ll T^0_K} \times \left( \frac{\pi \tau T}{\sin(\pi \tau T)} \right)^{1-x},$$

for $\tau^{-1} \ll T^0_K$, Fig. 3.3(b). Since $0 < 1 - x < 1$, the results for $\chi(\tau, T)$ imply that the order parameter susceptibility shows $\omega/T$-scaling. A similar conclusion applies to $G(\omega, T)$, as seen in Fig. 3.3(a). Our results yield $G(\tau, T \to 0) \sim \tau^{-\delta}$, with the exponent $\delta = 1 - r$, which is believed to be exact [95]. The fact that $2\delta \neq 1 - x$ signifies the importance of vertex corrections and in part reflects the interacting nature of the QCP (see below).

The boundary conformally-invariant form of $\chi$ and $G$ immediately imply that their dependence on real frequency satisfies $\omega/T$ scaling and that their relaxation rates, defined in the quantum relaxational regime, is linear in $T$. Expressed in terms of equation $\Gamma_M = i(\partial \ln M(\omega, T)/\partial \omega|_{\omega=0})^{-1}$ for a correlator $M$, the relaxation rates $\Gamma_{\chi} = aT$
and $\Gamma_G = bT$, where $a$ and $b$ are universal dimensionless constants. Such linear-in-$T$ form is consistent with what has been observed in quantum critical heavy fermion compounds, for both the single-particle Green function [?] and order parameter susceptibility [?]. A linear-in-$T$ relaxation rate signifies that the QCP is interacting, i.e., containing a nonzero nonlinear coupling among the critical modes. By contrast, at a Gaussian QCP (whose critical modes do not interact at the fixed point), the relaxation rate will be super-linear-in-$T$ because the nonlinear coupling itself vanishes as $T$ approaches zero (where the QCP lies) [40].

### 3.5 Discussion

It is instructive to compare our study with previous theoretical treatments of the finite-temperature scaling behavior of the pseudogap Anderson/Kondo model. One study [91] is perturbative in $r$, which not only becomes unreliable for finite $r$ but also does not allow the study of the single-particle Green’s function. Another study carries out calculations in real frequency at finite temperatures, but relies on the resummation of a perturbation series whose validity for the quantum critical regime is not clear [94]. Yet another study uses a Callan-Symanzik approach which requires analytic continuation that is problematic as reflected in the non-commutativity of the resummation and analytic continuation [95]; it will be important to check whether that procedure yields a $\mathcal{G}’(\omega, T)$ that is compatible in analyticity with $\mathcal{G}”(\omega, T)$. As a more specific illustration of our results, we note that $T^r \mathcal{G}”(\omega/T \to 0)$ is a nonzero constant, which is contrary to both the perturbative results of Ref. [94] and the results of the real-frequency Callan-Symanzik resummation for $\mathcal{G}”(\omega, T)$ [95].

The scaling of the local correlators in terms of $\pi T/\sin(\pi \tau T)$ suggests that the boundary critical state and the associated boundary operators are described by their counterparts in an effective model with conformal invariance. This is so in spite of
Figure 3.3: Scaling of (a) Green’s function $G(\tau, T)$ and (b) susceptibility $\chi(\tau, T)$ at the QCP for $r = 0.4$, $\Gamma_0 = 0.1D$ and $U_c(r = 0.4) = 0.085D$. The Kondo temperature in this case is $T_K^0 \approx 0.029D$ (for $r = 0$). For $T/D < 5 \cdot 10^{-3}$, we observe collapse of the data over several decades for more than two decades of the parameter $(\pi T)/\sin(\pi \tau T)$, i.e., $G_c(\tau, T) = \Psi(\pi T/\sin(\pi \tau T))$ and $\chi_c(\tau, T) = \Phi(\pi T/\sin(\pi \tau T))$. $\Psi(y \to 0) \propto y^{\delta}$ with $\delta = 0.57(5)$, and $\Phi(y \to 0) \propto y^{1-x}$ with $x = 0.68(3)$.

the fact that, for our problem, the pseudogap form of the DOS means that the bulk fermionic component of the Hamiltonian lacks conformal invariance. Thus, our results suggest an enhanced conformal symmetry that characterizes the QCP.

### 3.6 Summary

In this chapter, we have obtained the full finite-temperature scaling functions at the local quantum critical point of the pseudogap Anderson and Kondo models. Using the results directly obtained in real frequency ($\omega$) in the large-$N$ limit, and by showing that the imaginary-time local correlators of the physical $N = 2$ model have the form of a boundary conformally-invariant fixed point, we have succeeded in determining the full scaling function in both the quantum coherent and relaxational regimes without using any numerically ill-conditioned analytical-continuation schemes. We have demonstrated that the Kondo-breakdown QCP features a linear-in-$T$ relaxation rate for both spin and single-electron dynamics, which is consistent with the experimental
observations in quantum-critical heavy fermion metals.
In chapter 3 we have focused on the dynamical scaling and relaxational properties of a Kondo destroyed QCP at particle hole symmetry. In this chapter, we are interested in studying the different types of quantum critical points that may occur in the periodic Anderson model at mixed valence [see equation (2.7), as opposed to the Kondo lattice model]. Again, motivated by the EDMFT mapping (section 2.4), we focus on the universality class associated with the Kondo breakdown QCP in the single impurity pseudogap Anderson model. Breaking particle hole symmetry introduces charge fluctuations on to and off of the impurity, which allows us to study the critical point when the impurity occupation is not close to an integer value. Interestingly, we show charge excitations are not just bystanders, instead they are also driven critical. Guided by the dynamical scaling form we have established in chapter 3 we are able to show both spin and charge susceptibilities obey $\omega/T$ and $H/T$ scaling [114].
4.1 Introduction

Theoretical studies of critical Kondo destruction have largely been confined to the Kondo-lattice limit of integer valence. In rare-earth intermetallics, superconductivity is believed to arise in the vicinity of valence transitions [115, 116, 117], which have been found to be first order. Until recently, there has been no significant evidence for a QCP associated with valence fluctuations. Interestingly, the situation has changed with the observation of mixed valency in the ytterbium-based heavy-fermion superconductor $\beta$-YbAlB$_4$ [118], which is quantum critical under ambient conditions [119]. In an applied magnetic field, the magnetization obeys $H/T$ scaling [120], consistent with the $\omega/T$ scaling seen previously near the unconventional QCPs of antiferromagnetic heavy-fermion compounds. These properties implicate $\beta$-YbAlB$_4$ as a strong candidate for a mixed-valent heavy-fermion QCP, and raise the prospect that the material’s unusual scaling behavior can be understood in terms of critical Kondo physics.

At first glance, critical Kondo destruction at mixed valence appears unlikely. Kondo destruction in a Kondo lattice amounts to the localization of $f$ electrons. While unconventional, this is physically transparent, because localization can readily arise for a commensurate filling of an electronic orbital (one $f$-electron per site). At mixed valence, the situation is more subtle because the $f$ orbital has a fractional, generally incommensurate, per-site occupancy, and there is no mechanism known for electron localization at incommensurate fillings. This leads to important questions of principle: Can critical Kondo destruction occur in the presence of valence fluctuations and, if so, how does the criticality compare to its local-moment counterpart? For instance, are charge excitations part of the critical fluctuation spectrum?

In this chapter, we address these issues in the mixed-valence regime of an Anderson impurity model whose conduction-electron density of states features a pseudogap
centered on the Fermi energy. We focus on an impurity model because of the local nature of the Kondo-destruction physics (as discussed in detail in chapter 1, section 2.4); Given that the commensurate-filling (i.e., local-moment) limit of the model exhibits critical Kondo destruction \[91\] and as in shown in the previous chapter, the associated dynamical scaling properties \[88\], we consider the pseudogapped density of states to provide a prototype setting to search for a Kondo-destruction QCP at mixed valence. Our model has the advantage of being amenable to study using reliable methods: the continuous-time quantum Monte Carlo (CT-QMC) method \[87\] and the numerical renormalization group (NRG) \[91, 121, 90\].

Surprisingly, we do find critical Kondo destruction in this mixed-valent model. The critical properties in the spin sector reflect the collapse of an energy scale as the QCP is approached from the Kondo-screened side but not from the Kondo-destroyed side, much as in the integer-valent (local-moment) limit. By contrast, the charge sector shows a collapsing energy scale on both sides of the QCP. The critical point displays $H/T$ (and $\omega/T$) scaling. This existence proof for a Kondo destruction QCP at mixed valence makes it feasible to interpret the $H/T$ and related scaling properties of $\beta$-YbAlB$_4$ in terms of an interacting fixed point.

## 4.2 Methods

The Anderson impurity Hamiltonian is defined in equation (3.7). The band density of states vanishes in a power-law fashion at the Fermi energy ($\epsilon_F = 0$), i.e. has a pseudogap [equation (3.2)] As mentioned in the previous chapter, the impurity-band interaction is completely specified by the imaginary part of the hybridization function,

$$\Gamma(\epsilon) = \pi \sum_k |V_{dk}|^2 \delta(\epsilon - \epsilon_k) = \Gamma_0 |\epsilon/D|^r.$$ 

The critical properties of the model with particle-hole (p-h) symmetry ($\epsilon_d = -U/2$) and its Kondo limit ($U \gg \Gamma_0$, where local charge fluctuations are negligible)
Figure 4.1: (a) Binder cumulant \( B(U, \beta) \) vs. \( U \) for \( r = 0.6, \Gamma_0 = 0.1D, \) and \( \epsilon_d = -0.05D, \) and the labeled temperatures. Error bars were obtained from a jackknife analysis of the CT-QMC data. (b) Blow up of the same data around the intersection of curves, which determines \( U_c/D = 0.063125 \pm 0.0008. \)

have been investigated in a number of analytic and numerical studies \([90, 91, 89, 92, 93, 95, 122, 88]\), (. see the previous chapter for the dynamical scaling functions in the presence of particle hole symmetry \([88]\)). The breaking of p-h symmetry is irrelevant for pseudogap exponents \( r \) in the range \( 0 < r < r^* \approx 0.375, \) but becomes relevant for \( r > r^* \), leading to a mixed-valent QCP \([90]\); \( r = 1 \) serves as an upper critical “dimension”, above which the critical properties are mean-field like \([91, 122]\).

In the following chapter, we investigate the p-h-asymmetric pseudogap Anderson model by varying \( U \) for fixed \( \Gamma_0 \) and \( \epsilon_d \) to pass from a Kondo-screened strong-coupling phase \( (U < U_c) \) to a Kondo-destroyed local-moment phase \( (U > U_c). \) We apply the CT-QMC technique (see appendix B), which was recently shown to be able to reach temperatures \( T \) sufficiently low to access the quantum critical regime \([88]\). We measure the dynamical local spin and charge susceptibilities, \( \chi_s(\tau, \beta) = \langle T_\tau S_z(\tau)S_z(0) \rangle \) and \( \chi_c(\tau, \beta) = \langle T_\tau :n(\tau):n(0): \rangle, \) respectively, where \( S_z = \frac{1}{2}(n_\uparrow - n_\downarrow), \) \( :n: = \sum_\sigma n_\sigma - \langle \sum_\sigma n_\sigma \rangle, \) and \( \beta = 1/T \) (taking \( k_B \equiv 1 \)) plays the role of the system size. The corresponding static susceptibilities follow from \( \chi_{c,s}(\beta) = \int_0^\beta d\tau \chi_{c,s}(\tau). \) As mentioned in chapter 3, measuring powers of the local magnetization allows con-
Figure 4.2: Valence and local spin properties vs. $u = U/U_c - 1$ for $r = 0.6$, $\Gamma_0 = 0.1D$, and $\varepsilon_d = -0.05D$: (a) Occupancy $\langle n_d \rangle$ at the labeled temperatures. The QCP ($u = 0$) occurs at mixed valence, i.e., $\langle n_d \rangle \neq 1$. (b) Local magnetization $M_{\text{loc}}$, showing quenching of the impurity spin for $u < 0$ but the emergence of a free local moment for $u > 0$.

struction of the Binder cumulant [112] [see equation (3.8)]. We supplement our $T > 0$ (finite-$\beta$) CT-QMC results with static quantities calculated arbitrarily close to $T = 0$ ($\beta = \infty$) using the NRG method as adapted to treat pseudogap impurity problems [121, 90, 91]. NRG results presented below were obtained with Wilson discretization parameter $\Lambda = 9$, with $\Gamma_0$ corrected [90] to compensate for the band discretization, and retaining all many-body states up to 50 times the effective bandwidth of each iteration.

4.3 Phases

We focus our discussion on the representative case of one pseudogap exponent $r = 0.6$ with $\Gamma_0 = 0.1D$ and $\varepsilon_d = -0.05D$. Figure 4.1 plots the variation of the Binder cumulant with $U$ at different temperatures. For small $U$, charge fluctuations are strong and the Binder cumulant lies above the range $1 < B(U, \beta) < 3$ obeyed by a pure spin system [88, 112]; in this limit, the low-energy behavior is close to that of a pseudogap resonant level. As $U$ increases, charge fluctuations are suppressed
leading at low temperatures to $B(U, \beta) < 3$; this part of the strong-coupling phase exhibits a true pseudogap Kondo effect. For very large $U$, by contrast, $B(U, \beta)$ tends towards 1 at low temperatures, suggesting the presence of a decoupled impurity spin, characteristic of the local-moment phase. We locate the phase boundary by the intersection of $B(U, \beta)$ curves for different temperatures [88] at $U_c/D = 0.06313 \pm 0.0008$. The NRG gives $U_c = 0.06450D$, a small shift that can likely be attributed to residual effects of NRG discretization. The mixed-valent character of the QCP is demonstrated in Fig. 4.2(a), where the local occupation $\langle n_d \rangle$ is seen to differ from unity at $U = U_c$. Note also that $\langle n_d \rangle$ displays significant temperature dependence in the vicinity of the QCP.

### 4.4 Quantum Critical Properties

We are now in a position to look for a critical destruction of the Kondo effect in this mixed-valent QCP, i.e., the continuous vanishing of an effective Kondo energy scale signaled by the divergence of the zero-temperature static local spin susceptibility $\chi_s$ as $U$ approaches $U_c$ from below. We do find such a divergence in our zero-temperature $\chi_s$ vs. $U$ data [Fig. 4.3(a)] and in the temperature dependence of $\chi_s$ at $U = U_c$ [Fig. 4.3(b)]. Figure 4.2(b) shows the $U$ dependence of the local magnetization $M_{\text{loc}} = \lim_{h \to 0} \lim_{T \to 0} \langle M_z \rangle$, where $h$ is a local magnetic field entering a term $h(n_{\uparrow} - n_{\downarrow})/2$ (with $g\mu_B \equiv 1$) added to Eq. (3.7). Since $M_{\text{loc}} = 0$ throughout the strong-coupling phase, and $M_{\text{loc}}$ rises continuously from zero on entry to the local-moment phase, this quantity serves as an order parameter for the quantum phase transition. Our results
Figure 4.3: Local static spin susceptibility $\chi_s(T, U)$ for $r = 0.6$, $\Gamma_0 = 0.1D$, and $\varepsilon_d = -0.05D$, (a) vs. $u = U/U_c - 1$ at the labeled temperatures, and (b) vs. $T$ at the critical point $U = U_c$.

can be summarized as

\begin{align*}
\chi_s(T, U = U_c) &\sim T^{-x_s}, \\
\chi_s(T = 0, U < U_c) &\sim |u|^{-\gamma_s}, \\
M_{\text{loc}}(T = 0, U > U_c) &\sim u^{\beta_s},
\end{align*}

(4.1)

where $u = U/U_c - 1$. We find $x_s = 0.80(3)$ from CT-QMC, in excellent agreement with the NRG value $x_s = 0.7908(3)$; the NRG also yields $\gamma_s = 1.42(2)$ and $\beta_s = 0.1874(2)$. These power-law behaviors are all defining characteristics of critical Kondo destruction.

We now turn to the charge response. In order to probe valence fluctuations near the QCP, we turn to the static local charge susceptibility $\chi_c(T, U)$. As shown in Fig. 4.4(a), $\chi_c(T = 0, U)$ increases with $U$ in the strong-coupling phase and diverges as $U \rightarrow U_c^-$, in a manner similar to $\chi_s(T = 0, U)$. In the local-moment phase, the spin and charge responses are very different: $\chi_s(T = 0, U) = \infty$ but $\chi_c(T = 0, U)$ remains finite, although it diverges as $U \rightarrow U_c^+$. In other words, the valence fluctuation energy scale is nonzero in both phases, vanishing only when $U$ approaches $U_c$ from either
side. At $U = U_c$, $\chi_c$ has a singular temperature dependence as shown in Fig. 4.4(b). These behaviors are consistent with

$$\chi_c(T, U = U_c) \sim T^{-x_c},$$

$$\chi_c(T = 0, U) \sim |u|^{-\gamma_c}. \quad (4.2)$$

CT-QMC yields $x_c = 0.36(3)$, while the NRG gives $x_c = 0.120(1)$ (extracted at temperatures much lower than can be accessed by CT-QMC) and $\gamma_c = 0.21(1)$. The difference between the two $x_c$ values stems from a very slow crossover to the quantum critical regime [Fig. 4.4(b) inset]. The much wider crossover window for $\chi_c$ compared with $\chi_s$ [Fig. 4.3(b)] likely arises because $x_c < x_s$, meaning that lower temperatures must be reached before sub-leading contributions to $\chi_c$ become negligible. We stress that the singularity in the charge susceptibility is unique to the mixed-valence QCP, and does not appear at its integer-valence counterpart.

We now reach the important conclusions that the Kondo destruction occurs at a genuinely mixed-valent QCP and that valence fluctuations are part of the critical spectrum. Calculations for level energies $\varepsilon_d \neq -0.05D$ (and hence different critical occupancies $\langle n_d \rangle$) indicate that the critical exponents defined above depend on the band exponent $r$, but not on the impurity valence. This implies that the divergence of the static charge susceptibility is a universal property. At the same time, we find that the critical behavior in the spin sector coincides with the model in its integer valence limit, i.e., the p-h-asymmetric pseudogap Kondo model [91].

### 4.5 Dynamical Scaling at the QCP

We now discuss the dynamical scaling of $\chi_s(\tau, T)$ and $\chi_c(\tau, T)$. Guided by the dynamic scaling results of chapter 3 and in analogy with the spin response at the Kondo
Figure 4.4: Local static charge susceptibility $\chi_c(T,U)$ for $r = 0.6$, $\Gamma_0 = 0.1D$, and $\varepsilon_d = -0.05D$, (a) vs. $u = U/U_c - 1$ at the labeled temperatures, and (b) vs. $T$ at the critical point $U = U_c$, where the discrepancy between CT-QMC and NRG data is due mainly to the difference in $U_c$ values. Inset: $\chi_c(T,U_c)$ over a wider range of $T$, showing the slow crossover behavior.

destruction QCP in the usual Kondo limit [123, 88], we find that at $U = U_c$ both $\chi_s(\tau,T)$ and $\chi_c(\tau,T)$ collapse onto the conformal scaling form, showing a power-law dependence on $\pi T/\sin(\pi \tau T)$ with exponents $\eta_{c,s}$ (see section 5.1 for a detailed discussion of the imaginary time scaling form). For the temperatures considered, the charge susceptibility has not yet reached its asymptotic power-law behavior [based on Fig. 4.4(b)]. Our results thus imply that both leading and sub-leading terms of the critical $\chi_c(\tau,T)$ scale in terms of $\pi T/\sin(\pi \tau T)$. The scaling form means $\chi_s(\omega,T)$ and $\chi_c(\omega,T)$ obey $\omega/T$ scaling [88] at $U = U_c$.

We next consider the effect on the QCP of applying a finite local magnetic field $h$. Consistent with the $\omega/T$ scaling we find $T/h$ scaling for fields $|h| < T_K$, i.e.,

$$\chi_{c,s}(T,h,U_c) \sim h^{-y_{c,s}} f_{c,s}(T/h),$$

(4.3)

where $f_{c,s}(x)$ is a scaling function [see Figs. 4.5(c) and 4.5(d)]. Scaling collapse in $T/h$ further reflects the interacting nature of this mixed-valence QCP. At such an interacting QCP, critical exponents satisfy hyperscaling relations that imply $y_{c,s} =$
$x_{c,s}$, equalities confirmed by our results to within numerical accuracy.

Our results are to be contrasted with the generalization of the spin-density-wave QCP to the valence sector $[124, 125]$. Like its spin counterpart $[36, 37]$, such a mixed-valent QCP is Gaussian (noninteracting) and is not expected to obey either energy-over-temperature or field-over-temperature scaling.

4.6 Discussion

We now briefly consider the case $r = 1$, motivated by critical Kondo screening in graphene and d-wave superconductors. For $\Gamma_0 = 0.1D$ and $\varepsilon_d = -0.05D$, we find
$U_c/D = 0.05475 \pm 0.0006$ with CT-QMC, or 0.05562 with NRG. Both methods indicate that the local static charge susceptibility diverges at $U_c$, along with the spin susceptibility. We find $x_c$ to be an increasing function of $r$, but logarithmic corrections to scaling [91] prevent reliable determination of critical exponents for $r = 1$.

This work provides new insights into the unusual critical properties of $\beta$-YbAlB$_4$ [118], suggesting that Kondo destruction can occur in this material even though it is mixed valent. (Mixed valence is natural in this material given that its onset Kondo temperature is high—on the order of 200 K—and its mass enhancement is moderate.) The demonstration of $h/T$ scaling provides evidence that the experimentally observed field-over-temperature scaling signals Kondo destruction. Our finding of a rapid variation of $\langle n_d \rangle$ near the QCP, which can be tested experimentally [?], suggests that the concentrated lattice system is essentially quantum critical over a range of densities, leading to the exciting possibility of quantum criticality occurring over a region of parameter space rather than just at an isolated point. Finally, our work raises intriguing questions about the extent to which quantum-critical magnetic and valence degrees of freedom influence the superconductivity observed in $\beta$-YbAlB$_4$.

From a general theoretical perspective, how quantum criticality can go beyond the GLW framework of order-parameter fluctuations is a fundamental problem that is important not only for heavy-fermion metals but also for QCPs arising in insulating magnets and other strongly correlated systems. At present, there are few concrete theoretical examples for such unconventional QCPs. By identifying a new QCP in this category, our results provide another setting to gain intuition about beyond-GLW QCPs in general.
4.7 Summary

In this chapter, we have shown that mixed-valent quantum criticality can display the phenomenon of Kondo destruction. The quantum critical point has a collapsing Kondo energy scale and a singular charge-fluctuation spectrum. The valence varies strongly with temperature near the critical point. In the concentrated lattice case, similar quantum critical behavior is expected to occur over an extended range of parameters. Our results raise the prospect of unconventional quantum criticality in mixed-valent systems beyond $\beta$-YbAlB$_4$. 
In chapters 3 and 4 we have focused on the universality classes of Kondo destroyed quantum critical points in pseudogap Anderson impurity models. The EDMFT mapping in chapter 1 section 2.4, gives rise to an additional bosonic bath that we have not considered, up until now. In the following chapter, we consider the pseudogap Anderson and Kondo impurity models (at particle hole symmetry) with the $z$-component of the impurity spin Ising coupled to a bosonic bath with a sub ohmic density of states (defined below). In the following chapter, we go into detail describing each phase of the model, as well as the static and dynamic critical properties, which allows us to elaborate on the finite temperature dynamic scaling form established in chapters 3 and 4. As a result, we determine the different universality classes that accompany Kondo destroyed quantum critical points [126] and find they fall into three distinct classes (for impurities with particle hole symmetry).

5.1 Introduction

This chapter investigates the quantum-critical destruction of the Kondo effect in pseudogap variants of the Ising-symmetric (or easy-axis) Bose-Fermi Anderson (BFA)
and Bose-Fermi Kondo (BFK) models. In each model, a local degree of freedom couples to a band of conduction electrons having a density of states that vanishes as $|\epsilon|^r$ on approach to the Fermi energy ($\epsilon = 0$). The local degree of freedom is also coupled via the $z$ component of its spin to a bosonic bath having a density of states proportional to $\omega^s$ for frequencies up to some cutoff $\omega_c$ (i.e., for $0 < \omega < \omega_c$).

In the presence of a metallic conduction band (corresponding to an exponent $r = 0$), the BFA and BFK models with a sub-Ohmic bosonic bath characterized by a bath exponent $0 < s < 1$ feature a second-order quantum phase transition (QPT) [30, 127, 128, 129, 130, 131, 94, 132] between a Kondo-screened (fermionic strong-coupling) phase and a localized (Kondo-destroyed) phase in which the bosons asymptotically suppress spin-flip scattering and a residual impurity moment survives to $T = 0$. For $1/2 < s < 1$, the Ising-symmetry BFA and BFK models are thought [130, 131, 94, 132] to share the same critical properties as the corresponding sub-Ohmic spin-boson model, which features an interacting QCP characterized by critical exponents that vary continuously with the bath exponent $s$.

In the absence of the bosonic bath, by contrast, the pseudogap BFA and pseudogap BFK models reduce, respectively, to the pseudogap Anderson and pseudogap Kondo models, in which the depression of the low-energy density of states impedes the formation of a many-body Kondo screening cloud and gives rise to QPTs [89, 121, 90, 91, 133, 88] between a Kondo phase and a localized phase in which the impurity exhibits a free spin-$\frac{1}{2}$ at $T = 0$. In chapters 3 and 4, we have studied the dynamical scaling properties of the pseudogap Anderson model at and away from particle hole symmetry in some detail. The QPTs in the pseudogap Anderson and Kondo models belong to the same universality class [90, 91, 133, 88] and are described by critical exponents that vary with the band exponent $r$. The pseudogap versions of the BFA and BFK models offer fascinating possibilities for nontrivial interplay between
two different mechanisms for destruction of the Kondo effect; an interplay that we investigate in this chapter.

An SU(2)-symmetric version of the pseudogap BFK model (in which the Cartesian components of the impurity spin couple to different bosonic baths sharing the same exponent \( s \)) has been studied via perturbative renormalization-group (RG) methods, [134, 135] while the Ising-symmetric case of bosonic coupling to the \( z \) component of the impurity spin has been the subject of preliminary investigation using the numerical renormalization group (NRG) [136]. A spinless variant of the model (coupling the impurity charge to a bosonic bath) has been addressed by perturbative and numerical RG techniques [137]. In all these previous studies, the order-parameter susceptibility has been found to exhibit an anomalous \( T^{-x} \) variation in the quantum-critical regime with an exponent \( x = s \) independent of the band exponent \( r \). One of the objectives of the present chapter is to investigate more carefully the universality of this observation.

Another motivation for the present study is to expand our understanding of the conditions that lead to \( \omega/T \)- or dynamical scaling of critical correlation functions near unconventional quantum criticality. In the pseudogap Anderson model, the conduction-band density of states breaks conformal invariance, while in the metallic \((r = 0)\) BFK model, the conduction band is conformally invariant but the bosonic bath is not. Nonetheless, local correlators of each model have been found [123, 88, 114] to exhibit a boundary conformal scaling form in imaginary time, consistent with Eq. (3.5); such properties have been attributed to an enhanced symmetry at the QCPs. It is an intriguing question whether the scaling form Eq. (3.5) also applies to the critical correlators of the pseudogap BFA and BFK models, where the densities of states of the fermionic and bosonic baths both break conformal invariance in the bulk.

We address these questions through a combination of techniques. For the particle-
hole-symmetric pseudogap BFA model, we use a continuous-time quantum Monte Carlo (CT-QMC) method, [87] which stochastically samples a perturbation expansion in the Anderson hybridization, to probe static and dynamical quantities. We also use the Bose-Fermi extension of the NRG method [94, 132] to resolve the critical spectrum and extract static critical exponents of the pseudogap BFK model. Our results show that the two models are in the same universality class.

In particular, we find that within different ranges of the exponents $r$ and $s$, the measured critical exponents are determined by the fermionic band alone, by the bosonic bath alone, or by both the fermions and the bosons. We show that both the single-particle Green’s function and the local spin susceptibility obey the scaling form of Eq. (3.5) with exponents $2\lambda < 1$, proving that each correlator obeys $\omega/T$ scaling in both the quantum coherent ($\omega > T$) and the relaxational ($\omega < T$) regimes. Agreement with NRG results for static quantities confirms the ability of the CT-QMC approach to study quantum-critical properties of models involving bosons.

The remainder of the chapter is organized as follows: Section 5.2 introduces the pseudogap Bose-Fermi models and Sec. 5.3 briefly describes the numerical methods used to solve these models. An overview of the phase diagram in Sec. 5.4 is followed in Sec. 5.5 by a detailed description of the quantum-critical properties. These results are summarized and discussed in Sec. 5.6.
5.2 Models

The Bose-Fermi Anderson impurity model with Ising-symmetric bosonic coupling is described by the Hamiltonian

\[
H_{\text{BFA}} = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \epsilon_d (n_{d\uparrow} + n_{d\downarrow}) + U n_{d\uparrow} n_{d\downarrow} \\
+ \frac{V}{\sqrt{N_k}} \sum_{k,\sigma} (d_{\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger d_{\sigma}) \\
+ \sum_q \omega_q \phi_q^\dagger \phi_q + \frac{1}{2} g (n_{d\uparrow} - n_{d\downarrow}) \sum_q (\phi_q^\dagger + \phi_{-q}),
\]

where \(c_{k\sigma}\) annihilates a conduction-band electron with wave vector \(k\), energy \(\epsilon_k\), and spin \(z\) component \(\frac{1}{2}\sigma\) with \(\sigma = 1\) (or \(\uparrow\)) or \(-1\) (or \(\downarrow\)); \(d_{\sigma}\) annihilates an impurity electron with energy \(\epsilon_d\) and spin \(z\) component \(\frac{1}{2}\sigma\); \(n_{d\sigma} = d_{\sigma}^\dagger d_{\sigma}\); \(\phi_q\) annihilates a boson of energy \(\omega_q\); and \(N_k\) is the number of unit cells in the host (i.e., the number of distinct \(k\) points). The other energy scales entering Eq. (5.1) are the Coulomb repulsion \(U\) between two electrons in the impurity level, the local hybridization \(V\) between the impurity level and the conduction band, and the coupling \(g\) between the \(z\) component of the impurity spin and the bosonic bath. We focus in this paper on cases \(\epsilon_d = -\frac{1}{2} U\) corresponding to particle-hole-symmetric impurities, but briefly discuss the effect of breaking this symmetry in Sec. A.5.

Over a wide region of its parameter space, the low-energy properties of \(H_{\text{BFA}}\) can be mapped via a Schrieffer-Wolff transformation onto the Ising-symmetry Bose-Fermi Kondo Hamiltonian (see appendix A.1 for details):

\[
H_{\text{BFK}} = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J \mathbf{S} \cdot \mathbf{s}_c + \frac{W}{N} \sum_{k, k'} c_{k\sigma}^\dagger c_{k'\sigma} \\
+ \sum_q \omega_q \phi_q^\dagger \phi_q + g S_z \sum_q (\phi_q^\dagger + \phi_{-q}),
\]
where \( J \) is the Kondo coupling, \( W \) parameterizes nonmagnetic potential scattering, and

\[
s_c = \frac{1}{2N_k} \sum_{k,k',\sigma,\sigma'} \hat{c}_{k\sigma} \sigma_{\sigma\sigma'} \Gamma_{k'\sigma'}
\]

(5.4)
is the on-site conduction-band spin, with \( \sigma \) being a vector of Pauli spin matrices. For \( \epsilon_d = -\frac{1}{2} U \), the potential scattering vanishes for electrons on the Fermi surface, and we can set \( W = 0 \). Although the bare Kondo exchange term is SU(2) symmetric, the bosonic coupling breaks spin rotational invariance. As a result, the RG description of the BFK model in terms of renormalized couplings requires consideration of an anisotropic exchange \( J_z S_z s_c + \frac{1}{2} J_\perp (S^+ s_- + S^- s_+^\dagger) \).

For both models, we assume a conduction-band (fermionic-bath) pseudogap density of states as in equation (3.2) with a power-law pseudogap described by \( 0 < r < \frac{1}{2} \), and a sub-Ohmic bosonic bath specified by

\[
\rho_B(\omega) = \sum_q \delta(\omega - \omega_q) = K_0^2 \omega_c^{1-s} \omega^s \Theta(\omega) \Theta(\omega_c - \omega)
\]

(5.5)

with \( \frac{1}{2} \leq s < 1 \). The pseudogap density of states \( \rho_F(\epsilon) \) leads to a BFA model with the hybridization function \( \Gamma_F(\epsilon) = \pi V^2 \rho_F(\epsilon) = \Gamma |\epsilon/D|^r \Theta(D - |\epsilon|) \), where \( \Gamma = \pi \rho_0 V^2 \).

Various limiting cases of Eqs. (5.1) and (5.2) have been studied previously. For \( g = 0 \), the pseudogap Bose-Fermi models simplify to their pure-fermionic counterparts, in which a pseudogap critical point separates Kondo and free-moment phases; at particle-hole symmetry, this critical point exists only for \( 0 < r < \frac{1}{2} \) (Ref. [90]). In the absence of the conduction band, \( H_{BFA} \) and \( H_{BFK} \) both reduce to the sub-Ohmic spin-boson model in zero transverse field, which has two degenerate ground states in which the bosonic coupling localizes the impurity either in its up- or down-spin configuration. For \( r = 0 \), the pseudogap BFA and BFK models reduce to their metallic counterparts where the critical properties for Ising symmetry are thought [130, 131, 94, 132] to
coincide with those of the spin-boson model for $\frac{1}{2} \leq s < 1$. In the sections that follow we show that the quantum criticality in the full pseudogap Bose-Fermi models described by Eqs. (5.1) and (5.2) falls into one of three distinct types, depending on the values of the bath exponents $r$ and $s$, with one of these types being governed by a mixed Bose-Fermi QCP unlike those seen in any of the limiting cases.

5.3 Methods

5.3.1 Continuous Time Quantum Monte Carlo

To make $H_{\text{BFA}}$ suitable for application of the approach, we apply a canonical transformation to eliminate the term linear in bosonic operators. This is achieved by the generator $S = \frac{1}{2} g(n_{d\uparrow} - n_{d\downarrow}) \sum_q \omega_q^{-1}(\phi_q^\dagger - \phi_{-q})$, which transforms Eq. (5.1) to

$$\tilde{H}_{\text{BFA}} = e^S H_{\text{BFA}} e^{-S}$$

$$= \sum_{k\sigma} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \tilde{\epsilon}_d (\tilde{n}_\uparrow + \tilde{n}_\downarrow) + \tilde{U} \tilde{n}_\uparrow \tilde{n}_\downarrow$$

$$+ \frac{V}{\sqrt{N_k}} \sum_{k\sigma} (\tilde{d}_\sigma^\dagger c_{k\sigma} + c_{k\sigma}^\dagger \tilde{d}_{\sigma}) + \sum_q \omega_q \phi_q^\dagger \phi_q,$$  \quad (5.6)

where $\tilde{d}_\sigma = d_\sigma \exp[\frac{1}{2} \sigma g \sum_q \omega_q^{-1}(\phi_q^\dagger - \phi_{-q})]$, $\tilde{U} = U + \frac{1}{2} g^2 \sum_q \omega_q^{-1}$, and $\tilde{\epsilon}_d = -\frac{1}{2} \tilde{U}$. Physically, the canonical transformation can be viewed as dressing the impurity with a bosonic cloud, which in turn renormalizes $U$, $\epsilon_d$, $d_\sigma$, and $d_\sigma^\dagger$ without breaking particle-hole symmetry.

We are now in a position to calculate the partition function by expanding in the hybridization $V$. This is similar to the approach in Refs. [111] and [138], except that we couple the bosonic bath to the $z$ component of the impurity’s spin rather than to its occupancy. An extension of this method to the case of an SU(2)-symmetric spin-boson coupling has recently been proposed [139]. The resulting perturbation expansion is
then sampled stochastically using a Metropolis algorithm. Tracing out the fermionic band, which is unchanged by the presence of bosons, \[87\] allows the partition function to be recast as

\[
Z = \sum_k \int D[k] W_k,
\]

where at perturbation order \(k\) there are \(k\) segments along the imaginary time axis, each one defined by a pair of renormalized impurity operators, \(\tilde{d}_{\sigma_j}^{(\tau'_j)}(\tilde{\tau}''_j)\) and \(\tilde{d}^{\dagger}_{\sigma_j}(\tau''_j)\). The weight of a particular configuration of segments is

\[
W_k = w_F w_{\text{loc}} w_B,
\]

where \(w_F\) is the weight of the band fermions, \(w_{\text{loc}}\) is the weight of the local configuration and \(w_B\) is the weight of the bosonic bath. \(w_F\) can be obtained as a product of determinants and \(w_{\text{loc}}\) is calculated in terms of the length and overlap of imaginary time segments; for details see appendix B, and Ref. [87]. If the operators in a given segment configuration are time-ordered, with \(s_i = 1 (-1)\) indicating that the \(i\)th operator acts at time \(\tau_i\) to create (annihilate) an electron of spin \(z\) component \(\sigma_i\), then the bosonic weight is

\[
w_B = \langle e^{\frac{1}{2} g \sigma_2 k^s_2 \hat{B}(\tau_2) \ldots e^{\frac{1}{2} g \sigma_1 \hat{B}(\tau_1)}},
\]

which yields (see appendix A section A.2 for explicit details)

\[
B(\tau) = K_0^2 (\omega_c/T)^{1-s} \Gamma(s-1) \left[ \zeta(s-1, \tau T + T/\omega_c) + \zeta(s-1, 1 - \tau T + T/\omega_c) \right],
\]

where \(\Gamma(x)\) is the gamma function and \(\zeta(t, z)\) is the Hurwitz zeta function [140]. Now the local update procedure is identical to that in Ref. [111]. In all the CT-QMC calculations reported below, we have considered the low-temperature scaling limit.
\( T \ll \omega_c \) and consequently dropped the terms \( T/\omega_c \) from Eq. (5.8). We have checked that retaining or discarding these terms does not change any of the universal features at the QCP such as critical exponents.

We perform an unbiased CT-QMC study of the quantum-critical properties of the pseudogap BFA model by applying finite-temperature scaling to determine the location of the QCP. We measure powers of the local magnetization

\[
\langle M_z^n \rangle = \left\langle \left( T \int_0^{1/T} d\tau S_z(\tau) \right)^n \right\rangle,
\]

where \( S_z(\tau) = \frac{1}{2} [n_{d\uparrow}(\tau) - n_{d\downarrow}(\tau)] \), from which the Binder cumulant

\[
U_4(T, g) = \frac{\langle M_z^4 \rangle}{\langle M_z^2 \rangle^2}
\]

is obtained. Here, we have redefined the Binder cumulant as a function of \( g \), different then the definition in equation (3.8). Similar to the case without bosons \([88, 114]\) we find that swap moves \([87]\) are essential to accurately calculate the Binder cumulant. As briefly discussed in chapter 3, near classical phase transitions, the Binder cumulant is a function of system size and temperature, and finite-size scaling allows one to obtain the critical temperature in the thermodynamic limit from classical Monte Carlo simulations of finite systems \([112]\). For the current quantum-mechanical problem, the inverse temperature 1/T and coupling \( g \) play the roles of system size and temperature, respectively, so taking the zero-temperature limit allows one to determine the critical coupling \( g_c \). In the vicinity of the critical point, the Binder cumulant obeys the scaling form \([112]\)

\[
U_4(T, g) = \tilde{U}_4 \left( \frac{g/g_c - 1}{T^{1/\nu}} \right),
\]

where \( \nu \) is the correlation-length exponent defined in Eq. (5.16) below. Therefore, finite-temperature scaling applied to the Binder cumulant can be used to extract the
correlation-length critical exponent.

We also use CT-QMC to measure the single-particle Green’s function \( G_\sigma(\tau, T) = \langle T_\tau d_\sigma(\tau) d_\sigma^\dagger(0) \rangle \) [\( \equiv G(\tau, T) \) in zero magnetic field] and the local spin susceptibility \( \chi_{\text{loc}}(\tau, T) = \langle T_\tau S_z(\tau) S_z(0) \rangle \), as described in Ref. [87]. For the susceptibility calculations presented in this paper, we have used the segment representation, and have checked that the results are consistent with those calculated using a “matrix” formalism [87]. The static local spin susceptibility can then be determined as \( \chi_{\text{stat}}(T) = \chi_{\text{loc}}(\omega = 0, T) = \int_0^{1/T} d\tau \chi_{\text{loc}}(\tau, T) \), where we have set the Landé g factor and the Bohr magneton to unity. For the noninteracting problem (\( U = g = 0 \)), with \( r = 0.4 \), we find agreement within numerical accuracy between the exact and CT-QMC results for both the Green’s function and the local spin susceptibility [141].

The CT-QMC results reported below were obtained for \( r = 0.4, \omega_c = K_0^{-1} = D, \Gamma = 0.1D, U = 0.01D \), and for two different bath exponents: \( s = 0.6 \) and \( s = 0.8 \). It is known from chapter 3 (and ref. [88]) that in the absence of bosons, the QCP point for \( r = 0.4 \) and \( \Gamma = 0.1D \) occurs at \( U_c \simeq 0.085D \). Therefore, by fixing \( U = 0.01D \) and adjusting the bosonic coupling \( g \), we are able to ensure that we are accessing the pseudogap Bose-Fermi QCP and not the pure-fermionic pseudogap QCP (for \( g = 0 \)).

5.3.2 Numerical Renormalization Group

The Bose-Fermi NRG [94, 132] treatment of the Hamiltonian (5.2) entails three key steps: (i) Partition of the fermionic and bosonic baths described by \( \rho_F(\epsilon) \) and \( \rho_B(\omega) \) into logarithmic bins spanning the energy ranges \( \Lambda^{-j} < |\epsilon|/D, \omega/\omega_c \leq \Lambda^{-(j-1)} \), where \( j = 1, 2, 3, \ldots \) and \( \Lambda > 1 \) is the Wilson discretization parameter. Within each logarithmic bin, the continuum is replaced by a single state, namely, the linear combination of states that couples to the impurity. (ii) Tridiagonalization of the
baths, yielding the Hamiltonian

\[ H_{\text{BFK}} = D \sum_{n=0}^{\infty} \sum_{\sigma} [\epsilon_n f_{n\sigma}^\dagger f_{n\sigma} + \tau_n (f_{n\sigma}^\dagger f_{n-1,\sigma} + \text{H.c})] \]

\[ + \omega_c \sum_{m=0}^{\infty} [\epsilon_m b_m^\dagger b_m + t_m (b_m^\dagger b_{m-1} + \text{H.c})] \]

\[ + F^2 \rho_0 J S \cdot \sum_{\sigma, \sigma'} f_{0\sigma}^\dagger \bar{\sigma}_{\sigma'} f_{0\sigma'} + BK_0 g S_z (b_0 + b_0^\dagger). \]

(5.12)

All information about \( \rho_F(\epsilon) \) is encoded in \( D \) and the dimensionless coefficients \( F \) and \( \{ \epsilon_n, \tau_n \} \), while \( \rho_B(\omega) \) is parametrized by \( \omega_c \) and the dimensionless quantities \( B \) and \( \{ \epsilon_m, t_m \} \). For a particle-hole-symmetric \( \rho_F(\epsilon) \) such as that in Eq. (??), \( \epsilon_n = 0 \) for all \( n \). For large values of \( n \), the remaining tight-binding coefficients satisfy \( \tau_n \sim DA^{-n/2} \) and \( |\epsilon_m|, t_m \sim \omega_c \Lambda^{-m} \). (iii) Iterative solution of Eq. (5.12) on fermionic chains restricted to sites \( 0 \leq n \leq N \) with \( N = 0, 1, 2, \ldots \). As a result of the faster decay of the bosonic hopping coefficients with increasing index \( m \), the bosonic chain is restricted to \( 0 \leq m \leq N/2 \), meaning that a site is added to this chain only at even values of \( N \). As in the conventional (pure-fermionic) NRG, the \( N_s \) many-body states of lowest energy are retained to form the basis for iteration \( N + 1 \). In problems involving bosonic baths, it is also necessary to truncate the Fock space on each site of the bosonic chain. In this work we employed a basis of boson number eigenstates \( 0 \leq b_m^\dagger b_m \leq N_b \).

The NRG calculation of critical exponents in the vicinity of a QCP is carried out as described previously for the metallic \( (r = 0) \) BFK model [94, 132] and as illustrated in a preliminary publication on the pseudogap BFK model [136]. The local magnetization (equivalent to \( \langle M_z \rangle \) above) and the static local susceptibility are evaluated as

\[ M_{\text{loc}} = \langle S_z \rangle, \quad \chi_{\text{stat}} = \partial M_{\text{loc}}/\partial h_{\text{loc}}, \]

(5.13)
Figure 5.1: Schematic zero-temperature phase diagram for the pseudogap BFK model on the plane spanned by the bosonic coupling $g$ and the Kondo exchange coupling $J$. The system undergoes a QPT at any crossing of the solid line $J = J_c(g)$ representing the phase boundary between the two stable phases: Kondo and localized. In this study, we consider crossings achieved by varying just one model parameter, as shown by the horizontal and vertical dashed lines. The labels $g_u$ and $J_u = J_c(g_u)$ mark the point along the phase boundary at which the temperature $T_u$, the upper limit of the quantum-critical regime (see Fig. 5.2), takes its maximum value. The terminus of the phase boundary at $g = 0$, $J = J_c(0)$ corresponds to the QPT of the pure-fermionic Kondo model. The pseudogap BFA model has a very similar phase diagram on the $g$-$\Gamma$ plane at any fixed, positive value of $U = -2\epsilon_d$.

where $h_{\text{loc}}$ is a magnetic field that couples only to the impurity through an additional Hamiltonian term $h_{\text{loc}}S_z$. All results reported below were obtained for $\omega_c = \sqrt{\pi}/K_0 = D = \rho_0^{-1} = 1$, using Wilson discretization parameter $\Lambda = 9$ and a bosonic truncation parameter $N_b = 8$, and retaining after each iteration $N_s = 500$ many-body multiplets corresponding to approximately 900 eigenstates [?]. Experience from previous studies [94, 132, 136] indicates that critical exponents calculated for these NRG parameter choices are well-converged with respect to discretization errors (induced by the departure of $\Lambda$ from its continuum value 1) and truncation errors (arising from restricting the values of $N_s$ and $N_b$).
Over the range of bosonic exponents $0 < s < 1$, the Bose-Fermi NRG yields critical exponents for the case $r = 0$ that reproduce those obtained via NRG [142] for the spin-boson model having the same exponent $s$. It has been suggested in Refs. [143] and [144] that, for $0 < s < \frac{1}{2}$, errors associated with the NRG calculation on a finite bosonic Wilson chain lead to unphysical results with nontrivial exponents and hyperscaling. On the other hand, for this same range of $s$, Refs. [110]–[145] have demonstrated an $\omega/T$ scaling for both the leading and sub-leading components of the self-energy, which provides evidence for the interacting nature of the fixed point. Since this issue has yet to be fully resolved, we restrict ourselves in this paper to study the range $\frac{1}{2} \leq s < 1$.

### 5.4 Phases

In this section, we describe the two zero-temperature phases of the pseudogap BFA and BFK models that can be accessed by tuning one model parameter while holding all other parameters constant, as illustrated in the case of the BFK model by the horizontal and vertical dashed lines in Fig. 7.2. We will assume for the moment that the bosonic coupling $g$ is the parameter that is varied. It is important to emphasize that, if carried out at any temperature $T > 0$, such a variation invariably produces smooth crossovers in physical properties, represented schematically by the crossing of dashed lines on the $T$ vs. $g$ diagram in Fig. 5.2. Only at $T = 0$ is it possible to drive the pseudogap BFA or BFK model through a QPT at $g = g_c$ separating a Kondo phase (reached for $g < g_c$) from a localized phase (accessed for $g > g_c$).

The Kondo phase can be characterized by the vanishing (as $T \to 0$) of the long-imaginary-time value of the local spin susceptibility $\chi_{\text{loc}}(\tau = 1/2T, T)$. Correspondingly, the static local susceptibility $\chi_{\text{stat}}(T)$ approaches a constant at low temperatures (see, for example, the squares in Figs. 5.5 and 5.9), signaling that the impurity
Figure 5.2: Schematic $T$ vs. $g$ diagram in the vicinity of the pseudogap Bose-Fermi QCP studied in this work. The QCP dominates the physics in a temperature window between crossover scales $T_u$ and $T_l$ (dashed lines). For $g < g_c$ and $0 < T \lesssim T_l$, the system is in its Kondo regime, whereas for $g > g_c$ and $0 < T \lesssim T_l$, the spin becomes decoupled from the conduction band and the system is in the localized regime. At $T = 0$ (only), cases $g < g_c$ and $g > g_c$ correspond to different phases, distinguished by the value of the order parameter $\psi$ defined in Eq. (5.14).

spin is screened. Since these behaviors (and all other universal low-energy properties found for $g < g_c$) prove to be identical to those in the Kondo phase of the pseudogap Anderson and Kondo models, and independent of the bosonic bath exponent $s$, we associate them with an RG fixed point located at renormalized couplings $g = 0$ and either $\Gamma = \infty$ or $J = \infty$.

In the localized phase, by contrast, $\chi_{\text{loc}}(\tau = 1/2T, T)$ approaches a constant $C(g) > 0$ in the limit $T \to 0$ and the static local susceptibility assumes the Curie-law form $\chi_{\text{stat}}(T) = C(g)/T$ (triangles in Figs. 5.5 and 5.9) characteristic of a free spin whose size is $\propto \sqrt{C(g)}$. In this low-temperature regime, the impurity spin is essentially decoupled from the conduction band and follows the fluctuations of the bosonic bath. The asymptotic low-energy properties are governed by an RG fixed point located at renormalized couplings $g = \infty$ and either $\Gamma = 0$ or $J = 0$. 
The two phases described above are separated by a QPT occurring at bosonic coupling $g_c$ where the Curie constant $C(g)$ extrapolates continuously to zero as $g$ is decreased. As a result, $\lim_{T \to 0} T X_{\text{stat}}$ can serve as an order parameter for the QPT, [90, 91] vanishing throughout the Kondo phase and equaling the Curie constant in the localized phase. However, it is conventional instead to take as the order parameter

$$\psi = \lim_{h_{\text{loc}} \to 0} M_{\text{loc}}(T = 0),$$ (5.14)

which rises continuously from zero on entry into the localized phase.

If one fixes all parameters apart from $\Gamma$ and $g$ in the BFA model [$J$ and $g$ in the BFK model], then the function $g_c(\Gamma)$ [$g_c(J)$] defines the boundary between the Kondo and localized phases. This boundary, shown for the Kondo case as the solid line in Fig. 7.2, is anchored at $g = 0$ by the QCP of the pure-fermionic pseudogap models. One of the central questions addressed in our work is whether the critical behavior reached by crossing the phase boundary at $g > 0$ coincides with or differs from that for $g = 0$.

Our two numerical techniques lead to different approaches for locating the phase boundary. In the CT-QMC treatment of the pseudogap BFA model, similar to chapter 3, the low-temperature limit of the Binder cumulant $U_4$ evolves continuously from $U_4 = 3$ in the Kondo phase to $U_4 = 1$ in the localized phase. $U_4$ is independent of temperature at the critical bosonic coupling $g_c$, but not at other nearby values of $g$. Therefore, one can find $g_c$ by the intersection of curves $U_4$ vs. $g$ for different (low) temperatures (see Figs. 5.3 and 5.7).

Within the NRG, one can identify the phase boundary of the pseudogap BFK model through examination of the asymptotic low-energy many-body spectrum, the $T \to 0$ values of thermodynamic properties such as the impurity contribution to the entropy ($S_{\text{imp}} = 2r \ln 2$ in the Kondo phase, and $S_{\text{imp}} = \ln 2$ in the localized phase), or
the static local spin susceptibility $\chi_{\text{stat}}(T)$. In the present study of the pseudogap BFK model, rather than calculating $g_c$ as a function of $J$, we have instead determined the critical Kondo coupling $J_c$ for different values of $g$. For given bath exponents $r$ and $s$, points on the phase boundary at any $g > 0$ are all found to share the same many-body spectrum and the same power laws in the quantum-critical regime $0 \leq T \lesssim T_u$ (see Fig. 5.2). This universality strongly suggests that the quantum criticality is governed by a single QCP to which the system flows starting from any point on the curve $J_c(g)$. However, the upper temperature $T_u$, which marks the energy scale at which RG flow first brings the system under the influence of the QCP, varies widely along the boundary. In order to provide the most accurate possible account of the quantum-critical properties, we focus below on NRG results obtained for the boundary point $g = g_u$, $J = J_u \equiv J_c(g_u)$ that yields the highest value of $T_u$ for given $(r, s)$, and can therefore be assumed to lie closest to the QCP. An advantage of this approach is that for certain $(r, s)$ pairs we find $g_u = 0$, making clear that in such cases the QCP is of pure-fermionic character.

In what follows, we write $\Delta = g - g_c$ for the BFA model and $\Delta = J_c - J$ for the BFK model to denote the system’s distance from the phase boundary, with $\Delta < 0$ describing the Kondo phase and $\Delta > 0$ describing the localized phase.

5.5 Results Near the Quantum Critical Point

5.5.1 Static Critical Behavior

At any point lying on the phase boundary between the Kondo and localized phases, the static susceptibility exhibits a temperature dependence

$$\chi_{\text{stat}}(T; \Delta = 0) \simeq AT^{-x(r,s)}$$  \hspace{1cm} (5.15)
for all temperatures in the quantum-critical window $0 < T \lesssim T_u$. Here, the exponent $x$ is a universal property of the pseudogap Bose-Fermi QCP (i.e., $x$ depends only on the bath exponents $r$ and $s$), whereas the crossover temperature $T_u$ and the prefactor $A$ can vary from point to point along the phase boundary; as noted above, $T_u$ is highest for the boundary point that lies nearest to the QCP.

Close to but not precisely on the phase boundary, the system enters the quantum-critical regime once the temperature drops below roughly the same scale $T_u$ found for $\Delta = 0$. However, further lowering the temperature produces a second crossover to an asymptotic regime $T \lesssim T_l$ governed either by the Kondo fixed point (for $\Delta < 0$) or by the localized fixed point (for $\Delta > 0$); see Fig. 5.2. Unlike $T_u$, the lower crossover scale $T_l$ shows significant $\Delta$ dependence, and vanishes continuously upon approach to the phase boundary according to

$$T_l \propto |\Delta|^\nu,$$

where $\nu$ is the correlation-length exponent.

In the absence of bosons, the exponent $x(r, s)$ necessarily assumes the value $x_F(r)$ found at the QCP of the pure-fermionic pseudogap Anderson and Kondo models. With a constant fermionic density of states (i.e., $r = 0$) and isotropic, XY, or Ising symmetry of the bosonic couplings, it is known [130, 131] that $x(0, s)$ for $\frac{1}{2} < s < 1$ reduces to the exponent $x_B(s) = s$ of the spin-boson model. Based on perturbative RG, [134, 135] it has been concluded that $x(r, s)$ for a spin-isotropic version of the pseudogap BFK model is independent of $r$, an observation that agrees with asymptotically exact results obtained in the dynamical large-$N$ limit [99, 100] where the symmetry group of the spin-isotropic pseudogap BFK model is generalized from SU(2) to SU($N$) [146]. A preliminary NRG study [136] of the easy-axis pseudogap BFK model also found $x(r, s) = s$. However, that study considered only exponent
pairs \((r, s)\) for which \(x_B(s) < x_F(r)\), a regime in which it is quite plausible that the bosons should dominate the singular part of the spin response. In the present study we have also investigated cases where \(x_F(r) < x_B(s)\) that offer better prospects for finding fermion-dominated spin dynamics.

In what follows we show using both CT-QMC calculations and the NRG that the static magnetic critical exponent \(x\) is simply the smaller of the exponents governing the cases of pure-fermionic and pure-bosonic critical Kondo destruction:

\[
x(r, s) = \min[x_F(r), x_B(s)].
\]  

(5.17)

We focus primarily on the pseudogap exponent \(r = 0.4\) and two values of the bath exponent: \(s = 0.6\) and 0.8. For the pure-fermionic Kondo model, the critical susceptibility is described by a temperature exponent \(x_F(r = 0.4) = 0.688(1)\) obtained within the NRG, [91] consistent with the value \(x_F = 0.68(3)\) found using CT-QMC for the corresponding Anderson model [88]. (Here and throughout the remainder of the chapter, a number in parentheses indicates our estimated uncertainty in the last digit.) For the Bose-Fermi models, therefore, the cases \((r, s) = (0.4, 0.6)\) and \((r, s) = (0.4, 0.8)\) are representative of the regimes \(x_B < x_F\) and \(x_B > x_F\), respectively. For each of these cases, we present CT-QMC results for the pseudogap BFA model and NRG results for the pseudogap BFK model, finding the critical behavior of the two models to be fully equivalent.

In order to explore the full range of \(r\) and \(s\), we supplement the detailed results for \(r = 0.4\), \(s = 0.6\) and 0.8 with static critical exponents for a larger set of \((r, s)\) pairs as obtained for the BFK model using the NRG. In addition to \(x\) and \(\nu\) introduced in
Eqs. (5.15) and (5.16), we consider exponents $\beta$ and $\delta$ defined via the relations [132]

\[ M_{\text{loc}}(\Delta > 0; T = 0, h_{\text{loc}} \to 0) \propto \Delta^\beta, \]  
(5.18)

\[ M_{\text{loc}}(h_{\text{loc}}; \Delta = 0, T = 0) \propto |h_{\text{loc}}|^{1/\delta}. \]  
(5.19)

If the QPT occurs below its upper critical dimension, yielding an interacting QCP, one expects the singular component of the free energy to take the form

\[ F_{\text{crit}} = T f \left( \frac{|\Delta|}{T^{1/\nu}}, \frac{|h_{\text{loc}}|}{T^{(1+x)/2}} \right), \]  
(5.20)

where $f$ is a scaling function. With this ansatz, the exponents $\beta$ and $\delta$ are related to $\nu$ and $x$ by hyperscaling relations

\[ \beta = \nu(1 - x)/2, \]  
(5.21)

\[ \delta = (1 + x)/(1 - x). \]  
(5.22)

In each of the cases we have studied, the value of $x$ is consistent with Eq. (5.17), and wherever we have tested them, the hyperscaling Eqs. (5.21) and (5.22) are well obeyed. Based on the value of $\nu(r, s)$ [or alternatively, $\beta(r, s)$]—as well as an analysis of the many-body spectrum at the QCP—we are led to subdivide the region of the $(r, s)$ plane in which $x(r, s) = x_B(s)$ into two parts: one in which the fermions appear to play no role in the critical behavior, and another in which bosonic and fermionic fluctuations combine to produce critical behavior unlike that found in either the metallic $(r = 0)$ BFK model or the pseudogap Kondo model.
Figure 5.3: Binder cumulant $U_4$ vs. bosonic coupling $g$ for $r = 0.4$ and $s = 0.6$ at different inverse temperatures $\beta = 1/T$. There is a clear intersection all curves at the critical coupling $g_c/D = 0.225(7)$. Error bars for Binder cumulant calculations are obtained from a jackknife error analysis.

**Results for $r = 0.4$, $s = 0.6$**

Figure 5.3 shows the Binder cumulant $U_4$ as a function of the bosonic coupling $g$ of the of the pseudogap BFA model for $r = 0.4$, $s = 0.6$ at different temperatures as calculated using CT-QMC. The intersection of the curves places the QCP at $g_c/D = 0.225(7)$.

The scaling form Eq. (5.11) of the Binder cumulant in the vicinity of the QCP can be used to extract the correlation-length exponent defined in Eq. (5.16). As illustrated in Fig. 5.4, we obtain an excellent collapse of data taken at different temperatures with a fitted exponent $\nu(r = 0.4, s = 0.6)^{-1} = 0.25(3)$.

Having found $g_c$, we are able to establish that the static local susceptibility has the expected temperature dependence in each phase and at the critical coupling, as illustrated in Fig. 5.5. In particular, for $g = g_c$, $\chi_{\text{stat}}$ follows Eq. (5.15) with $x(r, s) = 0.61(2)$ over the lowest decade of temperature for which data were obtained:
2.5 \times 10^{-4} D \leq T \lesssim T_u \simeq 2.5 \times 10^{-3} D. \) (For comparison purposes, we note that for \( g = 0 \), the Kondo temperature is \( T_K^0 = 0.06 D \).) To within numerical accuracy, we find that \( x(r, s) = x_B(s) = s \), in agreement with previous perturbative and numerical RG studies \([134, 135, 136]\).

In the BFK model, the convergence of the NRG many-body spectrum to the critical spectrum is fastest (i.e., the crossover scale \( T_u \) is highest) for \( g_u/D = 0.84(4) \), with \( J_c(g = 0.84D)/2D \simeq 0.9666. \) (The value of \( J_c \) was determined to roughly 10 significant figures.)

Figure 5.6 shows the temperature dependence of the critical static local susceptibilities of the Anderson and Kondo models. The NRG results for the Kondo model exhibit small oscillations around the dependence predicted in Eq. (5.15). Such oscillations, which are periodic in \( \log T \) with period \( \log \Lambda \), are a known consequence of the NRG band discretization \([147]\) that can be reduced in amplitude by working with smaller values of \( \Lambda \). Over the two decades of temperature shown in the figure, the
Figure 5.5: Static spin susceptibility $\chi_{\text{stat}}$ from CT-QMC vs. temperature $T$ for $r = 0.4$ and $s = 0.6$ in the Kondo-screened phase (squares), at the critical coupling (circles), and in the localized phase (triangles). At the critical coupling $g_c \approx 0.225$, $\chi_{\text{stat}}$ diverges according to Eq. (5.15) with $x = 0.61(2)$.

NRG data are described by an exponent $x \approx 0.603$. However, a fit over the range $10^{-15} \leq T/D \leq 10^{-5}$ yields an improved estimate $x = 0.600(1)$, consistent to within numerical error with the CT-QMC result for the Anderson model. Like the CT-QMC estimate for the Anderson model, this value is consistent with the hypothesis that for $x_B(s) < x_F(r)$ spin fluctuations are primarily driven critical by the bosonic bath, and $x(r, s) = x_B(s) = s$.

The inverse of the correlation-length exponent extracted from the crossover in the NRG many-body spectrum is $\nu^{-1} = 0.233(1)$, again consistent with the value obtained for the Anderson model. It is very important to note, this value differs from that found in two other cases: in the metallic BFK model, [132] $\nu(r = 0, s = 0.6)^{-1} = 0.509(1)$, while in the pseudogap Kondo model, [91] $\nu_F(r = 0.4)^{-1} = 0.171(1)$. Although the critical spin fluctuations (and hence the exponent $x$) for $(r, s) = (0.4, 0.6)$ seem to be dominated by the bosonic bath, the RG flow away from the critical point described by the exponent $\nu$ is clearly different from that in cases of pure-bosonic or pure-fermionic
Figure 5.6: Static spin susceptibility $\chi_{\text{stat}}$ vs. temperature $T$ for $r = 0.4$ and $s = 0.6$ calculated within CT-QMC for the BFA model and using the NRG for the BFK model at the QCP. The curves run parallel over the temperature range shown and are fitted by consistent exponents.

criticality.

Results for $r = 0.4$, $s = 0.8$

Figure 5.7 shows the variation of the BFA-model Binder cumulant for $r = 0.4$, $s = 0.8$ as calculated using CT-QMC. The intersection of curves representing different temperatures places the QCP at $g_c/D = 0.28(1)$. This critical value is larger than that ($g_c/D \approx 0.225$) for $s = 0.6$ because the bosonic interaction between time segments falls off faster with increasing $s$. Figure 5.4 shows that the Binder cumulant scales according to Eq. (5.11) with an excellent collapse of data taken at different temperatures with a fitted exponent $\nu(r = 0.4, s = 0.8)^{-1} = 0.17(2)$.

Figure 5.9 illustrates the temperature dependence of the static local susceptibility in each phase and at the critical coupling. For $g = g_c$, $\chi_{\text{stat}}$ follows Eq. (5.15) with $x(r, s) = 0.68(2)$ over the lowest decade of temperature for which data were obtained, a clear departure from the behavior $x(r, s) = x_B(s) = s$ seen above for $(r, s) =$
Figure 5.7: Binder cumulant $B_4$ vs. bosonic coupling $g$ for $r = 0.4$ and $s = 0.8$ at different inverse temperatures $\beta = 1/T$. There is a clear intersection of the curves at the critical coupling $g_c/D = 0.28(1)$.

In the BFK model, the convergence of the NRG many-body spectrum to the critical spectrum is fastest (i.e., the crossover scale $T_u$ is highest) for $g_u = 0$, with $J_u = J_c(g_u)/2D \simeq 0.7908$. The value $g_u = 0$ means that the impurity is entirely decoupled from the bosons, and the QCP must be of pure-fermionic character. Indeed, the asymptotic low-energy many-body spectrum in the quantum-critical regime can be reproduced by taking every possible combination of (i) one state from the spectrum of free $s = 0.8$ bosons, and (ii) one state from the critical spectrum of the $r = 0.4$ pseudogap Kondo model. We summarize this spectral decomposition in the shorthand (BF critical) = (B free) $\otimes$ (F critical) and refer to it below simply as F-type criticality.

Figure 5.10 compares the temperature dependence of the critical static local susceptibilities of the BFA and BFK models. Over the two decades of temperature shown in the figure, the NRG data for the BFK model are described by an exponent $x \simeq 0.68$, identical to the CT-QMC value for the Anderson model. However, since
the QCP corresponds to $g = 0$, we know that the exponent must coincide exactly with that of the pseudogap Kondo model: \[ x_F(r = 0.4) = 0.688(1). \] This value clearly differs from the one $x = s = 0.8$ found within the spin-boson-model [142] and the metallic BFK model [94].

Similarly, we can be confident that the correlation-length exponent must be identical to that of the pseudogap Kondo model, $\nu_F(r = 0.4)^{-1} = 0.171(1)$, a result that is consistent with the CT-QMC value $\nu(r = 0.4, s = 0.8)^{-1} = 0.17(2)$ quoted above.

Our results suggest that in cases $(r, s)$ where $x_B(s) > x_F(r)$, the physics at and near the QCP is determined primarily by fermionic fluctuations, and that critical properties should coincide with those of the pseudogap Anderson and pseudogap Kondo models.
Figure 5.9: Static spin susceptibility $\chi_{\text{stat}}$ from CT-QMC vs. temperature $T$ for $r = 0.4$ and $s = 0.8$ in the Kondo-screened phase (squares), at the critical coupling (circles) and in the localized phase (triangles). At the critical coupling $g_c/D = 0.28(1)$, $\chi_{\text{stat}}$ diverges according to Eq. (5.15) with $x = 0.68(2)$.

Results for other $(r, s)$

In order to investigate more systematically the different types of quantum criticality exemplified in the cases $(r, s) = (0.4, 0.6)$ and $(0.4, 0.8)$, we have studied the particle-hole-symmetric pseudogap BFK model for 23 different $(r, s)$ pairs spanning the ranges $0.1 \leq r \leq 0.4$ and $0.5 \leq s \leq 0.9$. As shown in appendix A section A.3, Table A.1 summarizes the critical properties, one line per $(r, s)$ pair. In every case where it can be tested, spanning the full range of bath exponents $0 \leq r < \frac{1}{2}$ and $\frac{1}{2} \leq s < 1$, hyperscaling [Eq. (5.21)] holds to within our estimated numerical uncertainty. Thus, based on an examination of the critical spectra and the exponents $x$ and $\beta$ (and hence $\nu$ via hyperscaling), we are able to identify three distinct types of quantum criticality:

- **Fermionic (F)**—The asymptotic low-energy critical spectrum exhibits SU(2) spin symmetry and decomposes into a direct product of the spectrum of free bosons with bath exponent $s$ and the critical spectrum of the pseudogap Kondo model with band
Figure 5.10: Static spin susceptibility $\chi_{\text{stat}}$ vs. temperature $T$ for $r = 0.4$ and $s = 0.8$ calculated within CT-QMC for the BFA model and using the NRG for the BFK model at the QCP. The curves run parallel over the temperature range shown and are described by consistent exponents.

exponent $r$, i.e., (BF critical) = (B free) $\otimes$ (F critical). All static critical exponents that have been calculated are identical to those of the pure-fermionic pseudogap Anderson and Kondo models with the same $r$.

• Bosonic (B)—The asymptotic low-energy critical spectrum exhibits SU(2) spin symmetry and decomposes into a direct product of the critical spectrum of the spin-boson model with bath exponent $s$ and the strong-coupling spectrum of the pseudogap Kondo model with band exponent $r$, i.e., (BF critical) = (B critical) $\otimes$ (F strong-coupling). The strong-coupling spectrum of the particle-hole-symmetric pseudogap Anderson and Kondo models is characterized by a phase shift of $(1 - r)\pi/2$ for electrons at the Fermi energy (see Ref. [90]). All static static critical exponents that have been calculated in region B are identical to those of the spin-boson model and of the metallic ($r = 0$) BFA and BFK models with the same $s$. However, despite the asymptotic decomposition of the low-energy spectrum, the single-particle spectral function has a non-Fermi liquid form (at least for $r = 0$), as discussed in Sec. 5.5.2.
This may be related to the fact that the fermionic strong-coupling spectrum is not only found at the Kondo fixed point where the exchange couplings take renormalized values \( J_z = J_\perp = \infty \), but also is approached for \( J_z = \infty, J_\perp = \text{finite} \) in the limit of energy scales much smaller than \( J_\perp \). We will return to this observation in Sec. A.4.

- Mixed (M)—The critical spectrum exhibits broken SU(2) spin symmetry and does not decompose into a direct product of bosonic and fermionic parts. The exponents satisfy \( x = x_B(s) = s \) but the order-parameter exponent lies between the values for the spin-boson model and the pseudogap Kondo/Anderson models, i.e., \( \nu_F^{-1}(r) < \nu^{-1}(r, s) < \nu_B^{-1}(s) \).

The three types of quantum criticality are clearly revealed in plots of \( x \) and \( 1/\nu \) vs. \( s \) at fixed \( r \). As can be seen in Fig. 5.11, \( x(r, s) \) coincides with \( x_B(s) = s \) until the latter value exceeds its counterpart \( x_F(r) \) in the pure-fermionic pseudogap problem. The break in the slope of \( x \) vs. \( s \) marks the transition from M-type to F-type criticality. Fig. 5.12 shows that the Bose-Fermi correlation-length exponent equals the bosonic value \( \nu_B(s) \) for sufficiently small \( s \) (B-type criticality) and equals the fermionic value \( \nu_F(r) \) over precisely the range of \( s \) where \( x(r, s) = x_F(r) \) (F-type criticality), but between these regimes, \( \nu(r, s) \) takes values that differ from both \( \nu_B(s) \) and \( \nu_F(r) \) (M-type criticality).

Figure 5.13 summarizes the type of criticality found at different locations on the \( r-s \) plane, including points studied for the metallic case \( r = 0 \) where the behavior is always of the B type. It is seen that each type of criticality (F, B, or M) occupies a contiguous region. All the results are consistent with there being a boundary \( s = x_F(r) \) between the F and M regions (shown as a solid curve in Fig. 5.13). As argued at the beginning of this section, such a boundary arises from the assumption that the spin response at the Bose-Fermi critical point is dominated by the bath (bosonic or fermionic) that has the more singular dynamical spin fluctuations, corresponding
Figure 5.11: Static magnetic critical exponent $x$ vs. bath exponent $s$ for $r = 0.2$, 0.3, and 0.4. The diagonal line represents the pure-bosonic exponent $x_B(s) = s$, while each horizontal line segment shows the pure-fermionic value $x_F(r)$. For each $(r, s)$ pair, the Bose-Fermi exponent satisfies $x = \min[x_F(r), x_B(s)]$.

to the smaller value of $x$. The results in Fig. 5.13 are also consistent with there
being a boundary $s = 1 - 2r$ between the M and F regions (the straight line in the
figure). Such a boundary marks the line of equality of the frequency exponents of
the bare bosonic propagator and the fermionic particle-hole bubble, [?] although the
significance of this observation in the present context remains to be established.

5.5.2 Critical Dynamics

We now turn to the finite-temperature dynamics of the impurity Green’s function
and the local susceptibility calculated at the critical bosonic coupling $g = g_c$. Since
the NRG is unreliable in the regime $|\omega| \lesssim T$, we rely mainly on the CT-QMC for this
part of the study, focusing once more on the type-M case $r = 0.4$, $s = 0.6$ and on the
type-F case $r = 0.4$, $s = 0.8$.

Figs. 5.14 and 5.15 plot $G(\tau, T)$ and $\chi_{loc}(\tau, T)$, respectively, as functions of the
combination $\xi = \pi \tau_0 T / \sin(\pi \tau T)$, where $\tau_0 = 1/D$ renders the scaling function dimensionless. For both $(r, s)$ pairs, the critical correlation functions at temperatures well below the bare Kondo temperature, $T_K^0 \equiv T_K(g = 0) \approx 0.06 D$, exhibit excellent scaling collapse over two decades of $\xi$. The scaling collapse leads to the important conclusions that in the long-time limit $\tau T_K^0 \gg 1$,

$$G(\tau, T) = \Psi \left( \frac{\pi \tau_0 T}{\sin(\pi \tau T)} \right)^{\frac{T \ll T_K^0}{T_K^0}} \left( \frac{\pi \tau_0 T}{\sin(\pi \tau T)} \right)^{\eta_G},$$

$$\chi_{\text{loc}}(\tau, T) = \Phi \left( \frac{\pi \tau_0 T}{\sin(\pi \tau T)} \right)^{\frac{T \ll T_K^0}{T_K^0}} \left( \frac{\pi \tau_0 T}{\sin(\pi \tau T)} \right)^{\eta_\chi}. \quad (5.23)$$

We obtain $\eta_G = 0.58(4), \eta_\chi = 0.40(2)$ for $s = 0.6$ and $\eta_G = 0.58(4), \eta_\chi = 0.31(2)$ for
Figure 5.13: Summary of the pairs of bath exponents \((r, s)\) studied in this work. Results for \(r = 0\) describe a metallic conduction band, while those for \(r > 0\) correspond to pseudogapped problems. Squares, triangles, and circles respectively correspond to quantum criticality of the F, B, and M types, as described in the text. Filled symbols summarize NRG results for the BFK model while open symbols represent CT-QMC results for the BFA model. Solid lines show the conjectured boundaries \(s = 1 - 2r\) and \(x_B(s) = s = x_F(r)\) between the different types of criticality.

\(s = 0.8\). These exponents are consistent with the relations

\[
\eta_G = 1 - r, \quad \eta_x = 1 - x,
\]

where \(x(r, s)\) is defined in Eq. (5.15). In the zero-temperature limit, Eq. (5.23) and the first Eq. (5.24) give \(G(\tau, T \to 0) \sim \tau^{-(1-r)}\), reproducing an exact result [134, 135]. The quality of the scaling collapse in Figs. 5.14 and 5.15, as well as the reproduction of the correct zero-temperature limit, provide significant evidence that our results have reached the asymptotic low-energy scaling regime.

Since \(1 - r\) and \(1 - x\) are both less than one, each correlator obeys \(\omega/T\) scaling per the discussion of Eq. (3.5). Following the discussion around equation (3.4), similar to chapter 3, this then implies both spin and single particle relaxation rates are linear in
Figure 5.14: Single-particle Green’s function \( G(\tau, T) \) vs \( \xi = \pi \tau_0 T / \sin(\pi \tau T) \) for \( r = 0.4, s = 0.6, g = 0.225D \approx g_c \) (lower data) and for \( r = 0.4, s = 0.8, g = 0.28D \approx g_c \) (upper data, all \( G \) values multiplied by 1.75 to avoid overlap with the \( s = 0.6 \) data). One observes excellent collapse of the data for just under two decades of \( \xi \). Temperature labels are shared between this figure and Fig. 5.15.

Temperature. The observation that \( \eta_\chi \neq 2\eta_G \) implies that vertex corrections cannot be neglected, in line with the fully interacting nature of the QCP. Once again, similar to our results in chapters 3 and 4, we have found at the Kondo destroyed QCP scaling forms in imaginary time that are consistent with a boundary conformal field theory, which leads to \( \omega/T \) scaling and a linear in temperature relaxation rate.

For reasons discussed in Sec. 5.6, we have not been able to access low enough temperatures using CT-QMC to study cases of B-type quantum criticality. In this region of the \( r-s \) plane, we must rely on information from previous NRG studies of the \( r = 0 \) BFK and BFA models, [94, 132] which have demonstrated that at the critical coupling, the local susceptibility calculated for \( |\omega| \gtrsim T \) is consistent with the existence of \( \omega/T \) scaling, while the zero-temperature impurity spectral function shows a non-Fermi liquid form. The latter is also seen for \( r = 0 \) results in a dynamical large-\( N \) limit, [148] as a function of both frequency and temperature. It is reasonable to
attribute this non-Fermi-liquid behavior to the existence of an RG-irrelevant coupling between the fermionic and bosonic sectors of the Hilbert space.

5.6 Summary

In this chapter, we have applied a combination of continuous-time quantum Monte-Carlo (CT-QMC) and numerical renormalization-group (NRG) methods to study systematically the interplay between bosonic and fermionic baths, each of which on its own can induce critical Kondo destruction at a continuous zero-temperature transition. We have shown that at particle-hole symmetry, the quantum critical point (QCP) in the easy-axis pseudogap BFA model belongs to the same universality class as the QCP of the corresponding Kondo model. We have further shown the surprising result that the value of the exponent \( x \) for the temperature dependence of the...
critical local spin susceptibility [defined in Eq. (5.15)] of either model is sensitive to the exponents \( r \) and \( s \) characterizing the vanishing of the fermionic and bosonic densities of states. In the region of the \( r-s \) plane where \( s \geq x_F(r) \) (\( x_F \) being the thermal critical exponent of the pseudogap Anderson and Kondo models without bosons), all critical exponents of the Bose-Fermi models that we have calculated are identical to those of the pure-fermionic models, and the critical many-body spectrum decomposes into a direct product of a free bosonic spectrum and a critical pseudogap fermionic spectrum; this regime has eluded all previous studies. For \( s < x_F(r) \), the critical spin fluctuations are instead dominated by the bosonic bath, leading to \( x = x_B(s) = s \). However, the correlation-length exponent \( \nu \) [defined in Eq. (5.16)] coincides with that of the spin-boson model, and the asymptotic low-energy critical spectrum decomposes into a direct product of a critical bosonic spectrum and a pseudogap Kondo fermionic spectrum, only for \( s \leq 1 - 2r \). Within an intermediate region \( 1 - 2r < s < x_F(r) \), \( \nu(r, s) \) takes a value lying between those for the spin-boson model and for the pseudogap Anderson and Kondo models, and bosonic and fermionic degrees of freedom cannot be disentangled in the critical spectrum. In all three regions, other static critical exponents are related to \( x \) and \( \nu \) via hyperscaling relations that are expected to hold only at an interacting critical point.

We have also shown that at the QCP, the imaginary-time correlation functions \( G(\tau, T) \) and \( \chi_{\text{loc}}(\tau, T) \) scale as functions of \( \xi = \pi T \tau_0 / \sin(\pi \tau T) \) and that their real-frequency counterparts obey \( \omega/T \) scaling, consistent with the notion that the QCP is fully interacting. Scaling collapse of imaginary-time correlators as functions of \( \xi \) has previously been reported for the sub-Ohmic BFK model, [123] where the Kondo effect is critically destroyed by the bosonic bath, and in the pseudogap Anderson model at and away from particle-hole symmetry in chapters 3 and 4 (refs. [88, 114]) where criticality is driven by fermionic fluctuations of the band. That it generalizes to the
more complex case considered in the present work suggests that the scaling collapse may very well be a general feature of local quantum criticality. The scaling collapse in terms of $\xi$ implies (under conditions spelled out in Sec. 5.5.2) that the associated real-frequency correlator displays $\omega/T$ scaling, a property that has been reported in several experiments on unconventional quantum criticality in 4$f$-electron based magnets [65, 68]. A scaling collapse of the form observed here is natural for boundary-conformal quantum impurity systems. However, conformal symmetry is broken both by the bosonic bath (as in the sub-Ohmic BFK model), and the fermionic bath (as in the pseudogap Anderson model). Symmetry restoration frequently accompanies criticality. The case discussed here, however, has to be distinguished from this more standard situation of irrelevant symmetry-breaking fields, as the broken symmetry in the bulk induces boundary criticality with local correlators that are compatible with a boundary conformal critical theory. As discussed earlier, [123] a deeper understanding of this observation should help identify a critical field theory of unconventional quantum criticality.

From a methodological viewpoint, this chapter has shown that the CT-QMC method can attain sufficiently low temperatures in the presence of a bosonic bath to identify a quantum critical point lying between stable phases, and to obtain critical properties in agreement with those given by the NRG. Such study is possible using the CT-QMC only in cases where entry into the critical power-law regime takes place at a fairly high temperature $T_u$. The presence of a pseudogap in the fermionic density of states helps in this regard: the value of $T_u$ decreases as $r$ decreases, so larger $r$ values are optimal. Decreasing the bath exponent $s$ also reduces $T_u$, making it difficult to study the range $s < \frac{1}{2}$ without fine-tuning of the Hamiltonian.
Chapter 6

Cluster Extended Dynamical Mean Field Theory

In chapters 3, 4, and 5, we have systematically studied the different types of universality classes associated with critical Kondo destruction. We have shown these QCPs are accompanied by $\omega/T$ scaling and linear in temperature single particle relaxation rates, consistent with the experiments on CeCu$_{6-x}$Au$_x$ and YbRh$_2$Si$_2$. In addition, we have also shown the local Kondo energy scale $T^*$ vanishes continuously on approach to the QCP with a universal fractional exponent, consistent with the diverging effective mass in CeRhIn$_5$. As a result, we have gained a significant amount of intuition and understanding by studying Kondo destruction in simplified single impurity models.

In the following chapter, we begin to shift our focus to study the effect of Kondo breakdown quantum critical points on superconductivity. To do so, we must first formulate the effective theory that can describe both Kondo destruction and the formation of a superconducting ground state. This is achieved by developing a new cluster extended dynamical mean field theory approach that is distinct from previous developments [149] in symmetry broken phases. The scheme presented in the following chapter is the natural generalization of the EDMFT to the cluster case. As a result of the formalism presented in the following section we will be able to quantify pairing
correlations in the normal state of the locally critical point.

6.1 Introduction

In DMFT based approaches, incorporating real space correlations beyond a single site have naturally been done with the development of quantum cluster theories [149]. In this case, strongly correlated problems can be mapped to a quantum cluster model with self consistent fermionic baths and the interactions within the cluster are treated exactly. From a methodological point of view, a main advantage of dynamical cluster theories is that they incorporate non-perturbative corrections to DMFT without introducing a non-causal self energy [149]. This can be formulated in real space which leads to cluster DMFT (CDMFT) [150] or in momentum space which is known as the dynamical cluster approximation (DCA) [151] and there are numerous other cluster embedding schemes possible such as the variational cluster approximation (VCA) [152]. When the Weiss fields are neglected these cluster schemes are no longer self consistent and reduce to cluster perturbation theory (CPT), which approximates lattice quantities by expanding about the isolated cluster limit [153].

From a theoretical point of view, a main advantage of dynamical cluster theories is the ability to account for exotic types of order not possible within DMFT [109]. For example, a four site cluster can treat a d-wave superconducting order parameter as well as stripe charge or spin order. Such a pairing mechanism is expected to be appropriate for the cuprates, heavy fermion materials and possibly the iron pnictides. In this case, any superconducting ground state will have cooper pairs formed between sites which can lead to a variety of different pairing symmetries, such as extended s-wave, p-wave or d-wave.

These cluster schemes have also been generalized to extended CDMFT (ECDMFT) [154, 109] and extended DCA (EDCA) [155], by introducing self consistent bosonic baths
via a Hubbard-Stratonivich transformation decoupling the inter site interaction term. The Hubbard-Stratonivich field then becomes a self consistent dynamic bosonic Weiss field in the cluster limit. In addition, ECDMFT was also constructed for spin only models in ref. [156]

In this chapter, we present a new cluster extended dynamical mean field theory scheme that we dub C-EDMFT. We derive the equations by generalizing ref. [74] to the cluster case using a locator expansion about a dressed cluster limit. We formulate the equations in both real and momentum space, which in the absence of any broken symmetry, corresponds to an alternate derivation of ECDMFT and EDCA respectively. We introduce magnetic order in the same fashion as EDMFT in ref. [78] distinct from DMFT, and then generalize this approach to also include superconductivity. We also show how to quantify pairing correlations induced by magnetic interactions in the normal state within this approach. Lastly we use the formalism to derive effective impurity models associated with strongly correlated problems of central interest.

In the development of the formalism of C-EDMFT, for illustration purposes, we consider a one band Hubbard model with two body inter site interactions on a generic lattice.

\[
H = \sum_{\langle ij \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{\langle ij \rangle, \alpha} J_{ij}^\alpha S_i^\alpha S_j^\alpha \tag{6.1}
\]

where \(c_{i\sigma}\) destroys an electron of spin \(\sigma\) at site \(i\), \(n_i = \sum_\sigma n_{i\sigma}\), and \(n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}\). The index \(\alpha\) runs over 0, 1, 2, 3, where for \(\alpha = 1, 2, 3\) (or for \(\alpha = x, y, z\)) the operator \(S_i^\alpha = c_{i\mu}^\dagger (\sigma_{\mu\nu}^\alpha / 2) c_{i\nu}\), is the spin operator, where \(\sigma_{\mu\nu}^\alpha\) is the \(\alpha\)-Pauli matrix for \(\alpha = x, y, z\). In addition we consider the charge channel with \(\alpha = 0\), where the operator
\[
S^0_i = n_i \text{: denotes the normal ordered density : } n_i := n_i - \langle n_i \rangle. \]
We denote nearest neighbors by \( \langle i, j \rangle \) and only consider nearest neighbor hopping \( t_{ij} \) and two body exchange interaction \( J^\alpha_{ij} \). For \( J^\alpha_{ij} = 0 \), the model reduces to the standard Hubbard model with an onsite Coulomb repulsion of strength \( U \). It is natural to extend these techniques to multi-band models and longer range interactions.

A main focus of this work is a self consistent solution of the single particle Greens function \( G_{ij\sigma}(\tau) = -\langle T_{\tau} c^\dagger_{i\sigma}(\tau) c_{j\sigma} \rangle \) as well as the spin and charge susceptibilities \( \chi_{ij}^\alpha(\tau) = \langle T_{\tau} : S^\alpha_i(\tau) :: S^\alpha_j : \rangle \). In general, for the single particle Greens function, a perturbative expansion about the non-interacting limit yields the Dyson equation

\[
G(k, i\omega_n) = \frac{1}{i\omega_n - \mu - t_k - \Sigma_{\text{lat}}(k, i\omega_n)},
\]

where \( t_k \) is the Fourier transform of \( t_{ij}(= 1/N \sum_k e^{ik(r_i - r_j)}t_k) \), \( \mu \) is the chemical potential, \( \Sigma_{\text{lat}}(k, i\omega_n) \) is the single particle self energy, and we denote fermionic Matsubara frequencies as \( \omega_n \). Analogous to the single particle Greens function, we introduce a spin and charge self energy \( M^\alpha_{\text{lat}}(q, i\nu) \) which is defined in terms of each susceptibility as

\[
\chi^\alpha(q, i\nu_n) = \frac{1}{M^\alpha_{\text{lat}}(q, i\nu_n) + J^\alpha_q}
\]

where \( J^\alpha_q \) is the Fourier transform of \( J^\alpha_{ij} \) and \( \nu_n \) is a bosonic Matsubara frequency. The spin/charge self energies can be regarded as the how much their corresponding susceptibility differs from a Gaussian model where \( \chi_{ij}^\alpha \propto 1/J^\alpha_{ij}( \text{ref. [156]} ) \). In the following we will derive a self consistent dynamical cluster mean field theory to approximate the lattice quantities \( \Sigma_{\text{lat}}(k, i\omega_n) \) and \( M^\alpha_{\text{lat}}(q, i\nu) \) and in turn the single particle Greens function and spin/charge susceptibilities.

The remainder of the paper is organized as follows: in section 6.2 we review and develop extended cluster theories. We then extend these concepts to superconducting
order and normal state properties in section 6.4. We then use the formalism to derive an effective cluster model in section 6.5 and discuss alternate approaches and relevant solution methods in 6.6. Lastly we conclude the paper in section 6.7.

6.2 Extended Cluster Theories

We begin by dividing the lattice of $N$ sites into clusters of size $N_c$, where each lattice site is now labeled by $x = r + R$, where $r$ labels the cluster and $R$ labels the sites within the cluster (see figure 6.1). This is then Fourier transformed to $k = \tilde{k} + K$, where $K$ is the intra cluster momentum and $\tilde{k}$ is the inter cluster momentum. With this notation $t_{ij}$ and $J_{ij}^{\alpha}$ can be written as $A_{R_iR_j}(r_i - r_j) = A(r_i - r_j)$, where the bold $A$ denotes a matrix in cluster indices. We then separate $t_{ij}$ and $J_{ij}^{\alpha}$ into intra and inter cluster parts

\[
t(r_i - r_j) = t_c \delta_{r_i, r_j} + \delta t(r_i - r_j),
\]
\[
J^{\alpha}(r_i - r_j) = J_c^{\alpha} \delta_{r_i, r_j} + \delta J^{\alpha}(r_i - r_j),
\]

(6.4)

where $t_c$ and $J_c^{\alpha}$ are the interactions within the cluster, whereas $\delta t$ and $\delta J^{\alpha}$ are the interactions between clusters, note that by construction $\delta t(0)$ and $\delta J^{\alpha}(0)$ vanish.

6.2.1 Real Space Formulation

We will first derive the equations in real space and in the following section will then briefly discuss the necessary steps in order to specify the self consistent equations in momentum space. We first focus on a ground state with no broken symmetry, and will then generalize the equations to the case of magnetic order and superconductivity in sections 6.3 and 6.4. We perform a locator expansion in $\delta t$ and $\delta J$ about the cluster limit [149]. The isolated cluster single particle Greens func-
Figure 6.1: Division of the lattice into \( N/N_c \) clusters, of size \( N_c = L_c^2 \). The vector \( r \) labels each cluster, while sites within the cluster are labelled by \( \mathbf{R} \). Interactions are divided into within the cluster \( J_c \) and between clusters \( \delta J \), (which is also done for the hopping elements \( t_c \) and \( \delta t \).) We have omitted the channel index \( \alpha \) for clarity.

Correlation and susceptibilities are defined by

\[
C_0^G(X, Y; r, \tau) = -\langle T_r c_{rX\sigma}(\tau) c_{rY\sigma}^\dagger \rangle_{H_c}
\]

and

\[
C_0^{\chi\alpha}(X, Y; r, \tau) = \langle T_r S_{rX\sigma}(\tau) S_{rY\sigma}^{\alpha} \rangle_{H_c}
\]

respectively, where \( H_c \) is the isolated cluster Hamiltonian at cluster \( r \). In the following we consider problems that have translational invariance between clusters which implies each cluster correlation function is identical and we can drop the label \( r \).

We now generalize the effective cumulant expansion of Metzner [157] for the Greens function and Smith and Si [74] for the susceptibilities from a single site to a cluster, which leads to matrix quantities. Along these lines, we introduce the effective cluster Greens function \( C_G(X, Y; \tau) \) and spin/charge susceptibilities \( C^{\chi\alpha}(X, Y; \tau) \) which are defined as the isolated cluster Greens function and susceptibility (in the \( \alpha \) channel) with all local decorations that are irreducible by cutting a single \( \delta t \) and \( \delta J^\alpha \) line respectively (see figure 6.2). The effective cluster correlation functions can be regarded as “dressed” cluster correlation function, generalizing the dressed atom picture of Metzner [157] to the cluster case. Retaining this class of diagrams can be formally justified in the large dimensional limit after rescaling \( \delta t \) and \( \delta J^\alpha \) by the square root.
of the coordination raised to the manhattan distance between clusters while keeping the dimension and number of sites in the cluster fixed\[150\]. Performing the locator expansion about the effective cluster correlation functions we arrive at the following Dyson like equations

\[
G_{r_ir_j}(i\omega_n) = C_G(i\omega_n)\delta_{r_ir_j} + C_G(i\omega_n) \sum_{r_l} \delta t(r_l - r_j) G_{r_l|r_j}(i\omega_n) \tag{6.5}
\]

\[
\chi_{\alpha}^{r_ir_j}(i\nu_n) = C_{\chi}^{\alpha}(i\nu_n)\delta_{r_ir_j} - C_{\chi}^{\alpha}(i\nu_n) \sum_{r_j} \delta J^{\alpha}(r_i - r_j) \chi_{r_i|r_j}^{\alpha}(i\nu_n). \tag{6.6}
\]

We note that these are matrix equations and we are using a bold notation to denote matrices in cluster indices. Fourier transforming equations (6.5) and (6.6) to inter-
cluster momentum $\tilde{k}$ and $\tilde{q}$ we arrive at for the Greens function

$$G(\tilde{k}, i\omega_n) = C_G(i\omega_n) + C_G(i\omega_n)\delta t(\tilde{k})G(\tilde{k}, i\omega_n)$$

$$= \left[ C_G(i\omega_n)^{-1} - \delta t(\tilde{k}) \right]^{-1}$$

(6.7) and (6.8)

and for the susceptibility

$$\chi^\alpha(\tilde{q}, i\nu_n) = C_{\chi^\alpha(i\nu_n)} - C_{\chi^\alpha(i\nu_n)}\delta J^\alpha_{\tilde{q}}\chi^\alpha(\tilde{q}, i\nu_n)$$

$$= \left[ C_{\chi^\alpha(i\nu_n)}^{-1} + \delta J^\alpha_{\tilde{q}} \right]^{-1}.$$  

(6.9) and (6.10)

Rewriting the Dyson equations for $G$ and $\chi^\alpha$ in equations (6.2) and (6.3) in real space cluster indices we find the self energy and spin/charge self energies are $\tilde{k}$ and $\tilde{q}$ independent respectively, and only depend on cluster indices. We arrive at the following equations for the effective cluster correlation functions

$$C_G(i\omega_n)^{-1} = g^0_c(i\omega_n)^{-1} - \Sigma(i\omega_n)$$

$$C_{\chi^\alpha}(i\nu_n)^{-1} = J^\alpha_c + M^\alpha(i\nu_n),$$

(6.11) and (6.12)

where the free isolated cluster Greens function is $g^0_c(i\omega_n)^{-1} = (i\omega_n + \mu)1 - t_c$ and $1$ is the identity matrix in cluster indices.

The fact that both self energies are $\tilde{k}$ and $\tilde{q}$ independent implies they can be calculated by an effective cluster model. The effective cluster model can be obtained by a generalized cavity method [150], expanding the partition function in terms of $\delta t$ and $\delta J^\alpha$ about a particular cluster $o$ and effectively integrating out all other degrees
of freedom, this leads to the cluster action

\[
S_C = S_C^0 - \int_0^\beta d\tau d\tau' \sum_{X,Y,\sigma} c^\dagger_{X\sigma}(\tau) G^{-1}_{0,XY}(\tau - \tau') c_{Y\sigma}(\tau') \\
- \frac{1}{2} \int_0^\beta d\tau d\tau' \sum_{X,Y,\alpha} S^\alpha_X(\tau) \chi^{-1}_{00,XY}(\tau - \tau') S^\alpha_Y(\tau').
\]

(6.13)

We have dropped the cluster label \(o\), defined the isolated cluster action as

\[
S_C^0 = \int_0^\beta d\tau \sum_{X \in C} n_{X1}(\tau) n_{X1}(\tau) \\
+ \sum_{\langle X,Y \rangle,\alpha} J^\alpha_{c,XY} S^\alpha_X(\tau) S^\alpha_Y(\tau),
\]

(6.14)

and introduced the effective Weiss fields \(G^{-1}_{0,XY}\) and \(\chi^{-1}_{00,XY}\) that are related to lattice quantities by

\[
G^{-1}_{0}(i\omega_n) = g_{c}(i\omega_n)^{-1} - \sum_{r_i,r_j} \delta t_{r_{i}r_{j}} G^{(o)}_{r_{i}r_{j}o} (i\omega_n) \delta t_{r_{j}o}
\]

(6.15)

\[
\chi^{-1}_{0a}(i\nu_n) = \sum_{r_{i},r_{j}} \delta J^{\alpha}_{r_{i}r_{j}a} \chi^{(o)}_{r_{i}r_{j}o} (i\nu_n) \delta J^{\alpha}_{r_{j}o}.
\]

(6.16)

Where \(G^{(o)}\) and \(\chi^{(o)}\) are the Greens function and spin susceptibility of the lattice with the cluster \(o\) removed, and we have taken the cluster \(o\) to be at the origin. Generalizing the arguments of ref [74] to the case of matrix cluster quantities we can relate \(G^{(o)}\) and \(\chi^{(o)}\) to the full Greens function and spin/charge susceptibilities to obtain (omitting the frequency labels)

\[
G^{(o)}_{r_{i}r_{j}} = G_{r_{i}r_{j}} - G_{r_{i}o}(G_{oo})^{-1} G_{or_{j}}
\]

(6.17)

\[
\chi^{(o)}_{r_{i}r_{j}a} = \chi_{r_{i}r_{j}a} - \chi_{r_{i}o} \chi^{(o)}_{0o} \chi_{r_{j}o}.
\]

(6.18)

With these relations, equations (6.5) and (6.6), as well as the self consistency condi-
tions

\[ G_{\text{loc}}(i\omega_n) = \frac{N_c}{N} \sum_k G(k, i\omega_n), \tag{6.19} \]

\[ \chi^\alpha_{\text{loc}}(i\nu_n) = \frac{N_c}{N} \sum_{\tilde{q}} \chi^\alpha(\tilde{q}, i\nu_n), \tag{6.20} \]

the Weiss fields are completely determined by the self energies and the local correlation functions where

\[ G^{-1}_0(i\omega_n) = \Sigma(i\omega_n) + G_{\text{loc}}(i\omega_n)^{-1}, \tag{6.21} \]

\[ \chi^{-1}_{0\alpha}(i\nu_n) = M^\alpha(i\nu_n) + J^\alpha_c - \chi^\alpha_{\text{loc}}(i\nu_n)^{-1}. \tag{6.22} \]

We have used equations (6.5) and (6.6) to eliminate the dependence on the effective cumulants and use the subscript “loc” denote averages calculated with the effective cluster action in equation (6.13), which also corresponds to the lattice quantities within the cluster as enforced via the self consistent equations (6.19) and (6.20). These equations first appeared in reference [154], derived by an alternative method. It is possible to generalize the arguments in references [150, 151] to prove that the extended version leads to manifestly causal self energies for both \( \Sigma \) and \( M^\alpha \).

It is useful to consider a few limiting cases of the above equations. First, we note that setting \( G^{-1}_0(i\omega_n) = g^0_c(i\omega_n)^{-1} \) and \( \chi^{-1}_{0\alpha}(i\nu_n) = 0 \) implies the effective cluster correlation functions reduce to the isolated cluster quantities, and the self energies are then completely determined by solving the isolated cluster problem. Therefore, in the absence of Weiss fields this approach reduces to CPT for both \( G_{ij} \) and \( \chi^\alpha_{ij} \) and is no longer self consistent. This clarifies the meaning of keeping all local decorations for \( C_G \) and \( C_{\chi^\alpha} \) and is necessary to properly introduce the dynamic Weiss fields. In the limit of one site in the cluster \( N_c = 1 \), the equations reduce to EDMFT, which emphasizes
the cluster theories incorporate spatial fluctuations beyond standard dynamical mean field theories. Lastly, in the limit of large cluster sizes, $N_c \to \infty$ the theory becomes exact. In this sense, extended dynamic cluster theories interpolates between the EDMFT and the exact answer as the cluster size is increased.

After self consistency has been reached it is possible to restore translational invariance to the self energies and thereby the correlation functions by interpolating the cluster quantities. Since the self energies are only defined for sites within the cluster (or cluster momentum) the interpolation scheme must respect the symmetry of the original lattice. Following reference [149], after the self consistent solution has been reached we interpolate the cluster self energies to obtain the lattice quantities with the estimation

\begin{equation}
\Sigma_{\text{lat}}(k, i\omega_n) = \frac{1}{N_c} \sum_{X,Y} e^{-ik \cdot (X-Y)} \Sigma(X, Y, i\omega_n), \tag{6.23}
\end{equation}

\begin{equation}
M^\alpha_{\text{lat}}(q, i\nu_n) = \frac{1}{N_c} \sum_{X,Y} e^{-iq \cdot (X-Y)} M^\alpha(X, Y, i\nu_n). \tag{6.24}
\end{equation}

We then use these to determine the lattice Greens function and spin susceptibility in equations (6.2) and (6.3). Other interpolation schemes are possible as described in [158], where each scheme preserves the symmetry of the lattice.

### 6.2.2 Momentum Space Formulation

The momentum space construction follows the DCA formulation, which restores translation symmetry by giving the cluster periodic boundary conditions[151, 155]. This is achieved by modifying the cluster Fourier transform to

\begin{equation}
[J_D^{\alpha}(\mathbf{k})]_{x_i, x_j} = J^\alpha(\mathbf{k})_{X_i, X_j} e^{-i\mathbf{k} \cdot (X_i - X_j)} \tag{6.25}
\end{equation}

\begin{equation}
= \frac{1}{N_c} \sum_{\mathbf{K}} e^{i\mathbf{K} \cdot (X_i - X_j)} J^\alpha_{\mathbf{K} + \mathbf{k}} \tag{6.26}
\end{equation}
as described in detail in ref[149], in the following we will refer to this as the DCA Fourier transform. This leads to periodic boundary conditions in the cluster and a coarse graining of the cluster quantities $\bar{t}_K = N_c/N \sum_k t_{k+K}$ and $\bar{J}_Q = N_c/N \sum_q J_{q+Q}$ and in turn, the inter-cluster quantities become $\delta t_{k+K} = t_{k+K} - \bar{t}_K$ and $\delta J_{q+Q} = J_{q+Q} - \bar{J}_Q$. Applying the DCA Fourier transform to equations (6.5) and (6.6) leads to matrix equations that are diagonal in momentum space. Here we specify the equations for the spin susceptibility, with the equations for the Greens function being identical to standard DCA. We have for the Dyson like equation

$$\chi^\alpha(\tilde{q} + Q, i\nu_n) = \frac{1}{1/C_{\chi^\alpha}(Q, i\nu_n) + \delta J_{q+Q}^\alpha},$$

(6.27)

with an effective spin cumulant

$$1/C_{\chi^\alpha}(Q, i\nu_n) = M^\alpha(Q, i\nu_n) + \bar{J}_Q^\alpha,$$

(6.28)

and Weiss field specified by

$$\chi_0^{-1}(Q, i\nu_n) = M^\alpha(Q, i\nu_n) + \bar{J}_Q^\alpha - 1/\chi_{\text{loc}}^\alpha(Q, i\nu_n),$$

(6.29)

with the self consistent equation

$$\chi_{\text{loc}}^\alpha(Q, i\nu_n) = \frac{N_c}{N} \sum_q \chi^\alpha(\tilde{q} + Q, i\nu_n).$$

(6.30)

Lastly, the cluster action is now diagonal in cluster momentum, which leads to

$$S_C = S_C^0 - \int_0^\beta d\tau d\tau' \sum_{K,\sigma} c_{K,\sigma}^\dagger(\tau) \mathcal{G}_{0,\bar{K}}^{-1}(\tau - \tau') c_{K,\sigma}(\tau')$$

$$- \frac{1}{2} \int_0^\beta d\tau d\tau' \sum_{Q,\alpha} S_{Q}^\alpha(\tau) \chi_{0,\alpha,\bar{Q}}^{-1}(\tau - \tau') S_{Q}^\alpha(\tau'),$$

(6.31)
where the isolated cluster action [in equation (6.14)] is written in cluster momentum
\[ S^0_c = \int_0^\beta d\tau U \sum_{\mathbf{q}} n_{\mathbf{q}^+}(\tau)n_{\mathbf{q}^0}(\tau)+\sum_{\mathbf{q},\alpha} \tilde{J}^\alpha_{\mathbf{q}} S^0_{\mathbf{q},\alpha}(\tau) S^0_{\mathbf{q},\alpha}(\tau). \]
These equations were first specified in ref. [155] for inter site density density interactions following a different procedure.

6.3 Magnetic Order

Before we discuss the cluster generalization of symmetry broken phases within EDMFT, we find it very useful to review the different schemes used to introduce magnetic order in the single site case. In the context of the EDMFT, there are two ways to introduce magnetic order into the system, namely whether or not the magnetic order parameter polarizes the single particle Weiss field \( G_{\mathbf{q},\sigma}^{-1} \) (see reference [77] for details). It has been shown [77] that allowing \( G_{\mathbf{q},\sigma}^{-1} \) to polarize amounts to keeping the particle hole bubble contribution \( [\chi_{\text{ph}}(\mathbf{q},\omega)]^{-1} - [\chi_{\text{ph,loc}}(\omega)]^{-1} \), to the spin susceptibility [5] (where the particle hole bubbles are constructed using the full lattice and local Greens function respectively obtained with DMFT and the brackets [. . .] denote a matrix form [74]).

Within the context of DMFT, such a term will exist due to the distinction between “normal” and “special” \( \mathbf{q} \)'s, ref. [5]. However, due to promoting \( J_{ij} \) to the same level as \( t_{ij} \) within the EDMFT, strictly speaking, there are no special \( \mathbf{q} \)'s allowed, since this would make \( J(\mathbf{q}) \sim O(d) \) which would diverge in the large \( d \) limit. Due to absence of any special \( \mathbf{q} \)s leads to \( [\chi_{\text{ph}}(\mathbf{q},\omega)]^{-1} = [\chi_{\text{ph,loc}}(\omega)]^{-1} \) and the particle hole bubble contribution vanishes [74]. Keeping the particle hole bubble within the EDMFT amounts to double counting contributions from the spin-spin interaction [77].

In the following section, we focus on the EDMFT generalization to the cluster case. In the DCA solution of the Bethe-Salpeter equation [149], a similar particle hole contribution to the spin susceptibility exists, namely, \( [\chi_{\text{ph}}(\mathbf{q},\omega)]^{-1} - [\chi_{\text{ph,loc}}(\omega)]^{-1} \) (here the particle hole bubble is constructed with the full single particle lattice and
local cluster Greens function respectively, obtained within DCA and the bold denotes matrices in cluster momentum) \cite{149}. Since, we have promoted $\delta J$ to the same level as $\delta t$, generalizing the EDMFT argument \cite{74} to the cluster case we conclude, there should only be generic $\bar{q}$’s. This amounts to not allowing the single particle Weiss field $\mathcal{G}_{0\sigma}^{-1}$ to polarize (i.e. is $\sigma$ independent), and is equivalent to the suppression of the particle hole bubble contribution. This makes the C-EDMFT approach distinct from previous extended versions of CDMFT and DCA.

We now consider magnetic order with an ordering wave vector $\mathbf{q} = \mathbf{q}_{\text{or}} \equiv \mathbf{q}_{\text{or}} + \mathbf{Q}_{\text{or}}$ within the channel $\alpha = \lambda$ with $\lambda \neq 0$. The cluster chosen must be large enough to accommodate the type of magnetic order under consideration, for example a four site cluster can describe magnetic strip order with $\mathbf{q}_{\text{or}} = (0, \pi)$ whereas a two site cluster can only treat either ferro- or antiferromagnetic order. This then implies that the order pattern within each cluster must be the same and therefore $\mathbf{q}_{\text{or}} = 0$.

We will first specify the equations in real space and then momentum space. After separating $J_{ij}^\alpha$ into inter- and intra-cluster parts we treat the cluster interactions exactly and normal order the interaction between clusters, via $S_i^\alpha = S_i^\alpha + \langle S_i^\alpha \rangle$. Due to the absence of any special $\bar{q}$’s, the magnetic order parameter does not polarize the single particle Wiess field $\mathcal{G}_{0\sigma}^{-1}$. All of the previous steps apply, but now we perform the locator expansion in the normal ordered interaction between clusters $\delta J_{XY}^\alpha(r_i - r_j) : S_{X_{r_i}}^\alpha : S_{Y_{r_j}}^\alpha :$. This corresponds to adding an additional term to the cluster action

\[
S_C \rightarrow S_C - \int_0^\beta d\tau \sum_X h_{\text{loc}}^X S_X^\lambda(\tau) \tag{6.32}
\]

and the local magnetic field is determined self consistently from

\[
h_{\text{loc}}^X = - \sum_Y \left[ \delta J_{XY}^\lambda(\mathbf{q}_{\text{or}} = 0) + \chi_{0\lambda,XY}(i\omega_n = 0) \right] M_Y, \tag{6.33}
\]
where $M_Y = \langle S_Y^\lambda \rangle_C$ and the average is over the cluster action.

In momentum space this approach, amounts to adding to the action

$$S_C \to S_C - \int_0^{\beta} d\tau h_{\text{loc}} S_{Q_{\text{or}}}^\lambda(\tau).$$  \hfill (6.34)

Now the local field is given by

$$h_{\text{loc}} = - \left[ \delta J_{Q_{\text{or}}}^\lambda + \chi_{0\lambda}^{-1}(Q_{\text{or}}, i\omega_n = 0) \right] M$$  \hfill (6.35)

where $M = \langle S_{Q_{\text{or}}}^\lambda \rangle_C$ and in this case the inter-cluster interaction is $\delta J_{Q_{\text{or}}}^\lambda = J_{Q_{\text{or}}}^\lambda - \bar{J}_{Q_{\text{or}}}^\lambda$
where we have coarse grained the cluster interaction as described previously.

It is useful to note, that in the limit of no dynamic Weiss field, the mean field equations for the self consistent field $h_{\text{loc}}$ reduce to that of cluster Weiss mean field theory. Here, the dynamic Weiss field renormalizes the static field due to the dynamic interactions mediated by $\chi_{0\lambda}^{-1}$.

### 6.3.1 Static Spin Susceptibility

In the following section, we use the self consistent equations that incorporate magnetic order to provide an alternative way of deriving the $z$ component of the static lattice spin susceptibility at an ordering wavevector $Q_{\text{or}}$, which we define as $\chi^z(Q_{\text{or}}, i\omega_n = 0) \equiv \chi_{or}$. This approach will also provide insight on how to incorporate superconducting long range order in C-EDMFT and determine the static lattice pairing susceptibility. In order to naturally incorporate an ordering wave vector, we will consider the momentum space formalism.

We introduce an additional term $H_1$, to the lattice Hamiltonian which couples the
\[ \lambda = z \text{ component of the spin operators at wavevector } \pm Q_{\text{or}} \text{ to a source field} \]

\[ H_1 = - (h_{-Q_{\text{or}}} S^z_{Q_{\text{or}}} + h_{Q_{\text{or}}} S^z_{-Q_{\text{or}}}) \quad (6.36) \]

Mapping this into the cluster action, assuming that the Weiss fields cannot be polarized (due to the absence of any special \( \tilde{q} \)'s), results in only adding an extra term \( S_1 \) to equation (6.34), namely

\[ S_1 = - \int_0^\beta d\tau \sqrt{\frac{N_c}{N}} h (h_{-Q_{\text{or}}} S^z_{Q_{\text{or}}} (\tau) + h_{Q_{\text{or}}} S^z_{-Q_{\text{or}}} (\tau)) \quad (6.37) \]

Here \( S^z_{Q_{\text{or}}} \) defined in the cluster need to be distinguished from \( S^z(q = Q_{\text{or}}) \), which is defined on the lattice, since we have \( S^z_{Q_{\text{or}}} = 1/\sqrt{N_c} \sum_{k, \sigma} (\sigma/2) c_{k, \sigma}^\dagger c_{k+Q_{\text{or}}, \sigma} \) and \( S^z(q = Q_{\text{or}}) = 1/\sqrt{N} \sum_{k, \sigma} (\sigma/2) c_{k, \sigma}^\dagger c_{k+Q_{\text{or}}, \sigma} \) respectively (where \( \sigma = +/ - 1 \) for \( \uparrow / \downarrow \)). The \( \sqrt{N_c/N} \) factor in the coarse grained equation (6.37) is to ensure the self consistency condition on \( G_{\text{loc}} \) is satisfied, \( G_{\text{loc}, \sigma}(K, K + Q_{\text{or}}, \tau) = \frac{N_c}{N} \sum_k G_{\sigma}(K + \tilde{k}, K + \tilde{k} + Q_{\text{or}}, \tau). \)

Multiplying the self consistent equation by \( \sigma \), summing over \( K \) and \( \sigma \) and taking \( \tau \to 0^- \), leads to

\[ \langle S^z_{Q_{\text{or}}} \rangle_C = \sqrt{\frac{N_c}{N}} \langle S^z(q = Q_{\text{or}}) \rangle_L. \quad (6.38) \]

Where \( \langle \ldots \rangle_C \) denotes an average with respect to the cluster action of equation (6.34) plus \( S_1 \) and \( \langle \ldots \rangle_L \) denotes an average with respect to the lattice action in the presence of a finite \( H_1 \). For later convenience, we define \( \langle S^z_{Q_{\text{or}}} \rangle_C \equiv F(M(h), h) \), which is a function of both the magnetic order parameter \( M \) and the source field \( h \).

Differentiating both side of equation (6.38) with respect to \( h \) at \( h = 0 \), leads to
an equation for $\chi_{or}$. The right-hand side gives the lattice correlation function,

$$
\left. \frac{d\langle S^z_{Q_{or}} \rangle_L}{dh_{-Q_{or}}} \right|_{h=0} = \sqrt{\frac{N_c}{N}} \int_0^\beta d\tau \langle T_\tau : S^z_{-Q_{or}}(\tau) :: S^z_{Q_{or}}(0) : \rangle_L
= \sqrt{\frac{N_c}{N}} \chi_{or}
$$

(6.39)

where we have defined $\chi_{or}$ as the static lattice spin susceptibility at the ordering wave vector. Whereas the left-hand side gives the cluster correlation function, using

$$
\frac{df}{dh_{-Q_{or}}} = \left( \frac{\partial f}{\partial M} \right) dM/dh_{-Q_{or}} + \partial f/\partial h_{-Q_{or}}
$$

and,

$$
\frac{\partial f}{\partial h_{-Q_{or}}} = \sqrt{\frac{N_c}{N}} \int_0^\beta d\tau \langle : T_\tau S^z_{-Q_{or}}(\tau) :: S^z_{Q_{or}}(0) : \rangle_C
= \sqrt{\frac{N_c}{N}} \chi_{loc,or}
$$

(6.40)

$$
\frac{\partial f}{\partial M} = -(h_{loc}/M)\chi_{loc,or}
$$

(6.41)

where $h_{loc}$ is given by equation (6.35) and we have defined $\chi_{loc}^z(Q_{or}, i\omega_n = 0) \equiv \chi_{loc,or}$ as the static local spin susceptibility in the ordering channel $Q_{or}$. Finally, using equations (6.39), (6.40) and (6.41) we obtain

$$
1/\chi_{or} = \chi_{0z}^{-1}(Q_{or}, i\omega_n = 0) + \delta J_{Q_{or}}^z + 1/\chi_{loc,or}.
$$

(6.42)

We recognize immediately this result as the C-EDMFT self-consistent equation for the static spin susceptibility at the ordering wavevector $Q_{or}$ and spin component $z$, [see equation (6.27)]. Therefore, we can conclude a non-polarized Weiss field is internally consistent with the C-EDMFT treatment. The lack of any special $\tilde{q}$'s has important implications for incorporating superconductivity which we come in the following section.
6.4 Superconductivity

We now extend these concepts to deal with superconductivity, where the attractive pairing interaction is mediated by the spin-spin interaction in equation (9.1). We first focus on an antiferromagnetic Ising interaction with $J^z_{ij} \equiv J_{ij} > 0$ and set the other $J^a_{ij}$ to zero. The antiferromagnetic interaction $J_{ij}$ leads to opposite spin pairing whereas these techniques can also be generalized to ferromagnetic interactions and same spin pairing. We then discuss the case of a full antiferromagnetic Heisenberg interaction where $J^a_{ij} \equiv I_{ij} > 0$ is only non-zero for $a = 1, 2, 3$.

Following the discussion of magnetic order in section 6.3, in the context of pairing, the absence of special $\mathbf{q}$'s implies we should not include a contribution from the particle particle bubble that arises in the Bethe-Salpeter equation solution within DCA. This amounts to not allowing the conduction electron band to become “polarized” by a finite superconducting order parameter. This makes our cluster scheme distinct from previous work [149, 109], because we treat superconductivity at the mean field level within an extended dynamical cluster scheme as described in the following sections. In the appendix, we also discuss the details of allowing the conduction electrons to include anomalous Weiss fields and how this effects the normal state properties.

6.4.1 Ising Spin Interaction

Conceptually, we would like to keep the strong inter site interactions (that give rise to the dynamic bosonic bath) while promoting a single mode in the static pairing channel giving it the chance to condense. We do so, by singling out the static, attractive pairing interaction between the paring operators $\hat{\Delta}_{i a j a}$ and $\hat{\Delta}_{i a j a}$ (defined
as $\hat{\Delta}_{i\sigma j\sigma}^\dagger(\tau) = c_{i\sigma}^\dagger(\tau) c_{j\sigma}^\dagger(\tau)$. We rewrite the spin-spin interaction as

$$\int_0^\beta d\tau \sum_{\langle i,j \rangle} J_{ij} S_i^\sigma(\tau) S_j^\sigma(\tau)$$

$$= - \sum_{\langle i,j \rangle, \sigma} J_{ij} \frac{4\beta}{1} \int_0^\beta d\tau_1 d\tau_2 \hat{\Delta}_{i\sigma j\sigma}^\dagger(\tau_1) \hat{\Delta}_{i\sigma j\sigma}(\tau_2)$$

$$+ \sum_{\langle i,j \rangle} \frac{1}{1} \frac{\beta}{2} \sum_{\omega_1, \omega_2} J_{ij} \frac{4}{1} (1 - \delta_{\omega_1, -\omega_2} \delta_{\alpha, \gamma}) c_{i\sigma}^\dagger(i\omega_1 - i\omega)$$

$$\times \sigma_{\alpha\beta} c_{i\beta}(i\omega_1) c_{j\gamma}(i\omega_2 + i\omega) \sigma_{\gamma\delta} c_{j\delta}(i\omega_2), \quad (6.43)$$

where the repeated indices $\alpha, \beta, \gamma, \delta$ are summed over. We then introduce a Hubbard-Stratonovich transformation to decouple the attractive interaction in the pairing channel

$$\exp \left( \sum_{\langle i,j \rangle, \sigma} \frac{J_{ij}}{4\beta} \int_0^\beta d\tau_1 d\tau_2 \hat{\Delta}_{i\sigma j\sigma}^\dagger(\tau_1) \hat{\Delta}_{i\sigma j\sigma}(\tau_2) \right)$$

$$= \int \mathcal{D}[\Delta, \bar{\Delta}] \exp \left[ - \sum_{\langle i,j \rangle, \sigma} \left( \frac{4\beta}{1} |\Delta_{i\sigma j\sigma}|^2 \right) \right.$$

$$\left. + \int_0^\beta d\tau \Delta_{i\sigma j\sigma} \hat{\Delta}_{i\sigma j\sigma}^\dagger(\tau) + \bar{\Delta}_{i\sigma j\sigma} \hat{\Delta}_{i\sigma j\sigma}(\tau) \right]. \quad (6.44)$$

We note that we would arrive at the same result of the right hand side of equation (6.44) if we perform the H-S transform directly to the left hand side of equation (6.43) and make the static mean field approximation. In this sense, the information that is left out in the mean field approximation is actually contained in the second term of the RHS of eq (6.43). This then can be interpreted as the fluctuations of the magnetic interaction around the superconducting mean field, which is then treated by C-EDMFT.

Now we take the saddle point approximation of $\Delta$ and follow the steps in section 6.2.1 to carry out a generalized cavity construction. Up to additional constants,
we obtain the effective cluster action, (where we have not allowed the single particle Weiss field to acquire anomalous terms consistent with the absence of any special \( \tilde{q} \)'s)

\[
S_{C,I} = S_{C,I}^0 - \sum_{\langle X,Y \rangle, \sigma} \int_0^\beta d\tau \left( \Delta_{X \sigma Y \sigma} \Delta_{X \sigma Y \sigma}^\dagger (\tau) + \text{h.c.} \right) - \int_0^\beta d\tau d\tau' \sum_{X,Y,\sigma} c_{X \sigma}^\dagger (\tau) G_{0,XY}^{-1}(\tau - \tau') c_{Y \sigma}(\tau') - \frac{1}{2} \int_0^\beta d\tau d\tau' \sum_{X,Y} S_X^Z(\tau) \chi_{0,XY}^{-1}(\tau - \tau') S_Y^Z(\tau') + \delta S. \quad (6.45)
\]

The saddle point equation leads to an additional self consistent equation for the superconducting order parameter

\[
\Delta_{X_i \sigma X_j \sigma}^c = \frac{J_{\tilde{X}_i X_j}}{4 \beta} \int_0^\beta d\tau \langle \hat{\Delta}_{X_i \sigma X_j \sigma}(\tau) \rangle_C, \quad (6.46)
\]

where the average is with respect to the effective cluster model in equation (6.45). The additional term in the action, \( \delta S \) represents all the modifications in the effective action caused by separating the zero frequency pairing interaction. The exact expression of \( \delta S \) can be found in the Appendix. We see that all terms in \( \delta S \) are suppressed by factors of \( 1/\beta \), and therefore at sufficiently low temperatures as well as quantum critical properties, \( \delta S \) can be safely neglected. In the following we only consider the low temperature limit and make the approximation that \( \delta S \approx 0 \). Working in this approximation guarantees the self consistency conditions for both \( G_{0,XY}^{-1} \) and \( \chi_{0,XY}^{-1} \) remain the same as the previous sections.

It is useful to note, this formulation can also be done in momentum space. Since using the DCA Fourier transform defined in equation (??), amounts to replacing \( J_{ij} \)
by $J_{ij}^{\text{DCA}} = N_c/N \sum_{\mathbf{q}} e^{i\mathbf{q} \cdot (\mathbf{x}_i - \mathbf{x}_j)} [J_{\text{DCA}}^{\delta}(\tilde{\mathbf{q}})] \mathbf{x}_i, \mathbf{x}_j$ in the spin channel. In order to treat the pairing channel on the same footing, we use $J_{ij}^{\text{DCA}}$ starting in equation (6.43). This then amounts to replacing $J_{X_iX_j}^c$ in equation (6.46) with $|J_{\text{DCA}}^c| \mathbf{x}_i \mathbf{x}_j$, which is the coarse grained interaction in cluster momentum ($\tilde{J}_Q$) that is Fourier transformed back to real space cluster variables (see ref. [149]) $[J_{\text{DCA}}^c] \mathbf{x}_i, \mathbf{x}_j = 1/N_c \sum_{\mathbf{Q}} e^{i\mathbf{Q} \cdot (\mathbf{x}_i - \mathbf{x}_j)} \tilde{J}_Q$.

In addition, this leads to periodic boundary condition on the cluster in real space.

### 6.4.2 Heisenberg Spin Interaction

We now consider the case of an antiferromagnetic Heisenberg spin $\sigma_i$ spin interaction $I_{ij}$. The derivation follows in parallel with the previous Ising case. Here, we separate out the singlet term with an attractive interaction [159]

$$
\int_0^\beta d\tau \sum_{\langle i,j \rangle} I_{ij} \vec{S}_i(\tau) \cdot \vec{S}_j(\tau)
= - \sum_{\langle i,j \rangle} I_{ij} \beta \int_0^\beta d\tau_1 d\tau_2 \hat{\Delta}_{ij}^\dagger(\tau_1) \hat{\Delta}_{ij}(\tau_2)
+ \sum_{\langle i,j \rangle, \omega_1, \omega_2} \frac{I_{ij}}{4\beta^3} (\sigma_{\mu\beta}^\alpha \sigma_{\beta\gamma}^\nu - \delta_{\omega_1, -\omega_2} (2\delta_{\mu\delta} \delta_{\beta\nu} - 2\delta_{\mu\beta} \delta_{\gamma\nu}))
\times c_{i\mu}^\dagger (i\omega_1 - i\omega) c_{i\beta} (i\omega_1) c_{j\gamma}^\dagger (i\omega_2 + i\omega) c_{j\nu} (i\omega_2),
$$

(6.47)

we have defined the singlet creation operator between sites $i$ and $j$ as

$$
\hat{\Delta}_{ij}^\dagger = \frac{1}{\sqrt{2}} \left( c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger \right),
$$

(6.48)

and its hermitian conjugate $\Delta_{ij} = (c_{j\downarrow} c_{i\uparrow} - c_{j\uparrow} c_{i\downarrow}) / \sqrt{2}$. As before, we then introduce a static Hubbard-Stratonovich field to decouple the singlet interaction $\hat{\Delta}_{ij}^\dagger \hat{\Delta}_{ij}$, the
saddle point equation for \( \Delta_{ij} \) now becomes

\[
\Delta_{X_i X_j} = \frac{I_{cX_i X_j}}{\beta} \int_0^\beta d\tau \langle \hat{\Delta}_{X_i X_j}(\tau) \rangle_C. \tag{6.49}
\]

with an effective action,

\[
S_{C,H} = S_{C,H}^0 - \sum_{\langle X,Y \rangle} \int_0^\beta d\tau \left( \Delta_{XY} \hat{\Delta}_Y^\dag (\tau) + \text{h.c.} \right)
- \int_0^\beta d\tau d\tau' \sum_{X,Y,\sigma} \chi_{X\sigma}(\tau) G_{0,XY}^{-1}(\tau - \tau') c_{Y\sigma}(\tau')
- \frac{1}{2} \int_0^\beta d\tau d\tau' \sum_{X,Y, \sigma \neq 0} S_{X\sigma}(\tau) G_{0,XY}^{-1}(\tau - \tau') S_{Y\sigma}(\tau'). \tag{6.50}
\]

Again, we have not allowed the single particle Weiss field to become polarized from the finite superconducting order parameter. The Heisenberg isolated cluster action \( S_{C,H}^0 \), is equation (6.14) with \( J^a_c = 0 \) for \( \alpha = 0 \) and \( J^a_c = I_c \) for \( \alpha = 1, 2, 3 \). We have also ignored the additional part of the action \( \delta S_H \) that is suppressed by a factor of \( 1/\beta \) (see the appendix for a discussion of the Ising case). We remark, it possible to use this formalism to describe states that have both magnetic order and superconductivity by including a finite \( h_{\text{loc}} \) as described in section 6.3.
### 6.4.3 Static Pairing Susceptibility

In this section we derive the static, zero momentum, lattice pairing susceptibility  
\[ \chi_{SC} \equiv \chi_{\text{lat}}^{\text{pair}}(q = 0, i\omega_n = 0), \]  
which is defined as

\[
\chi_{SC} = \frac{1}{N(z/2)} \sum_{(i,j),\sigma} \sum_{(k,l),\lambda} f_{i,j}^* f_{k,l} g_{\sigma\lambda} g_{\bar{\sigma}\bar{\lambda}} \times \int_0^\beta d\tau \langle T_\tau : \hat{\Delta}_{i\sigma j\bar{\sigma}}(\tau) :: \hat{\Delta}^\dagger_{k\lambda \bar{\lambda}} :: C \rangle,
\]

(6.51)

where \( N(z/2) \) is the number of bonds in the lattice, with \( z \) being the number of nearest neighbors. We will focus on the case of an Ising spin interaction \( J_{ij} \) but this can be easily generalized to the case of a Heisenberg interaction. We first project the superconducting gap onto a particular symmetry channel assuming the gap amplitude \( \Delta_0 \), is uniform across each bond, i.e. \( \Delta_{X\sigma Y\bar{\sigma}} = f_{XY} g_{\sigma\bar{\sigma}} \Delta_0 \) (and complex conjugate \( \Delta_{X\sigma Y\bar{\sigma}}^* = f_{XY}^* g_{\sigma\bar{\sigma}}^* \Delta_0^* \)), where the phase factor in real space is given by \( f_{XY} \) and that in spin space is \( g_{\sigma\bar{\sigma}} \), and they have the property \( |f_{XY}|^2, |g_{\sigma\bar{\sigma}}|^2 = 1 \) (see ref. [12]).

Following a similar procedure as described in in section 1.1 for magnetism, however in this case we have to project into a particular symmetry channel (through \( f_{ij}, g_{\sigma\bar{\sigma}} \)), we arrive at the following expression for the static zero momentum lattice pairing susceptibility.

\[
\chi_{SC} = \frac{1}{1/\chi_{\text{loc}}^{\text{pair}} - 1/J_{SC}},
\]

(6.52)

where we have defined the effective pairing interaction \( 1/J_{SC} = \frac{4}{N_b} \sum_{(X_i,X_j),\sigma} 1/J_{X_iX_j}^c \), and the static cluster pairing susceptibility \( \chi_{\text{pair}}^{\text{loc}} \equiv \chi_{\text{pair}}^{\text{loc}}(Q = 0, i\omega_n = 0) \), where

\[
\chi_{\text{pair}}^{\text{loc}} = \frac{1}{N_b} \sum_{(X_i,X_j'),\sigma} \sum_{(Y_i,Y_j'),\lambda} f_{X_iX_j'}^* f_{Y_iY_j'}^* g_{\sigma\lambda} g_{\bar{\sigma}\bar{\lambda}} \times \int_0^\beta d\tau \langle T_\tau : \hat{\Delta}_{X\sigma Y'\bar{\sigma}}(\tau) :: \hat{\Delta}^\dagger_{X'\sigma Y'\bar{\lambda}} :: C \rangle
\]

(6.53)
where \( N_b = \sum_{\langle X,Y \rangle} \) is the number of individual bonds in the cluster. Previous treatment of two particle response functions in various cluster theories demands much more computational effort because it involves the inversion of the Bethe-Salpeter equation, which is in principle a matrix equation of infinite dimension in the space of three wave vectors and frequencies. In our approach, static cluster susceptibilities, completely determine the corresponding lattice quantity.

We note that this can also be formulated in momentum space after the symmetry factors are first coarse grained in momentum space \( \tilde{f}(\mathbf{K}) = N_c/N \sum_{\mathbf{k}} f(\mathbf{k} + \mathbf{K}) \) (where \( f(\mathbf{k}) \) is the Fourier transform \( f_{ij} \)) and then Fourier transformed to real cluster space \( \tilde{f}_{X_i X_j} = [f_{DCA}]_{X_i X_j} = 1/N_c \sum_{\mathbf{K}} e^{i\mathbf{K} \cdot (\mathbf{X}_i - \mathbf{X}_j)} \tilde{f}_{\mathbf{K}} \). In this case, the coarse grained symmetry factors no longer have to satisfy \( |\tilde{f}_{X_i X_j}|^2 = 1 \), and as a result the effective pairing interaction becomes \( 1/J_{SC} = \frac{4}{N_b} \sum_{\langle X_i, X_j \rangle, \sigma} |f_{X_i X_j}|^2 / J_{X_i X_j} \).

6.5 Effective Cluster Models

The formalism we have discussed so far can be applied to a variety of strongly correlated problems vastly different from the Hamiltonian we have been considering in equation (9.1). One such example of a two band model is the Anderson lattice Hamiltonian, appropriate for the description of heavy fermion materials [9]. The model describes a band of conduction electrons hybridized with a band of localized, highly correlated \( f \)-electrons and is defined as

\[
\begin{align*}
H_{AL} &= \sum_{\langle i,j \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + \sum_i (\epsilon_f n_{fi} + U n_{fi\uparrow} n_{fi\downarrow}) \\
&+ \sum_{i, \sigma} \left( V c_{i\sigma}^\dagger f_{i\sigma} + h.c. \right) + \sum_{\langle i,j \rangle} J_{ij} S^z_{fi \uparrow} S^z_{fj \downarrow}
\end{align*}
\]

(6.54)
we have explicitly included an Ising RKKY interaction between the $f$-electron spins. The RKKY and Kondo interactions compete, and tuning their ratio can lead to a quantum phase transition between a heavy fermi liquid and an antiferromagnet. In certain cases it is quite clear that the QCP is of the spin density wave (SDW) type, where the heavy quasiparticles remain intact across the transition and undergo a SDW transition. In other cases, the SDW description fails, and the physics of critical Kondo destruction comes into play.

Focusing on the normal state properties, applying the extended dynamical cluster theory of section 6.2.2 in momentum space we arrive at the effective cluster action

\[
S_{C}^{\text{AL}} = \int_{0}^{\beta} d\tau \sum_{Q} U_{n_{f}Q_{1}}(\tau)n_{f-Q_{1}}(\tau) + \epsilon_{f}n_{fQ}(\tau) + \int_{0}^{\beta} d\tau \sum_{Q} J_{Q}S_{fQ}^{z}(\tau)S_{f-Q}^{z}(\tau) - \int d\tau d\tau' \sum_{K,\sigma} J_{K,\sigma}(\tau)G_{1}^{-1}(\tau - \tau')f_{K,\sigma}(\tau') - \frac{1}{2} \int_{0}^{\beta} d\tau d\tau' \sum_{Q} S_{fQ}^{z}(\tau)\chi_{0}(\tau - \tau')S_{f-Q}^{z}(\tau').
\] (6.55)

For the case of antiferromagnetic 2-d magnetic fluctuations, the divergence of the spin susceptibility at the ordering wave vector implies [through the self consistent equation (6.30)] the local spin susceptibility with cluster momentum $Q_{cr}$ is also logarithmically divergent [73]. This leads to a spin Weiss field associated with the critical momentum channel $\chi_{0}(Q_{AF}, i\nu_{n})$ that develops a sub-ohmic spectral density $\text{Im}\chi_{0}(Q_{AF}, \omega + 0^{+}) \sim \omega^{\delta}$. Based on universality, we can regard the effective cluster model in equation (6.55) with a sub-ohmic density of states for the ordered channel, as an effective model that contains both Kondo destruction and pairing correlations induced from antiferromagnetic interactions. For the simplest case of $N_{c} = 2$, and keeping only the critical degrees of freedom [i.e. only keeping the Wiess field in the ordered channel
we arrive at a toy model to study pairing correlations in the vicinity of a Kondo destroyed QCP. This model will be discussed in detail and solved in chapter 7 using a combination of continuous time quantum Monte Carlo and the numerical renormalization group [126]. In chapter 8, we consider the full self consistent solution and determine if the LQC survives finite size cluster corrections and, in addition how large $1/r_{pair}$ is at the QCP point.

Another strongly correlated problem of central interest is the extended Hubbard model, which adds to the standard Hubbard model an inter site density density interaction. We note that incorporating a spin orbit coupling can lead to topologically non-trivial ground states in the presence of interactions [160, 161]. The extended Hubbard model is thought to be the appropriate model to describe certain types of organic superconductors, strip charge order in the cuprates and different types of Mott transitions [154]. The extended Hubbard model is defined as

$$H = \sum_{i,j,\alpha,\beta} t_{ij}^{\alpha\beta} (c_{i\alpha}^\dagger c_{j\beta} + \text{h.c}) + U \sum_i n_{i\uparrow}n_{i\downarrow} + \sum_{(i,j)} V_{ij} : n_i : : n_j :,$$  \hspace{1cm} (6.56)

we have generalized the tight binding to a spin dependent hopping matrix $t_{ij}^{\alpha\beta}$ which allows for a spin orbit coupling term and $i,j$ no longer have to be nearest neighbors. Tuning the ratio of $U/V$ can lead to a variety of quantum phase transitions between a fermi liquid, a band insulator, and a Mott insulator. In contrast, tuning the strength of the spin orbit coupling can lead to topological transitions between a band and topological insulator. Applying the formalism of section 6.2.1 leads to the effective
cluster action

\[
S_{C}^{EH} = \int_{0}^{\beta} d\tau \sum_{x \in C} U n_{X\uparrow}(\tau) n_{X\downarrow}(\tau) + \int_{0}^{\beta} d\tau \sum_{(X,Y)} V_{c} : n_{X}(\tau) :: n_{Y}(\tau): - \int_{0}^{\beta} d\tau d\tau' \sum_{X,Y,\mu,\nu} c_{X,\mu}^{\dagger}(\tau) G_{0,XY,\mu\nu}^{-1}(\tau - \tau') c_{Y,\nu}(\tau') - \frac{1}{2} \int_{0}^{\beta} d\tau d\tau' \sum_{X,Y} : n_{X}(\tau) : \chi_{0ch,XY}^{-1}(\tau - \tau') : n_{Y}(\tau'): \quad (6.57)
\]

Studying the different types of quantum phase transitions in the effective cluster model alone can lead to significant new insights regarding the QCPs in the lattice problem. Such as, determining the nature of the transitions within the effective cluster model, will shed significant light on the transition in the lattice problem. In addition, by introducing an attractive inter site interaction \( V_{ij} < 0 \) can also lead to inter site pairing and in the presence of a spin orbit coupling topological superconductivity \[162\]. Therefore, the effective cluster model of equation (6.57) serves as a toy model to study different types of Mott transitions, superconductivity and interacting topological phase transitions.

6.6 Discussion

In this work we have derived extended cluster theories by a locator expansion about a dressed cluster limit. Distinct from the previous approaches we have described, an alternative derivation can also be done using a Baym-Kadanoff functional \[149, 156\]. In this case the generating functional of the grand potential is (focusing on one of the
two particle channels)

\[
\Gamma_{BK}[G, \chi] = \text{Tr} \left[ \log(G) \right] - \text{Tr} \left[ G(G_0^{-1} - G^{-1}) \right] - \frac{1}{2} \text{Tr} \left[ \log(\chi) \right] + \text{Tr} \left[ \chi(\chi_0^{-1} - \chi^{-1}) \right] + \Phi[G, \chi],
\]

(6.58)

with the stationary conditions \( \delta \Gamma / \delta G = \delta \Gamma / \delta \chi = 0 \). The self energies are then given by \( \delta \Phi[G, \chi] / \delta G = \Sigma, \delta \Phi[G, \chi] / \delta \chi = M \). Within the cluster approximation, the self energies are calculated from an effective cluster model. Therefore, the approximation that the functional \( \Phi \) is only a functional of \( G_{\text{loc}} \) and \( \chi_{\text{loc}} \) leads to the cluster EDMFT equations. This then implies that extended version of cluster methods are conserving [163].

The self consistent cluster dynamical mean field equations form a set of highly non-linear equations. Their solution require an accurate and reliable solution of the cluster impurity model, which is iteratively solved. Due to the self consistent dynamic Weiss fields there are very limited analytic tools and computational methods play a central role. The cluster model can be solved using the exact diagonalization (ED), the numerical renormalization group (NRG), the density matrix renormalization group (DMRG) and quantum Monte Carlo methods.

Including bosonic baths in diagonalization based techniques can be done, but it requires a truncation of the infinite bosonic Hilbert space. In this regard, the recently developed continuous time quantum Monte Carlo (CT-QMC) has the advantage that the bosons are traced out and the algorithm is numerically exact. These methods have been adapted to treat scalar bosonic baths that interact with the impurities charge [111, 138] and or spin [141, 126] degrees of freedom. Recently, the hybridization expansion has been generalized to incorporate a vector bosonic bath [139] and in the
presence of more than one impurity [126].

From a computational perspective, solving the cluster impurity models is the most time consuming part of solving the self consistent equations. In the presence of a phase transition, the number of iterations necessary to solve the equations can become quite large due to a “critical slowing down”. In this case, it is very useful to use mixing techniques that are well known in the context of density functional theory, in order to reduce the number of self consistent solutions [164].

6.7 Conclusions

In this chapter we have presented a new cluster extended dynamical mean field approach. We have developed the equations in both real and momentum space, incorporating magnetic order and superconductivity. We have also determined the normal state superconducting properties. We have then used the formalism to derive effective cluster models relevant to heavy fermion metals and Mott insulators. In conclusion, we have developed the framework to study unconventional superconductivity within an extended dynamical mean field theory, which will be relevant to quantum critical heavy fermion metals. In the proceeding two chapters, we will use the formalism derived in this chapter to construct an effective toy model and a framework to calculate pairing correlations in the vicinity of Kondo destroyed QCP.
In the following chapter, we study the effect of Kondo breakdown quantum criticality on pairing correlations in an effective cluster impurity model. We do so by introducing a two impurity model that serves as a “toy model” that has both Kondo destruction physics and pairing correlations. The model was rigorously derived in equation (6.55) of the previous chapter, where in the following we only keep the bosonic bath in the ordering channel. We first determine the critical properties of this model, and then focus on the local pairing susceptibility (defined below) across the phase diagram and determine how the critical suppression of Kondo screening, effects pairing correlations. This chapter aims to determine the physics of the effective cluster model we need to solve self consistently in order to understand the full lattice problem. The self consistent solution will be the focus of chapter 8.
7.1 Introduction

Theoretically, it remains an open question whether a Kondo-destruction QCP promotes unconventional superconductivity [18]. To make progress, it is essential to identify simplified models in which this issue can be addressed and insights can be gained. Because an on-site Coulomb repulsion does not favor conventional s-wave pairing, this issue can only be studied in models that incorporate correlations among different local-moment sites.

In this chapter, we study perhaps the simplest models that support Kondo-destruction physics and allows the study of superconducting correlations: two local moments that interact with each other through a direct exchange interaction and are also coupled both to a conduction-electron band and to a bosonic bath. This model was derived rigorously in section 6.5, (see the effective action in equation (6.55)). Intuitively, we have been led to these models by the significant insights gained from solving single-impurity models as in chapters 3, 4, and 5, where Kondo-destruction QCPs are characterized by a vanishing Kondo energy scale, which in turn gives rise to $\omega/T$ scaling in the local spin susceptibility and a linear-in-temperature single-particle relaxation rate [94, 91, 123, 141, 88, 114, 126]. Such properties are reminiscent of the aforementioned experiments near the antiferromagnetic QCPs of heavy-fermion metals.

We solve the two-impurity Bose-Fermi Anderson models using a continuous-time quantum Monte-Carlo (CT-QMC) approach [87] in the form applied in Refs. [141] and [126], as well as the numerical renormalization group (NRG) [35, 94]. We determine the magnetic quantum critical properties and compute pairing susceptibilities across the phase diagram. We find that pairing correlations are in general enhanced near the Kondo-destruction QCP. This suggests a new mechanism for superconductivity near antiferromagnetic quantum phase transitions (QPTs).
7.2 Model

The two-impurity Bose-Fermi Anderson models, illustrated in Fig. 9.1, are defined by Hamiltonians of the form

$$H = \sum_{i=1,2} \left( \epsilon_d \sum_\sigma n_{d_i\sigma} + U n_{d_i\uparrow} n_{d_i\downarrow} \right) + H_{12}$$

$$+ \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{V}{\sqrt{N_k}} \sum_{i,k,\sigma} \left( e^{ik \cdot r_i} d_{i\sigma}^\dagger c_{k\sigma} + \text{H.c.} \right)$$

$$+ \sum_{q} \omega_q \phi_q^\dagger \phi_q + g (S_1^z - S_2^z) \sum_q (\phi_q^\dagger + \phi_{-q}).$$

(7.1)

Here, $d_{i\sigma}$ destroys an electron on impurity site $i = 1$ or $2$ with spin $\sigma = \uparrow$ or $\downarrow$, energy $\epsilon_d$, and on-site Coulomb repulsion $U$; $n_{d_i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$, and $S_i = \frac{1}{2} \sum_{\alpha,\beta} d_{i\alpha}^\dagger \sigma_{\alpha\beta} d_{i\beta}$ where $\sigma^{x,y,z}_{\alpha\beta}$ are the Pauli matrices. The operator $c_{k\sigma}$ destroys a conduction electron with wave vector $k$, spin $\sigma$, and energy $\epsilon_k$ that has a hybridization $V$ with each impurity, while $\phi_q$ destroys a boson with energy $\omega_q$ that couples with strength $g$ to the difference of impurity spin $z$ components. $N_k$ is the number of $k$ values.

To control the interimpurity exchange interaction, we take the limit of infinite impurity separation $|r_1 - r_2|$ to ensure the indirect Ruderman-Kittel-Kasuya-Yosida exchange interaction between $S_1$ and $S_2$ vanishes. Then impurities 1 and 2 hybridize with linearly independent combinations of band states, and interact only through their coupling to the bosonic bath and via a direct exchange term $H_{12}$, either of the Ising form $H_{12} = I_z S_1^z S_2^z$ or the Heisenberg form $H_{12} = I S_1 \cdot S_2$. We note that integrating out the bosonic bath will induce a retarded antiferromagnetic exchange of Ising symmetry.

We assume a flat electronic density of states $\rho_c(\epsilon) = \rho_0 \Theta(D - |\epsilon|)$ and a sub-Ohmic
Figure 7.1: Schematic representation of the two-impurity Bose-Fermi Anderson models considered in this work. The impurity spins interact via a direct exchange coupling $I$ (or $I_z$ for Ising exchange), and the difference of their $z$ components couples with strength $g$ to a dissipative sub-Ohmic bosonic bath having dispersion $\omega_q$. For very large impurity separation, each impurity effectively hybridizes with strength $V$ with its own conduction band of dispersion $\epsilon_k$.

bosonic density of states

$$
\rho_\phi(\omega) = K_0^2 \omega_c^{1-s} \omega_s \Theta(\omega) f(\omega/\omega_c).
$$

(7.2)

For the CT-QMC calculations we have used a cutoff function $f(x) = \exp(-|x|)$ and chosen $K_0^{-2} = \omega_c^2 \Gamma(s+1)$ so that the density of states is normalized to unity. Within the NRG, we use $f(x) = \Theta(1 - |x|)$ with $K_0 = 1$. In this work we restrict ourselves to the range $1/2 < s < 1$.

In the absence of the bosonic bath, the pure-fermionic two-impurity Anderson model can be mapped via a Schrieffer-Wolff transformation to a two-impurity Kondo model with a direct exchange interaction [165, 166]. In the case of Heisenberg exchange, both the Anderson and Kondo formulations are well studied [167, 168, 169, 170, 171, 172, 173, 174], displaying a critical point at an antiferromagnetic exchange $I_c > 0$ in the presence of particle-hole symmetry; at this point, the static
singlet-pairing susceptibility diverges [175]. For an Ising $H_{12}$, the model possesses a Kosterlitz-Thouless (KT) QPT at $|I_z^c| > 0$ between a Kondo-screened phase and an interimpurity Ising-ordered phase [176, 177]. Without the conduction band, Eq. (7.1) reduces to a two-spin boson model; studies of this model with $S^z_1 + S^z_2$ coupled to a spin bath found a QCP separating a delocalized phase and a ferromagnetically localized phase [178, 179].

7.3 Methods

We have solved Eq. (7.1) with $H_{12}$ of Ising form by extending the CT-QMC approach [87, 141, 126], the details can be found in appendix B. After a generalized Lang-Firsov transformation [141, 126], the CT-QMC performs time-dependent perturbation theory in the hybridization and stochastically sums the resulting series via a Monte-Carlo algorithm. In order to locate the $T = 0$ transition via calculations performed at $T \equiv 1/\beta > 0$, we compute the staggered Binder cumulant [112, 88, 114, 126] $U^s_4(\beta, I_z, g) = \langle M^4_s \rangle / \langle M^2_s \rangle^2$, where the staggered magnetization $M_s = \beta^{-1} \int_0^\beta d\tau S^z_s(\tau)$ with $S^z_s = \frac{1}{2} (S^z_1 - S^z_2)$. It is important to note, this is a generalization of the single impurity Binder cumulant used in chapters 3, 4, and 5, where now the Binder cumulant detects both the Kondo destroyed QCP and the antiferromagnetic order of the two impurities. We also calculate the staggered static spin susceptibility $\chi_s(T) = \beta \langle M^2_s \rangle$.

To measure the pairing correlation between the $d$-electrons at different impurity sites, we study dynamic singlet ($d$-wave) and triplet ($p$-wave) pairing susceptibilities

$$\chi_\alpha(T, \beta) = \langle T_\tau \Delta_\alpha(\tau) \Delta^{\dagger}_\alpha \rangle, \quad \alpha = d \text{ or } p,$$

(7.3)

where $\Delta^\dagger_d = \frac{1}{\sqrt{2}} (d_{1\uparrow}^d d_{2\downarrow}^d - d_{1\downarrow}^d d_{2\uparrow}^d)$, $\Delta^\dagger_p = \frac{1}{\sqrt{2}} (d_{1\uparrow}^p d_{2\downarrow}^p + d_{1\downarrow}^p d_{2\uparrow}^p)$, and $T_\tau$ orders in imaginary time. The static pairing susceptibilities follow via $\chi_\alpha(T) = \int_0^\beta d\tau \chi_\alpha(T, \beta)$. In the
Figure 7.2: (a) Phase diagram for an Ising $H_{12}$ determined via CT-QMC from the staggered Binder cumulant. A square marks the Kosterlitz-Thouless QPT and circles denote second-order Kondo-destruction QPTs governed by the QCP at $I_z = 0$. (b) Phase diagram for a Heisenberg $H_{12}$ found with the NRG. Squares represent QPTs governed by the critical point at $g = 0$, while circles represent Kondo-destruction QPTs induced by the coupling to the bosonic bath. Kondo-screened (Kondo), interimpurity-singlet (IS), and local-moment (LM) phases all meet at a tricritical point. Generic particle-hole asymmetry eliminates the Kondo-IS transition, leaving a single line of Kondo-destruction QPTs induced by the bosonic coupling $g$.

presence of a bosonic coupling to $S_s$, the Heisenberg form of $H_{12}$ is beyond the reach of the CT-QMC.

Both forms of $H_{12}$ can be solved using the Bose-Fermi extension [94] of the NRG [35]. The staggered spin susceptibility is calculated as $\chi_s(T) = -\lim_{H_s \to 0} \langle S_s^z \rangle / H_s$ with an additional Hamiltonian term $H_s S_s^z$. The static pairing correlations are obtained by Hilbert transformation of the imaginary part of the dynamical susceptibilities, computed on the real frequency axis in the usual manner [180]. The NRG results presented below were obtained using discretization parameter $\Lambda = 9$, allowing up to 4 bosons per site of the Wilson chain, and keeping up to 1300 many-body eigenstates after each iteration.

In the following, we work with fixed $\Gamma_0 = 0.25D$ and $U = -2\epsilon_d = 0.001D$. This choice places the Anderson impurities at mixed valence with a high Kondo temperature $T_K \simeq 1.39D$ (for $g, I_z, I = 0$), ensuring a correspondingly high temperature
of entry into the quantum critical regime [126]. We also take $\omega_c = D$ and focus on sub-Ohmic bath exponents [see Eq. (7.2)] $s = 0.8$ for Ising exchange and $s = 0.6$ for the Heisenberg case.

### 7.4 Quantum Critical Properties

#### 7.4.1 Ising $H_{12}$

Figure 7.2(a) shows the $T = 0$ phase diagram for the case of Ising exchange, as obtained using CT-QMC. For $0 \leq g, I_z \ll D$, each impurity spin is locked into a Kondo singlet with the conduction band and $\chi_s(T)$ approaches a constant at low temperatures [e.g., Fig. 7.3(a)]. Upon increasing $g$ and/or $I_z$, the system passes through a QPT into an Ising-antiferromagnetic local-moment phase (LM) in which the impurity spins are anti-aligned and decoupled from the conduction band, as seen through a Curie-Weiss behavior of the staggered spin susceptibility: $\chi_s(T) \sim T^{-1}$ [Fig. 7.3(a)]. The Kondo energy scale vanishes continuously on the Kondo side of the QPT, characteristic of a Kondo-destruction QCP. The staggered Binder cumulant $U_4(\beta, I_z, g)$ varies from 3 deep in the Kondo phase to 1 far into the LM phase. For
fixed $I_z$, the cumulant near the QCP has a scaling form

$$U_4^s(\beta, I_z, g) = U_4^s(\beta^{1/\nu}(g/g_c - 1); I_z), \quad (7.4)$$

identifying $g_c$ as the point of temperature independence of $U_4^s$ vs $g$ [Fig. 7.5(a)]. Optimizing the scaling collapse according to Eq. (7.4) gives a correlation-length exponent $\nu(s = 0.8)^{-1} = 0.45(8)$ [Fig. 7.5(b)].

For $g = 0$, the Ising critical point is KT-like, characterized by a divergence

$$\chi_s(T, I_z = I^c_z, g = 0) \sim T^{-1}. \quad \text{(7.5)}$$

Consequently, the coupling $g$ has a scaling dimension $[g] = (1 - s)/2$ and is relevant for $s < 1$. This dictates a flow away from the KT fixed point along the phase boundary in Fig. 7.2(a) toward the $I_z = 0$ critical point. Tuning $g$ to the boundary at fixed $I_z > 0$, we find that the staggered spin susceptibility diverges as

$$\chi_s(T, I_z, g = g_c(I_z)) \sim T^{-x} \quad \text{(7.5)}$$

with $x = 0.79(3), 0.78(3), 0.80(3), 0.82(3), 0.82(3), 0.83(3), 0.83(4)$ for increasing $I_z$. These values are consistent with $x = s$, suggesting that the staggered channel exhibits the same critical properties as the single-impurity Ising-symmetric Bose-Fermi Kondo model [94].

### 7.4.2 Heisenberg $H_{12}$

For Heisenberg exchange, the NRG gives the phase diagram shown in Fig. 7.2(b). For small $g$ and $I$, the model is in the Kondo phase. Tuning $I$ for $g = 0$, we pass through a critical point into an interimpurity singlet (IS) phase, in which the impurity spins are locked into a singlet and decoupled from the conduction band. At the particle-hole-symmetric critical point [167, 168, 169, 170, 171, 172, 173, 174], the staggered spin
Figure 7.4: Schematic RG flow on the $g$-$I_z$ plane for the two-impurity Bose-Fermi Anderson model with Ising interimpurity exchange $H_{12}$. Trajectories with arrows represent the flows of the couplings ($g$ and $I_z$) with the decrease of energy. There are two stable fixed points, indicated by filled circles, which govern the Kondo-screened (Kondo) phase and the local-moment (LM) phase. The Kondo fixed point is at $(g, I_z) = (0, 0)$, while the LM fixed point is at $(g, I_z) = (\infty, 0)$. On the phase boundary, the RG flow is from the Kosterlitz-Thouless (KT) fixed point toward the Kondo-destruction (KD) fixed point. The KT and KD fixed points are both unstable and are shown by open circles. The direction of the RG flow on the phase boundary reflects the discussion in the text, i.e., all the points for nonzero $g$ on the phase boundary have the same critical behavior as the KD QCP on the $g$ axis.

susceptibility diverges as $\chi_s(T, I = I_c, g = 0) \sim \ln(T_K/T)$. Using the corresponding scaling dimension of the staggered impurity spin, along with the scaling dimension of the bosonic operator, we determine that the bosonic coupling has scaling dimension $[g] = -s/2$ and is irrelevant for $s > 0$. Indeed, we find that the NRG spectrum along the phase boundary is independent of $g$ for small values of $g$ (see figure ?? for the RG flow), indicating that the critical behavior is governed by the $g = 0$ QCP.

For small $I > 0$, tuning the bosonic coupling $g$ yields a QPT from the Kondo phase to the LM phase [Fig. 7.5(c)]. The Kondo energy scale vanishes continuously on approach from the small-$g$ side of this Kondo-destruction QCP. At the QCP, the
Figure 7.5: (a) Binder cumulant $U_4^s(\beta, I_z, g)$ vs $g$ for an Ising $H_{12}$ with $I_z = 1.25D$, $s = 0.8$, and at the labeled temperatures. Error bars come from a jackknife analysis of CT-QMC data. The intersection of curves gives the critical bosonic coupling $g_c/D = 0.465(5)$. (b) A scaling collapse of the same data near $g_c$ according to Eq. (7.4) yields a correlation-length exponent $\nu(s = 0.8)^{-1} = 0.45(8)$. (c) Flow of a low-energy NRG eigenstate vs iteration number $N$ for a Heisenberg $H_{12}$ with $I = 0.2D$, $s = 0.6$, and six values of $\Delta g \equiv 10^6(g - g_c)$, where $K_0g_c = 1.08742545(1)$. (d) Low-energy crossover scale from the NRG, fitted to $T^* \propto |g - g_c|^\nu$ yielding $\nu(s = 0.6)^{-1} = 0.40(2)$.

staggered spin susceptibility obeys Eq. (7.5) with $I_z$ replaced by $I$ and $x = s.61(2)$ [Fig. 7.3(b)], again consistent with $x = s$. Nearby, the correlation-length exponent is $\nu(s = 0.6)^{-1} = 0.40(2)$ [Fig. 7.5(d)]. Within numerical accuracy, we find that the Kondo-destruction QCPs for Ising and Heisenberg exchange fall within the same universality class. In both cases, the Kondo destruction QCPs are insensitive to breaking of particle-hole symmetry via setting $U \neq -2\epsilon_d$, as well as to a finite impurity separation (results not shown).
Figure 7.6: Schematic RG flow on the $g$-$I$ plane for the two-impurity Bose-Fermi Anderson model with Heisenberg inter-impurity exchange $H_{12}$. There are three stable fixed points corresponding to the three phases. The Kondo-screened (Kondo), local-moment (LM) and interimpurity-singlet (IS) phases are respectively located at $(g, I) = (0, 0)$, $(g, I) = (\infty, 0)$ and $(g, I) = (0, \infty)$, and are marked by filled circles. On the Kondo-LM phase boundary, the RG flow is from the triple-point (where the three phases meet) to the Kondo-destruction (KD) fixed point. Likewise, the RG flow on the Kondo-IS phase boundary is from the triple-point toward the fixed point KI, which separates the Kondo and IS phases on the $I$-axis.

We turn next to the transition between the IS and LM phases. Fixing $I$ at a large value and tuning $g$, the bosonic bath decoheres and destroys the interimpurity singlet state at a QCP, where we find similar critical properties to those on the Kondo-LM boundary: $\chi_s$ diverging according to Eq. (7.5) with $x = 0.61(3)$, and a correlation length exponent $\nu(s = 0.6)^{-1} = 0.40(2)$.

In the particle-hole symmetric case that is the focus of this paper, the Kondo, IS, and LM phases all meet at a tricritical point, as shown in Fig. 7.2(b). Generic particle-hole asymmetry is known to turn the Kondo-to-IS transition into a crossover [167, 168, 169, 170, 171, 172, 173, 174], leaving only a single line of Kondo-destruction QPTs.
7.5 Pairing Susceptibilities

We now consider the singlet and triplet pairing susceptibilities defined in Eq. (7.3). For both the Ising and Heisenberg forms of the interimpurity exchange, the static triplet pairing susceptibility \( \chi_p \) (not shown) is reduced by any nonzero value of \( g, I_z, \) or \( I. \)

More interesting is the singlet susceptibility, which we illustrate along paths on the \( g-I_z \) and \( g-I \) phase diagrams that start from \( g = I_z = I = 0 \) and cross the Kondo-LM boundary. Figure 7.7(a) plots \( \chi_d \) vs Ising exchange coupling at a sequence of temperatures along the cut \( g = 0.372I_z. \) The pairing susceptibility grows as \( I_z \) increases from zero, is peaked for \( I_z \) slightly below \( I_z^c, \) and then falls off within the LM phase as the \( d \) electrons localize and decouple from the conduction band. The singlet pairing susceptibility saturates at temperatures \( T \lesssim 0.004D \simeq 0.003T_K. \)

Figure 7.7(b) illustrates the Heisenberg form of \( H_{12}, \) plotting the \( T = 0 \) singlet pairing susceptibility vs \( I \) at \( T = 0 \) along a path \( g = 2.54I \) that crosses the Kondo-LM boundary. Very much as in the Ising case, \( \chi_d \) rises from \( I = 0 \) and peaks just below \( I = I_c. \)

The enhancement of the static singlet pairing susceptibility near a Kondo-destruction QCP is one of the principal results of this work. Although \( \chi_d \) peaks just inside the Kondo phase, the pairing correlation at the QCP is significantly higher than at \( g = I_z = I = 0. \) We stress that these results are associated with the critical destruction of the Kondo effect. They differ from those for \( g = 0, \) where for Heisenberg exchange \( \chi_d(T = 0) \) diverges at the Kondo-IS QPT [175]. We have found (by following the path \( g = 0.717I, \) not shown) that the singlet pairing susceptibility also diverges on crossing the Kondo-IS boundary at some \( g > 0, \) consistent with the picture that this boundary is governed by the \( g = 0 \) critical point.

The models considered here have both a dynamic (induced by \( g \)) and a static
Figure 7.7: (a) Static singlet pairing susceptibility $\chi_d(T, I_z, g)$ vs $I_z$ for an Ising $H_{12}$ with $s = 0.8$ along the line $g = 0.372I_z$, which crosses the Kondo-LM phase boundary at $I_z^c = 1.25D$. Note that $\chi_d$ saturates for temperatures $T \leq D/250$. (b) Static singlet pairing susceptibility $\chi_d(T = 0, I, g)$ vs $I$ for a Heisenberg $H_{12}$ with $s = 0.6$ along the line $g = 2.54I$, which crosses the Kondo-LM phase boundary at $I_z^c = 0.40D$. In both (a) and (b), $\chi_d$ is peaked just on the Kondo side of the phase boundary and remains elevated at the QCP over its value for $g = I_z = I = 0$.

$(I_z$ or $I$) exchange interaction between the impurities. The combination of dynamic and static antiferromagnetic interactions enhances the singlet pairing susceptibility between the impurities and gives rise to a peak near the Kondo-destruction QCP. This behavior is likely to have significant effects in lattice systems. Within an extended dynamical mean field approach [74, 75], for example, the enhanced pairing susceptibility in the impurity model may give rise to a pairing instability near a Fermi-surface-collapsing QCP of a Kondo lattice [72, 73, 63]. This would represent a new mechanism for superconductivity in the vicinity of antiferromagnetic order, and would be of considerable interest in connection with the superconductivity observed in the Ce-115 materials [69] and related heavy-fermion superconductors [50].

7.6 Summary

We have introduced and solved two variants of the two-impurity Bose-Fermi Anderson model using robust numerical methods. We have mapped out the phase diagrams
for these models and shown that each possesses a line of Kondo-destruction QCPs. The QCPs in the two models belong to the same universality class despite the differing symmetries of the interimpurity exchange interaction. Just as importantly, we have shown that the Kondo-destruction quantum criticality in these models enhances singlet pairing correlations. Our results hold promise for elucidating the superconductivity observed in heavy-fermion metals whose normal state shows characteristics of Kondo-destruction quantum criticality. In the following chapter we use the results and insights we have gained on the two impurity Bose Fermi Anderson model, in order to solve the full periodic Anderson model within a C-EDMFT approach (described in chapter 6).
In chapters 3, 4, and 5, we studied the properties of Kondo destroyed quantum critical points in detail and in the previous chapter we have studied their effect on local pairing correlations. Now that we have a much deeper understanding of the quantum critical properties of the effective cluster model, we can use the formalism developed in chapter 6 to solve the periodic Anderson model within a C-EDMFT approach. In the following chapter, using a two site cluster we determine the phase diagram of the model and study in detail, its superconducting properties for antiferromagnetic fluctuations in two and three dimensions. We show, the locally critical point gives rise to a significantly enhanced lattice pairing susceptibility, which may lead to a superconducting transition. Lastly, we are able to incorporate finite size corrections from the cluster model and determine the momentum dependence of the spin susceptibility.
8.1 Introduction

A considerable amount of insight has come out of the EDMFT solution of the Kondo lattice. For the case of two dimensional magnetic fluctuations, this has lead to the theory of the local critical point (LCP) \cite{72} (as described in section 2.4). Using the results of section 6, we have shown how to incorporate real space corrections beyond the single site approximation that leads to the EDMFT. It is therefore a very natural question to ask, does the LCP survive finite size corrections from a cluster generalization of EDMFT? In the following chapter we show the answer is indeed yes, the LCP is stable against two site cluster corrections and leads to a local spin susceptibility that is only critical in the ordering channel.

In the previous chapter we have shown the local pairing susceptibility is enhanced in the vicinity of a Kondo destroyed quantum critical point. However, the question still remains, how does this enhancement effect the lattice pairing susceptibility in the vicinity of the LCP? In the following chapter we answer this question using the formalism developed in chapter 6, and the CT-QMC as the impurity solver (as discussed in appendix B). We calculate the lattice pairing susceptibility $\chi_{SC}$ in the normal state using the formalism discussed in chapter 6 (see equation [6.52]). As we will show, $\chi_{SC}$ is significantly enhanced in the vicinity of the quantum critical point.
8.2 Method

We now aim to solve the periodic Anderson model within C-EDMFT using a two site cluster, here we rewrite the model for ease of reading

\[ H_{AL} = \sum_{\langle i,j \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + \sum_i (\epsilon_f n_{fi} + U n_{fi\uparrow} n_{fi\downarrow}) + \sum_{i, \sigma} \left( V c_{i\sigma}^\dagger f_{i\sigma} + \text{h.c.} \right) + \sum_{\langle i,j \rangle} I_{ij} S_{fi}^z S_{fj}^z. \]  

(8.1)

We have explicitly added an Ising RKKY interaction between the \( f \) impurities. Tuning the ratio of the antiferromagnetic RKKY interaction \( I > 0 \), and the bare Kondo temperature \( T_K^0 \), we can tune the model through a quantum critical point.

Using the C-EDMFT formalism in momentum space of section 6.2.2, this model reduces to the effective cluster action in equation (6.55) (in the paramagnetic state). Using the two site cluster, we tile the Brillouin zone so that all ferromagnetic fluctuations are confined to the zone center (more precisely \( I_q > 0 \)) with cluster momentum \( Q \equiv + \), and the antiferromagnetic fluctuations on the zone corners (\( I_q < 0 \)) with cluster momentum \( Q \equiv - \), see figure 8.1. This amounts to the cluster momentum in two dimensions \( Q = (0,0) = + \) and \( Q = (\pi, \pi) = - \) (as well as \( Q = (0,0,0) = + \) and \( Q = (\pi, \pi, \pi) = - \) in three dimensions). This tiling of the Brillouin zone leads to a density of states per patch, for magnetic fluctuations we have, \( \rho_I(\omega) = \frac{1}{N} \sum_{\mathbf{q}} \delta(\omega - I_{\mathbf{q}+\mathbf{Q}}) = \frac{1}{N_c} \sum_{\mathbf{Q}} \rho_I(\mathbf{Q}, \omega) \) and we have defined the density of states in patch \( \mathbf{Q} \)

\[ \rho_I(\mathbf{Q}, \omega) = \frac{N_c}{N} \sum_{\mathbf{q}} \delta(\omega - I_{\mathbf{q}+\mathbf{Q}}). \]  

(8.2)

As we will show, similar to the case of EDMFT, the self consistent solution \([76, 132]\) depends crucially on the dimensionality of magnetic fluctuations.
Figure 8.1: Tiling of the two dimensional Brillouin zone with the two site cluster (a), where the ferromagnetic fluctuations are confined to the zone center [the blue region (+)] and the antiferromagnetic region at the zone corners [the red region (-)]. The magnetic density of states in two dimensions (b) and three dimensions (c) corresponding to the tiling used.

As described in detail in section 6.3, within our C-EDMFT scheme we do not allow the electron bath to become polarized, this is achieved by taking a featureless density of states for the conduction band \( \rho(\epsilon) = \rho_0 \Theta(D - |\epsilon|) \) for a half bandwidth \( D \) and only enforcing self consistency on the bosonic baths (see references [78, 77, 80] for the one site case). In addition, in the C-EDMFT construction we have to be careful not to double count the RKKY interaction. It is well known in the periodic Anderson model an RKKY interaction is dynamically generated due to hybridization events that connect impurities [9]. Therefore, since we have already added the RKKY interaction “by hand”, we drop the dynamic inter-impurity interaction in the lattice model. This is achieved within the effective cluster model, by taking the two impurities to be infinitely far apart (see chapter 7), and they are then only coupled by \( \bar{I}_Q(= \)
\[ \sum_{\mathbf{q}} \bar{I}_{q+\mathbf{Q}} \] and the bosonic baths. This then corresponds to the cluster Hamiltonian

\[ H_C = \sum_{i=1,2} H_{i, AI}^i + \sum_{\mathbf{q}} \bar{I}_Q S_i^z f_i^z s_i^z + h_{\text{loc}} S_i^{\perp} \]  

(8.3)

\[ + \sum_{\mathbf{q}, \mathbf{Q}} \omega_{\mathbf{q}, \mathbf{Q}} \phi_{\mathbf{q}, \mathbf{Q}}^f \phi_{\mathbf{q}, \mathbf{Q}}^i + \sum_{\mathbf{q}, \mathbf{Q}} g_{\mathbf{q}}(\mathbf{Q}) S_i^z f_i^z (\phi_{\mathbf{q}, \mathbf{Q}}^f + \phi_{-\mathbf{q}, -\mathbf{Q}}^f) \]  

(8.4)

where we have explicitly included \( h_{\text{loc}} = [\delta I(Q_{AF}) + \chi_0, -(i \omega_n = 0)] \langle S_i^{\perp} \rangle \), with an ordering wave vector \( Q_{AF} \) to study antiferromagnetic order. The Greens function of the bosonic baths give rise to the dynamic Weiss fields through

\[ \chi_{0, Q}^{-1}(i \omega_n) = \sum_{\mathbf{q}} \frac{2 g_{\mathbf{q}}(\mathbf{Q})^2 \omega_{\mathbf{q}, \mathbf{Q}}}{\omega_{\mathbf{q}, \mathbf{Q}}^2 - \omega_n^2}. \]  

(8.5)

Due to the coarse graining, the relevant energy scale for the RKKY interaction is the inter site interaction at the ordering wave vector, which we take to be \( I_{Q_{AF}} \equiv -2I \) (note, this serves as a definition of \( I \)). The spin operators in cluster momentum are \( S_\perp^z = (S_1^z \pm S_2^z)/\sqrt{2} \) that each couple to two self consistent bosonic baths that represent ferro- (\( \phi_{\mathbf{q}, \mathbf{Q}}^f + \phi_{-\mathbf{q}, -\mathbf{Q}}^f \)) and antiferro-magnetic (\( \phi_{\mathbf{q}, \mathbf{Q}}^i - \phi_{-\mathbf{q}, -\mathbf{Q}}^i \)) fluctuations in the lattice model.

We have defined \( H_{i, AI}^i \) with \( i = 1, 2 \), which are two independent Anderson impurity models,

\[ H_{AI}^i = \sum_{\mathbf{k}, \sigma} [\epsilon_{\mathbf{k}} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} + V (f_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} + \text{H.c.})] + \epsilon_{i, f} n_{i, f} + U n_{i, f}^\dagger n_{i, f}^\dagger, \]  

(8.6)

which is a result of taking the infinite separation limit, and as we have previously discussed, \( n_{i, f} = f_{\mathbf{k}, \sigma}^\dagger f_{\mathbf{k}, \sigma} \), \( n_{i, f} = \sum_{\sigma} n_{i, \sigma, f} \), and \( S_i^z = (n_{i, \uparrow, f} - n_{i, \downarrow, f})/2 \). We take the Anderson parameters of each impurity to be the same and therefore they each have the same Kondo temperature. Since, the two impurities are independent, we can characterize the bare Kondo temperature through \( T_K^0 \equiv 1/\chi_{\text{loc}, i}(T \to 0) \), where \( \chi_{\text{loc}, i} = \int_0^\beta d\tau \langle T, S_i^z(\tau)S_i^z \rangle \) is the local static spin susceptibility of impurity \( i \). In all
of the calculations that follow we fix $U = 0.25D = -2\epsilon_f$ at particle hole symmetry, and take a hybridization $\Gamma_0 = \pi \rho_0 |V|^2 = 0.25D$. This leads to a relatively high bare Kondo temperature $T_K^0 \approx 1.0D$, where a high $T_K^0$ is advantageous to try and reach the quantum critical regime (which can be quite challenging \[126\] as described in chapter 5).

Using the fact that the two bosonic baths commute, we are still able to use the CT-QMC approach described in appendix B to solve the cluster model. We then iteratively solve the C-EDMFT equations self consistently. Away from the critical regime, we find relatively fast convergence taking roughly 30 iterations, where as near the critical point we find a critical slowing down and the number of iterations can become very large (even exceeding 1000 iterations). Therefore, we find it useful to employ simple mixing techniques \[164\] to reduce the number of iterations necessary.

### 8.3 Two Dimensional Magnetic Fluctuations

In the following section we consider the case of two dimensional magnetic fluctuations, which we approximate as a step function

$$\rho_I(\omega) = \frac{1}{N} \sum_q \delta(\omega - Iq) = \frac{1}{4I} \Theta(2I - |\omega|). \quad (8.7)$$

We note, this approximation neglects the Van-Hove singularity \[181\] present at $\omega = 0$ for the density of states corresponding to a two dimensional nearest neighbor interaction on a square lattice, yet keeps the key feature present in two dimensions of a jump in the density of states at the lower band edge at $I_{QAF} (= -2I)$ \[73\]. In two dimensions, the ordering wave vector corresponds to $Q_{AF} = (\pi, \pi)$, setting the lattice spacing to unity, (note that $Q_{AF} = -$). This leads to the density of states per patch $\rho_I(\pm, \omega) = \frac{1}{4I} \Theta(\pm \omega) \Theta(2I \mp \omega)$. and the coarse grained interactions $\bar{I}_\pm = \pm I$ and
\( \delta I(Q_{AF}) = -I \). Using the self consistent equation 6.30 and the density of states per patch, we perform the momentum sum to obtain the equations that the local spin susceptibilities satisfy once the self consistent solution has been obtained

\[
\chi_{\text{loc}}(\pm, i\omega_n) = \pm \frac{1}{2I} \log \left| \frac{\pm 2I + M(\pm, i\omega_n)}{M(\pm, i\omega_n)} \right|. \tag{8.8}
\]

The local spin susceptibilities are defined as \( \chi_{\text{loc}}(\pm, \tau) = \langle T_\tau S^z_\pm(\tau)S^z_\pm \rangle \), and then Fourier transformed to Matsubara frequencies \([38], \chi_{\text{loc}}(\pm, i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \chi_{\text{loc}}(\pm, \tau) \). We now coarse grain the spin self energy following reference \([149]\), to obtain \( M_{\text{lat}}(q, i\omega_n) = \alpha(+, q)M(+, i\omega_n) + \alpha(-, q)M(-, i\omega_n) \), where we have defined \( \alpha(\pm, q) = 1/2 \{1 \pm 1/2[\cos(q_x) + \cos(q_y)] \} \). We remark, this is a natural embedding of the two site cluster that preserves the symmetry of an underlying square lattice. Using the expression for the lattice spin susceptibility at the ordering wave vector \( 1/\chi_{\text{lat}}(Q_{AF}, i\omega_n) = -2I + M(-, i\omega_n) \), leads to the important relation for a two dimensional density of states

\[
\chi_{\text{loc}}(-, i\omega_n) = \frac{1}{2I} \log |1 + 2I\chi_{\text{lat}}(Q_{AF}, i\omega_n)|. \tag{8.9}
\]

Therefore, when the lattice orders antiferromagnetically [signaled by a divergence of the static \( \chi(Q_{AF}, i\omega_n = 0) \equiv \chi_{AF} \)], the local spin susceptibility in the ordering channel is also divergent. Since the local spin susceptibility is related to the local Kondo energy scale (as described in detail in the previous chapters 3, 4, and 5), we reach the important conclusion, if there is a continuous antiferromagnetic transition, the C-EDMFT equations in two dimensions guarantee it is accompanied by a critical breakdown of the Kondo effect.
8.3.1 Phase Diagram

We now consider the C-EDMFT solution in the temperature range \( T/T_K^0 = 0.0333, 0.0222, 0.0167, 0.0111, 0.0083, 0.0056 \). For a small RKKY interaction \( I < I_c \), we find the model in equation (8.1), is in the heavy fermi liquid (HFL) phase. This is signaled by \( \chi_{\text{loc}}(\pm, T) \) saturating to a finite value as \( T \to 0 \), as discussed in detail in chapters 3, 4, and 5, this implies the local moments are screened by the conduction electrons. In addition, the antiferromagnetic order parameter \( M_{\text{AF}}(\omega_n) = \langle S^z \rangle / \sqrt{2} = (\langle S^z_1 \rangle - \langle S^z_2 \rangle) / 2 \) is zero to within numerical accuracy, (even if we start initially with a large \( h_{\text{loc}} \)). At finite temperature, for increasing \( I \), the model crosses over into a non fermi liquid phase (NFL). We determine the cross over boundary from the HFL to NFL phase by considering when the dynamic local spin susceptibility in the ordered channel, develops a logarithmically divergent non fermi liquid form at low frequencies, i.e. \( \chi_{\text{loc}}(-, i\omega_n) \sim \log |i\omega_n/T_K^0| \), in the range \( \omega_n/T_K^0 \ll 1 \), as shown in figure 8.2. This determines the local Kondo energy scale \( E_{\text{loc}}^* \), shown in the phase diagram of figure 8.5.

![Figure 8.2: Dynamic local spin susceptibility vs ln|\(i\omega_n/T_K^0|\) in the ordering channel (\(Q = -\)) at a temperature \(T/T_K^0 = 0.0056\), on approach to the QCP from the HFL (left plot) and AF (right plot) phase. We find a clear ln|\(i\omega_n/T_K^0|\) dependence in the low frequency behavior of \(\chi_{\text{loc}}(-, i\omega_n)\) in the vicinity of the QCP \([I_c = 0.420(13)]\), in both phases. In particular, in the HFL phase, we find the logarithmic dependence develop in the range \(0.35T_K^0 \lesssim I \lesssim I_c\) and in the AF phase \(I_c \lesssim I \lesssim 0.46T_K^0\).](image-url)
For sufficiently large $I$, the model develops antiferromagnetic order at the Neel temperature, $T_N$, (which we refer to as the AF phase). As shown in figures 8.3, we see $\chi_{AF}$ diverges when approaching $T_N$ from either side of the phase diagram, and $M_{AF}$ jumps when the system orders at $T_N$. The jump in $M_{AF}$ implies the finite temperature magnetic transition is first order.

![Graph showing static lattice spin susceptibility and antiferromagnetic order parameter as functions of RKKY interaction $I$.](image)

Figure 8.3: Static lattice spin susceptibility at the ordering wave vector $\chi_{AF}$ and antiferromagnetic order parameter $M_{AF}$ as a function of the RKKY interaction $I$, for temperatures $T/T_K^0 = 0.0167$ (left plot) and $T/T_K^0 = 0.0111$ (right plot). We see $\chi_{AF}$ diverging on approach to the thermal phase transition and $M_{AF}$ jumping at the transition temperature $T_N$, to a finite value, displaying a first order thermal phase transition.

It is useful to note, in the one site EDMFT case [78], where the finite temperature transition is first order, the quantum critical point is indeed continuous [76, 132] and must be as dictated by the EDMFT equations per se [77]. Similarly, we find the size of the jump of $M_{AF}$ at $T_N$, gets smaller as the temperature is lowered (see figure 8.4). In addition, extrapolating both phase boundaries $E_{loc}^*(T)$ and $T_N(T)$ to zero temperature, yields $E_{loc}^*(T = 0)/T_K^0 = 0.415(8)$ and $T_N(T = 0) = 0.43(1)$, which agree to within numerical accuracy and we find a quantum critical point at $I_c = 0.420(13)$, see figure 8.5. Lastly, zero temperature NRG calculations of the present
Figure 8.4: Magnetic order parameter $M_{AF}$ (left plot) and the static local susceptibility in the ordered channel $\chi_{loc}(−,i\omega_n = 0)$ (right plot) as a function of $I$ for various temperatures.

model (with only one bosonic bath in the $Q = −$ channel) also yield a continuous zero temperature transition.¹ We conclude, even though the finite temperature transition is first order, the zero temperature transition is indeed continuous.

At finite temperatures, the divergence of the lattice spin susceptibility $\chi_{AF}$ is cut off at the cross over boundary $E^{*}_{loc}(T)$ (as in figures 8.3), which in turns cuts off the divergence of $\chi_{loc}(−,i\omega_n = 0)$ [through equation (8.8)] (see figures 8.3 and 8.4). However, at zero temperature we find the phase boundaries $E^{*}_{loc}(T = 0)$ and $T_N(T = 0)$ merge (as in figure 8.5), and the zero temperature transition is continuous. Therefore, at zero temperature, the lattice spin susceptibility $\chi_{AF}$ diverges concomitant with $\chi_{loc}(−,i\omega_n = 0)$ at the quantum critical point. To summarize, we find the quantum critical point is consistent with a LCP, which survives finite size corrections from the C-EDMFT approach.

Due to the breakdown of the Kondo effect, in the AF phase the local moments are no longer screened by the conduction band. This then implies that the static

¹Lili Deng and Kevin Ingersent, private communication, (2014).
Figure 8.5: Finite temperature phase diagram of the periodic Anderson model solved within a C-EDMFT approach. We find the HFL and the AF phases are separated by a non fermi liquid quantum critical regime. The boundary $E_{*\text{loc}}$ is a cross over at finite temperature, where as $T_N$ is a finite temperature classical transition. At zero temperature, the two phase boundaries merge at the quantum critical point, and $E_{*\text{loc}}(T = 0)$ becomes a true transition.

Kondo energy scale has vanished, nonetheless in the vicinity of $T_N$, their is still a “dynamical” Kondo effect [50] which entangles the local moments and the conduction electrons at energies away from the Fermi energy. As shown in figure 8.2, this can be seen in $\chi_{\text{loc}}(-, i\omega_n)$ in the AF phase, where the logarithmic scaling form holds in the vicinity of the QCP. The logarithmic scaling is cut off due to $\chi_{\text{lat}}(q, i\omega_n)$ saturating due to a large $M_{AF}$ [78], and through the self consistency condition $\chi_{\text{loc}}(-, i\omega_n)$. It is interesting to recognize, the weaker divergence of $\log(x) vs x$ for large $x$ (i.e. $\chi_{\text{loc}}(-, i\omega_n = 0)$ vs $\chi_{AF}$) is responsible for both the critical Kondo destruction from the HFL phase and the dynamical Kondo screening in the AF phase. Lastly we remark, dynamical Kondo screening develops into conventional Kondo screening when magnetic order is suppressed due to a large Kondo interaction, and is therefore an
essential part of the AF phase [50]. To contrast, in mean field treatments of the Kondo lattice [61], (see section 2.2 of the introduction), any phase without static Kondo screening will always have a zero mean field hybridization and as a result cannot describe dynamical Kondo screening.

We now come to the momentum dependence of the static lattice spin susceptibility $\chi_{\text{lat}}(q, i\omega_n = 0)$, in figure 8.10. In the HFL phase, we see broad peaks spread out through the Brillouin zone with close to equal weight in the zone center $q = (0,0)$ and corners $[q = \pm(\pi, \pi) and q = \pm(\pi, -\pi)]$. Where as, in the NFL phase, the excitations are completely confined to the region around the zone corners and the amplitude is significantly enhanced. In the AF phase, the finite value of $M_{AF}$ cuts off the divergence of $\chi_{AF}$ and as a result the amplitude of $\chi_{\text{lat}}(q, i\omega_n = 0)$ is much smaller, but the excitations remained pinned to the zone corners due to the antiferromagnetic ground state.

### 8.3.2 Pairing Susceptibilities

Now that we have determined the phase diagram, and shown the critical point is consistent with the LCP, we are in a position to study the superconducting properties in the normal state. Due to the antiferromagnetic interaction $I_{ij}$, as the results of the previous chapter have shown, opposite spin pairing is favored while equal spin pairing is suppressed. Similar to the previous chapter 7, we calculate the singlet and triplet pairing susceptibilities defined in the equation (7.3), and shown in figure 8.6. Similar to the conclusions of the previous chapter, we find the local singlet pairing susceptibility is enhanced in the vicinity of the antiferromagnetic transition.

Using the C-EDMFT formalism in section 6.4.3, we are able to calculate the static zero momentum lattice pairing susceptibility through equation 6.52. Since we are using the momentum space construction of C-EDMFT, we need to coarse grain
the gap symmetry factor in real space $F_{ij}$ as in equation 6.51 (with $f$ replaced with $F$) and the discussion below. Due to the fact that we only have two sites, we assume an extended $s$-wave gap symmetry, unfortunately we cannot treat a $d$-wave gap symmetry since the coarse grained symmetry factor vanishes. An extended $s$-wave gap symmetry corresponds to a symmetry factor in momentum space $F_s(k) = \cos(k_x) + \cos(k_y)$. Since this is the same symmetry as $I_q$ we can use the density of states in equation (8.7) (with $I = 1$) to perform the coarse graining. We obtain $ar{F}_s(K) = \frac{N_c}{N} \sum_{k} F_s(k + K) = \pm 1$, Fourier transforming $\bar{F}_s(K)$ and $\bar{I}_Q$ back to cluster real space, results in $\bar{F}_s(1,2) = 1$ and $\bar{I}_c(1,2) = I$ but with periodic boundary conditions on the cluster in real space. Lastly, using equation (6.52) we obtain

$$\chi_{SC} = \frac{4|\bar{F}_s|^2}{1/\chi_{\text{loc}}^{\text{pair}} - I/2}. \quad (8.10)$$

We have defined $\chi_{\text{loc}}^{\text{pair}} = \int_0^\beta d\tau \chi_d(\tau, T)$ as in equation (7.3). We are interested in how close the system is to being unstable towards the superconducting ground state, i.e. we are interested in the enhancement of $\chi_{SC}$ across the QCP. In figure 8.7, we show $\chi_{SC}$ for various temperatures. We find a common trend, where $\chi_{SC}$ is increasing.
on approach to the transition from both the HFL and AF phases, which leads to \( \chi_{SC} \) being significantly enhanced in the vicinity of the critical point. We now reach one of our key results: the quantum critical fluctuations of the LCP significantly enhances the lattice pairing susceptibility, and this represents a new mechanism for superconductivity on the border of magnetism and electronic localization, which is particularly pertinent to heavy fermion superconductors such as \( \text{CeRhIn}_5 \). It will be very interesting to see what happens when a finite superconducting order parameter is included along the lines of section 6.

![Figure 8.7: Pairing susceptibility across the QCP for two dimensional magnetic fluctuations, showing a large pairing enhancement at the LCP.](image)

8.4 Three Dimensional Magnetic Fluctuations

We now study the effect of three dimensional magnetic fluctuations. For the one site EDMFT solution, a three dimensional magnetic density of states leads to a spin density wave (SDW) transition and the impurity model is not critical at the antifer-
romagnetic QCP [132, 76]. Therefore, in the following chapter we step away from the LCP, and focus on the physics of the SDW transition in the context of C-EDMFT. We approximate the three dimensional density of states as a semicircle, where the density of states vanishes at the zone edge at \[ I(Q_{AF}) \equiv -2I, \]

\[
\rho_I(\omega) = \frac{1}{N} \sum_q \delta(\omega - I_q) = \frac{1}{2\pi I^2} \Theta(2I - |\omega|) \sqrt{(2I)^2 - \omega^2}. \tag{8.11}
\]

Note, in three dimensions the antiferromagnetic wave vector is \( Q_{AF} = (\pi, \pi, \pi) \).

We generalize the Brillouin zone tiling we used in two dimensions to three, namely the cluster region \( Q \equiv + \) corresponds to \( I_q > 0 \) (ferromagnetic fluctuations) and \( Q \equiv - \) is the region \( I_q < 0 \) (antiferromagnetic interactions). This corresponds to splitting the density of states per patch as

\[
\rho_I(\pm, \omega) = \frac{1}{\pi I^2} \Theta(\pm \omega) \Theta(2I \mp \omega) \sqrt{(2I)^2 - \omega^2},
\]

and the coarse grained interactions \( \bar{I}_\pm = \pm 8I/(3\pi) \), and \( \delta I_{Q_{AF}} = -2I[1 - 4/(3\pi)] \). This density of states then leads to the following self consistent solutions of \( \chi_{loc}(\pm, i\omega_n) \), where the integrals are done with contour integration (the \( Q = - \) region has a pole at the lower zone edge)

\[
\chi_{loc}(+, i\omega_n) = \frac{1}{\pi I^2} \left( -2I + \frac{1}{2} \pi M(+, i\omega_n) - A_+(i\omega_n) \tan^{-1} \left( \frac{A_+(i\omega_n)}{2I} \right) \right) \tag{8.12}
\]

\[
\chi_{loc}(-, i\omega_n) = \frac{1}{\pi I^2} \left( 2I + \frac{1}{2} \pi M(-, i\omega_n) + A_-(i\omega_n) \left[ \pi + \tan^{-1} \left( \frac{A_-(i\omega_n)}{2I} \right) \right] \right) \tag{8.13}
\]

where we have defined \( A_\pm(i\omega_n) = \sqrt{M(\pm, i\omega_n)^2 - (2I)^2} \), which is always real. At the antiferromagnetic zero temperature transition \( I = I_c \), the static spin self energy is pinned to \( M(-, i\omega_n = 0) = 2I_c \), (which is the relation for a diverging \( \chi_{AF} \)) and
therefore the local spin susceptibility in the ordering channel becomes

\[ \chi_{\text{loc}}^{\text{crit}}(-, i\omega_n = 0) = \frac{1}{I_c} \left( \frac{2}{\pi} + 1 \right), \tag{8.14} \]

and is finite at the QCP. Therefore, we reach the important conclusion, that the C-EDMFT equations for three dimensional magnetic fluctuations, guarantee the Kondo energy scale is finite at the antiferromagnetic transition and is therefore a SDW QCP.

The Hertz-Millis approach presented in section 1.2, is the correct description of this QCP because it includes the anomalous spatial dimension \( \eta \), which is neglected in the two site C-EDMFT treatment [78, 154]. However, it is based on a weak coupling approach, where as C-EDMFT takes the local (and cluster) interactions into account correctly, therefore it is still worthwhile to determine the properties of the SDW transition using the present technique. Lastly we remark, it is possible for the C-EDMFT treatment to incorporate an anomalous spatial dimension if the cluster size is big enough [149].

In three dimensions, we focus on the same Anderson impurity model parameters as we did for the two dimensional case, and only focus on the two temperatures \( T/T_K = 0.033, 0.011 \). For a small RKKY interaction \( I \), we find the system is in the HFL phase, where the local spin susceptibility saturates as the temperature is lowered, implying the moments are screened. For sufficiently large \( I \), the model orders antiferromagnetically at a temperature \( T_N \). As shown in figures 8.8, the magnetization sets in with a small but finite jump. When comparing the local spin susceptibility, to the \( 2-d \) case, we find \( \chi(-, i\omega_n = 0) \) is much less enhanced at the magnetic transition and has a much weaker temperature dependence (as shown in figure 8.8).

We now turn to the superconducting properties. In three dimensions we consider extended \( s \)-wave pairing, \( F_s(k) = \cos(k_x) + \cos(k_y) + \cos(k_z) \). For the extended \( s \)-wave case, we can use the same density of states as in equation (8.11), with \( I \).
Figure 8.8: Magnetic order parameter $M_{AF}$ as a function of $I$ for a variety of temperatures (left plot) and the static local spin susceptibility in the ordering channel as a function of $I$, for $3-d$ magnetic fluctuations. We have plotted $\chi_{\text{loc}}$ on the same scale as the $2-d$ case, to show the much weaker temperature dependence across the transition.

Figure 8.9: Static local pair susceptibility in the singlet channel across the SDW transition (left plot). Lattice pair susceptibility in the singlet extended $s$-wave pairing channel (right plot). We find the lattice pair susceptibility is strongly enhanced across the SDW transition, consistent with the notion of quantum critical SDW fluctuations providing the “glue” for cooper pairs [45].

replaced with $3/2$ (just because we are using $I(Q_{AF}) = -2I$), this yields $\bar{F}_s(K) = \frac{N}{N} \sum_{\mathbf{k}} F_s(\mathbf{k} + K) = \pm 4/\pi$. Following the same procedure as the two dimensional
case, we have
\[ \chi_{SC} = \frac{4|F_4|^2}{1/\chi_{\text{pair}} - 4I/(3\pi)}. \] (8.15)

Due to the two site cluster, the different gap symmetries only change the overall amplitude, but do not shift the location of the pole of the lattice pairing susceptibility.

We show, both the local (\(\chi_{\text{pair}}^{\text{loc}}\)) and the lattice (\(\chi_{SC}\)) singlet pairing susceptibility in figures 8.9. We again find the local triplet pairing susceptibility is monotonously suppressed for increasing \(I\) (not shown). We see the common trend in both the impurity model and the lattice, namely, the signet pairing susceptibility is enhanced on approach to the antiferromagnetic transition from both phases. In addition, comparing figures 8.7 and 8.9, we find the pairing enhancement in the the three dimensional case is slightly stronger than the two dimensional case (for the same symmetry channel).

8.5 Summary

In this chapter we have solved the periodic Anderson model with a two site C-EDMFT approach in momentum space, using the numerically exact, CT-QMC method as the cluster solver. For two dimensional magnetic fluctuations, we have found the Kondo effect is destroyed at the antiferromagnetic QCP, i.e., the LCP survives finite size corrections from the cluster approach. In addition, we have determined the momentum dependence of the lattice pairing susceptibility in the vicinity of the LCP. For the three dimensional case we have shown the Kondo energy scale is finite at transition and the antiferromagnetic QCP is of the SDW type.

Turning to our results for superconductivity, we have found for an extended s-wave symmetry, within the C-EDMFT approximation both the LCP and the SDW QCP give rise to a large pairing enhancement in the vicinity of the critical point.
Within the C-EDMFT treatment, we are neglecting spatial fluctuations beyond the limit of the cluster, but include the local quantum critical modes. Our results can therefore be understood as measuring the local quantum critical contribution to the pairing susceptibility. It is very exciting to realize the quantum critical fluctuations of the LCP within just a two site cluster generates such a strong pairing enhancement for an extended s wave symmetry, without incorporating enough spatial fluctuations to consider the most favorable symmetry channel $d_{x^2-y^2}$. In addition, it has been shown [45], quantum critical SDW fluctuations enhance the pairing susceptibility and our results are consistent with this. It will be very interesting to consider a four site cluster, where the full $d$ wave symmetry can be considered.

Our results make it plausible to understand the superconducting transition in CeRhIn$_5$, appearing as a result of being in the vicinity to a Kondo breakdown antiferromagnetic quantum critical point. As we have shown, the combination of the destruction of the Kondo effect and antiferromagnetic interactions gives rise to a significant pairing enhancement in the lattice model, which should be representative of the quantum critical normal state properties of CeRhIn$_5$. The large pairing enhancement due to the LCP provides a natural setting for superconductivity to form below the upper critical field in CeRhIn$_5$.

In conclusion, we have studied the magnetic, local, and superconducting properties of the antiferromagnetic quantum critical point in the periodic Anderson model within a two site C-EDMFT approach. We have found the results depend drastically on the dimensionality of the problem. In other words, our results have shown the types of phase transitions possible within heavy fermion systems depends crucially on the strength of quantum fluctuations present in the system. In the next chapter, we will explore this in detail by considering the effect of magnetic frustration on the Kondo lattice. Interestingly, this will allow us to connect the results of this chapter
for two and three dimensional magnetic fluctuations, in the perspective of a global phase diagram for heavy fermion metals [84, 85, 182].
Figure 8.10: Momentum dependence of the static spin susceptibility $\chi_{\text{lat}}(\mathbf{q}, \omega_n = 0)$ at a temperature $T = 0.0167T_K$ in the full Brillouin zone $-\pi \leq q_x \leq \pi$, and $-\pi \leq q_y \leq \pi$ in the HFL phase (top plot), in the NFL phase (middle plot), and in the AF phase (bottom plot).
In this thesis up until now, we have primarily focused on two different types of quantum critical points. We have discussed the SDW transition, which we reviewed in chapter 1 using the generalization of Landau theory to zero temperatures, then in the context of C-EDMFT in chapter 8. But, first and foremost, we have primarily been interested in the unconventional scaling and superconducting properties of Kondo destroyed quantum critical points in the context of impurity models and a cluster extended dynamical mean field theory. We have found the dimensionality, or strength of quantum fluctuations, have a significant impact on the types of phase transitions that can occur.

In this chapter we explore the effect of quantum fluctuations on phase transitions in the Kondo lattice Hamiltonian [equation (2.6)], by introducing magnetic frustration into the model. We do so, by considering the model on the Shastry-Sutherland lattice (described below), where the Heisenberg model on such a geometry is know to possess a valence bond solid ground state as a result of a large amount of magnetic
frustration [183]. This allows us to consider the interplay of magnetic frustration and Kondo screening, and in particular we will study the phase transition between a valence bond solid and a heavy fermi liquid. We use our results to determine a quantitative global phase diagram, which is pertinent to understand and classify a variety of heavy fermion materials and other strongly correlated electron systems.

9.1 Introduction

Geometrical frustration in insulating quantum antiferromagnets can lead to a variety of quantum phases, such as valence bond solids (VBS) and quantum spin liquids [82]. Recent studies have discovered intriguing properties in a growing list of metallic systems with local magnetic moments residing on frustrated lattices. In these heavy fermion compounds, the interplay of Kondo screening and magnetic frustration may give rise to entirely new ground states and quantum phase transitions [49]. For example, the compounds Yb$_2$Pt$_2$Pb [184, 185, 186] and CePd$_{1-x}$Ni$_x$Al [187] have spin-1/2 local moments located on the Shastry-Sutherland and Kagome lattices respectively. Likewise, both YbAgGe [188] and YbAl$_3$C$_3$ [189] feature triangular lattices. All these compounds show an enhanced specific heat coefficient, implying a large effective mass and the presence of Kondo screening.

General theoretical considerations of the competition between Kondo and RKKY interactions have led to a proposal for the global phase diagram of heavy fermion metals as a function of frustration or quantum fluctuations ($G$) on the one hand, and the Kondo coupling ($J_K$) on the other [84, 85, 86]; see Fig. 9.1(a). This phase diagram incorporates not only antiferromagnetic (AF) order, but also the physics of Kondo destruction [72, 63, 190]. From the Kondo-destroyed antiferromagnetic phase (AF$_S$), the transition to the heavy fermi liquid phase (P$_L$) could take place directly (type I), via the spin-density-wave phase (AF$_L$) (type II), or through the Kondo-destroyed
paramagnetic phase ($P_S$) (type III). The heavy fermion compounds CeCu$_{6-x}$Cu$_x$, YbRh$_2$Si$_2$ and CeRhIn$_5$ have shown strong evidence for realizing the type I transition [65, 68, 71, 70]. CePd$_3$Si$_{20}$, which is cubic and therefore would have a smaller $G$, has properties consistent with a type II transition [191]. Geometrical frustration is expected to enhance the quantum fluctuation parameter $G$, raising the prospect of realizing a type III transition. There is a recent surge of heavy-fermion materials that appear to be suitable for exploring this large-$G$ portion of the global phase diagram. In particular, Yb$_2$Pt$_2$Pb and its homologues such as Ce$_2$Pt$_2$Pb [184, 185, 186], featuring the geometrically-frustrated Shastry-Sutherland lattice, may involve an intermediate VBS $P_S$ phase.

In this chapter, we study the effect of frustration on the Kondo-Heisenberg model.
by considering it on the Shastry-Sutherland lattice (SSL) [183], as illustrated in Fig. 9.1(b). We determine the phase diagram as a function of frustration and Kondo coupling within a slave-fermion approach. We identify and clarify the role of intermediate low energy states that break the symmetry of the SSL and exhibit partial Kondo screening (PKS). In addition, we show that the phase diagram we determine provides the first concrete realization of the global phase diagram (see Figs. 9.1(a) and 9.4) previously advanced based on general theoretical considerations.

9.2 Model

The Kondo-Heisenberg Hamiltonian on the SSL is defined as

$$H = \sum_{(i,j)\sigma} t_{ij}(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + J_K \sum_i \mathbf{S}_i \cdot \mathbf{s}_i^c + \sum_{(i,j)} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

(9.1)

where \((i, j)\) denote the nearest neighbors (NN) and next nearest neighbors (NNN) on the SSL as shown in Fig. 9.1(b). The NN and NNN tight binding parameters for the conduction electrons, denoted by \(c_{i\sigma}\), are \(t_1\) and \(t_2\), respectively. The spins of the conduction electrons are \(\mathbf{s}_i^c = c_{i\alpha}^\dagger (\sigma_{\alpha\beta}/2)c_{i\beta}\) at site \(i\), where \(\sigma_{\alpha\beta}\) are the Pauli spin matrices. They are coupled to spin-1/2 local moments, \(\mathbf{S}_i\), through an antiferromagnetic Kondo coupling \(J_K\). We have explicitly included the RKKY interactions, incorporating \(J_1\) and \(J_2\), the NN and NNN terms respectively [Fig. 9.1(b)]. The degree of frustration is measured by the ratio \(G = J_2/J_1\). We represent the local moments using fermionic spinons [192], \(f_{i\sigma}\) such that \(\mathbf{s}_i = f_{i\alpha}^\dagger (\sigma_{\alpha\beta}/2)f_{i\beta}\) with a constraint \(\sum_{\sigma} f_{i\alpha}^\dagger f_{i\sigma} = 1\) at each lattice site. The spin-1/2 Heisenberg model on the SSL was extensively studied (e.g., Refs. [183, 193, 194, 195]). For \(J_2/J_1 > 2\), it possesses an exact VBS ground state, where singlets form across each disconnected diagonal bond [183]. Whereas for small \(J_2/J_1\), the model has an AF ground state [193, 194]. The transi-
tion between these two states has not been completely determined [193, 194]. The
model in the presence of Kondo coupling was studied in some detail by Bernhard et
al. [196], and was also discussed qualitatively [86]. As we will discuss, our work here
reports the first complete analysis of the relevant phases, and this is essential both
in realizing the global phase diagram and in shedding light on the experimentally
observed PKS phase.

9.3 Mean Field Theory in the Large-\(N\) limit

Generalizing the spin symmetry from \(SU(2)\) to \(SU(N)\), we arrive at
\[
H = \sum_{(i,j),\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - J_K/N \sum_i : B_i^\dagger B_i : - \sum_{(i,j)} (J_{ij}/N) : D_{ij}^\dagger D_{ij} : ,
\]
where
\[
B_i = \sum_{\sigma} c_{i\sigma}^\dagger f_{i\sigma}, \quad D_{ij} = \sum_{\sigma} f_{i\sigma}^\dagger f_{j\sigma}.
\]
The sum now runs over \(\sigma = 1, \ldots, N\), and the constraint becomes \(\sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma} = N/2\). We have also used \(\cdots\) : to denote normal
ordering. The large-\(N\) mean field Hamiltonian can be expressed as:
\[
H_{MF} = E - \sum_{(i,j),\sigma} (Q_{ij}^\dagger f_{i\sigma}^\dagger f_{j\sigma} + \text{h.c.}) + \sum_{i,\sigma} \lambda_i f_{i\sigma}^\dagger f_{i\sigma}
+ \sum_{(i,j),\sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - \sum_{i,\sigma} (b_i^\dagger c_{i\sigma}^\dagger f_{i\sigma} + \text{h.c.}).
\]
(9.2)

We have used a Hubbard-Stratonovich transformation decoupling \(B_i\) and \(D_{ij}\) in the
Kondo singlet and resonating valence bond (RVB) channels respectively [197, 190],
and the constraint is enforced by \(\lambda_i\). The constant term is \(E/N = \sum_i (|b_i|^2/J_K - \lambda_i/2) + \sum_{(i,j)} |Q_{ij}|^2/J_{ij}\). The Kondo parameter \(Nb_i = J_K \langle B_i \rangle\) can be taken to be real by
absorbing its phase into the constraint field \(\lambda_i\) [61], whereas the RVB parameters
\(NQ_{ij} = J_{ij} \langle D_{ij} \rangle\) are in general complex.

We solve Eq. (9.2) by using a four-site unit cell, where each site is labeled by
\[ i \rightarrow (r, X), \text{ with } X = A, B, C, D \text{ marking the sublattice [see Fig. 9.1(b)], and } r \text{ specifying a unit cell. We introduce Fourier transforms per sublattice [198] as } c_{rX\sigma} = \frac{1}{\sqrt{N_u}} \sum_k e^{-ik \cdot (r + \delta_X)} c_{kX\sigma}, \text{ where } \delta_X \text{ points to each sub lattice } X \text{ from sub-lattice } A. \]

Keeping the full generality of the four-site unit cell we introduce sublattice dependent Kondo parameters and constraint fields \( b_X, \lambda_X \), and use ten complex RVB parameters \( Q_{ij} \) as shown in Fig. 9.1(c). We consider the metallic case \( 0 < n_c < 1 \), where \( n_c = \frac{1}{4N_u} \sum_{i,\sigma} \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle \) is the filling of the conduction band.

### 9.4 Large \( N \) Phase Diagram

The zero temperature phase diagram is shown in figure 9.2. Without loss of generality, we have chosen \( t_1/t_2 = 1.0 \) and \( n_c = 0.5 \) for Figs. 9.2 and 9.3. For small Kondo coupling and a large \( J_2/J_1 \) ratio, a VBS ground state arises for which only \( Q_{x+y} = Q_{x-y} \) are nonzero. The singlet bonds are the same as in the pure Heisenberg model on the Shastry-Sutherland lattice at large \( J_2/J_1 \), and we label it as SSL-VBS. This solution does not break any symmetry of the SSL.

Keeping \( J_K/t_1 \) small and decreasing \( J_2/J_1 \), we find a first order transition at \( J_2/J_1 = 1 \) from the SSL-VBS to a plaquette VBS (P-VBS) ground state where only \( Q_{x2} = Q_{x4} = Q_{y3} = Q_{y2} \) are nonzero. The P-VBS ground state breaks a reflection symmetry about either of the diagonal bonds in the the SSL. It is degenerate with the conventional VBS on the square lattice with only \( Q_{x1} = Q_{x4} \) being nonzero.

For a large Kondo coupling we find a heavy Fermi liquid (HFL) ground state, which has a nonzero Kondo parameter \( b_A = b_B = b_C = b_D \). The singlet bond parameters are also nonzero: \( Q_{xi} = Q_{yi} \), for \( i = 1 - 4 \) and \( Q_{x+y} = Q_{x-y} \). We also obtain \( \lambda_A = \lambda_B = \lambda_C = \lambda_D \), so the solution does not break any symmetry of the SSL. Here, we find that each \( Q_{ij} \) acquires a finite phase \( Q_{ij} = |Q_{ij}|e^{i\phi_{ij}} \). Correspondingly, we define a gauge independent flux through the triangular and square plaquettes as \( \Phi_{\triangle} = \sum_{\triangle} \Phi_{\triangle} \).
Figure 9.2: Large-$N$ phase diagram as a function of frustration ($J_2/J_1$) and Kondo coupling ($J_K/t_1$), for a metallic filling $n_c = 0.5$. The phases are described in the main text. The solid lines represent first-order transitions, and the dashed lines surrounding the grey area locate the boundaries of the intermediate phases that exhibit partial Kondo screening (PKS).

$$\sum_{\triangle} \phi_{ij} \text{ (mod } 2\pi) \text{ and } \Phi_{\square} = \sum_{\square} \phi_{ij} \text{ (mod } 2\pi),$$ respectively, where the summation is over the bonds around a plaquette. For the range of fillings $0 < n_c \lesssim 0.75$, we find $\Phi_{\triangle} = \pi$ and $\Phi_{\square} = 0$, whereas for $0.75 \lesssim n_c < 1$ we obtain $\Phi_{\triangle} = 0$ and $\Phi_{\square} = 0$. The finite flux through each triangular plaquette is a consequence of the spinons acquiring a finite kinetic energy from their hybridization with the conduction-electron band; we can therefore consider this as a hybridization induced flux phase. However, even though the flux through each triangular plaquette is $\pi$, the total flux through each square plaquette is still zero (mod $2\pi$); the flux does not affect the electronic band structure in the HFL phase.

We now turn to the transition among the two VBS phases and the HFL phase. Restricting the solution to these three states, we obtain the phase boundary in Fig. 9.2(a) and the mean field parameters shown in Fig. 9.3(a). Unexpectedly, when considering the general solution we find a number of intermediate states that break the lattice
symmetry, in the region shown as the grey shaded area in Fig. 9.2(a). In some cases, for example the intermediate phase between the SSL-VBS phase and the HFL phase we find a state with partial Kondo screening (PKS): some (half) of the moments in the unit cell are still locked into valence bonds, while the other spins are Kondo screened. This is discussed in detail in appendix C. Tuning $t_1/t_2$ only affects the location of the phase boundary; a smaller ratio of $t_1/t_2$ makes it easier for the Kondo singlets to form and therefore the transition between each VBS phase and the HFL phase occurs for smaller values of $J_K/t_1$.

### 9.5 Magnetism at $N = 2$

We now incorporate long range AF order into our approach. To do so, we no longer have access to the large-$N$ limit and are restricted to $N = 2$. We rewrite the Heisenberg term in Eq. (9.1) as follows: $J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j = x J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + (1 - x) J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$; the term proportional to $x$ is treated within the RVB decoupling described previously. The additional term is decoupled in terms of Néel order: $(1 - x) J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j = (1 - x) J_{ij} (2 \mathbf{M}_i \cdot \mathbf{S}_j - \mathbf{M}_i \cdot \mathbf{M}_j)$, where $\mathbf{M}_i = \langle \mathbf{S}_i \rangle$. We consider the Néel ground state with an ordering wave vector $\mathbf{Q} = (\pi/a, \pi/a)$ . This AF order corresponds to $\mathbf{M}_A = -\mathbf{M}_D = \mathbf{M}_C = -\mathbf{M}_B = \mathbf{M}$ within the four site unit cell. In the absence of a Kondo coupling, $J_K = 0$, the Heisenberg phase diagram as a function of $x$ and $J_2/J_1$ is presented in appendix C.

We present the results for the metallic case with $x = 0.7$ in Fig. 9.4. For $J_K = 0$ we find a quantum AF phase as a self consistent solution. This state, corresponding to a free energy local minimum, is taken as a candidate of the true Néel ground state. The AF phase is described by a finite Néel order parameter $\mathbf{M}$ and finite RVB mean field parameters along the horizontal and vertical bonds that do not break any lattice symmetry, $Q_{xi} = Q_{yi}$ for $i = 1 − 4$. For $x = 0.7$, this candidate state does have a lower
Figure 9.3: (a) The bond and Kondo singlet parameters at a fixed ratio $J_2/J_1 = 2.0$ as a function of $J_K$, displaying a first order transition from the SSL-VBS to the HFL phase. We have rescaled the parameters so that they are dimensionless and show the three independent quantities for the solution that breaks no lattice translational symmetry. Band structure along high symmetry directions in the reduced Brillouin zone in the SSL-VBS phase with $J_K = 0$ and $J_2/J_1 = 2.0$ (b) and in the HFL phase with $J_K = 2.1 t_1$ and $J_2/J_1 = 2.0$ (c). The thick blue lines are the gapped spinon dispersion in the SSL-VBS phase, whereas the other bands are those of the conduction electrons on the SSL. In (c) the bands in the vicinity of the Fermi energy ($\epsilon_F = 0$) have small velocity, displaying the renormalized heavy mass in the HFL phase.

free energy than the classical Néel state ($Q_{xi} = Q_{yi} = 0$); the finite RVB parameters can be thought of as fluctuations about the classical ground state. Incorporating fluctuations further will reduce the free energy even more, making the AF phase the true ground state in the limit $J_2/J_1 \ll 1$. 
The resulting phase diagram is given in Fig. 9.4, for parameters \( n_c = 0.5 \) and \( t_1/t_2 = 1 \). We have restricted the solutions to states that do not break any lattice symmetries. For small \( J_K/t_1 \) and tuning the ratio of \( J_2/J_1 \), we find a first order transition from the AF phase to the SSL-VBS phase. For small \( J_2/J_1 \), and tuning the Kondo coupling, the AF phase has a continuous transition (we are not able to discern between a continuous and a very weakly first order transition), into a spin density wave (SDW) phase characterized by the onset of Kondo screening: \( b_A = b_B = b_C = b_D \) increases continuously from zero with nonzero values of \( M \), \( Q_{xi} = Q_{yi} \) for \( i = 1 − 4 \) and \( Q_{x+y} = Q_{x-y} \). Upon increasing \( J_K \) further, there is a first order transition from the SDW phase into the HFL phase with \( M = 0 \).

Our results demonstrate a rich interplay between Kondo and RKKY interactions. In addition to the AF order and its suppression, there is also the competition between the Kondo effect and VBS order in the magnetically-disordered region. In the notation of Fig. 9.1(a), we associate Kondo hybridization \((b \neq 0)\) with a large Fermi surface (subscript \( L \)) and Kondo destruction \((b = 0)\) with a small Fermi surface (subscript \( S \)). The phase diagram we have calculated, Fig. 9.4, represents a remarkable realization of the global phase diagram that had been advanced on qualitative considerations [84, 49, 86]. It will be instructive to study Kondo lattice models in other geometrically frustrated cases, for example Kagome lattices (pertinent to CePd\(_{1-x}\)Ni\(_x\)Al [187]) and triangular lattices (relevant to YbAgGe [188] and YbAl\(_3\)C\(_3\) [189]), and explore the generality of the global phase diagram. Compared to those cases, the Kondo model on the SSL has the main advantage that the magnetically frustrated regime is accessible by a large-\( N \) approach.

Several remarks are in order. First, in the phase diagram of Fig. 9.4, we find a line of direct transitions from \( AF_S \) to \( P_L \). However, whether this is a line of transitions or a single point is sensitive to the model parameters in our approach and
for $x = 0.75$ we find the transition collapsing to a single point (see appendix C). It is important to consider how further quantum fluctuations will affect the topology of the phase diagram in Fig. 9.4. Recently, insights have been gained from calculations on a quantum impurity model incorporating local quantum fluctuations [83]; within an extended dynamical mean field context [72], the results of Ref. [83] imply this direct transition to be a line in the phase diagram.

Second, due to an even number of spins per unit cell, the spinon bands are either empty or completely full [86]. Hence the volume of the Fermi surface will not change when the system goes from the SSL-VBS to the HFL phase. Nonetheless, the topology of the Fermi surfaces reflects the incorporation ($L$) or absence ($S$) of the Kondo resonances in the Fermi volume and can be different for the two cases. We show the Fermi surfaces for $n_c = 0.5$ in both the VBS-SSL and HFL phases in appendix C.

Third, it is instructive to compare our results to those of Ref. [196]. Where there is overlap, the results of that work and ours are largely consistent. We are able to draw substantially new implications by studying the competitions of all the phases pertinent to the global phase diagram, including the $AF_L$ phase. Furthermore, our work has also uncovered PKS phases in this Kondo lattice model. In a similar vein, we note that the Shastry-Sutherland Kondo lattice was also considered in Ref. [86], with a particular focus on possible superconducting pairings. The implications of our systematic study for superconductivity is an intriguing issue, but is beyond the scope of the present work.

The systematic nature of our results is important not only for comparing our calculated phase diagram with the proposed global phase diagram of the antiferromagnetic Kondo lattice systems, but also to drawing implications of our results for experiments in heavy-fermion metals. Our phase diagram in Fig. 9.4 opens up a trajectory from the $AF_S$ to the HFL phase via a sequence of quantum phase transitions.
that passes through a VBS phase without Kondo screening. This result has implications for Yb$_2$Pt$_2$Pb, which is metallic, and contains a sizable Kondo coupling as evidenced by the observation of a large specific-heat [184, 185, 186]. Indeed, experiments [184, 185, 186] appear to have realized such a sequence of transitions; evidence for the VBS phase has come from the determination of the spin-dimerization gap.

In addition, we have provided evidence for intermediate, partially Kondo screened phases. Such a phase has also been discussed in a variational quantum Monte Carlo approach in related Kondo lattice models [199]. In this regard, it is intriguing that experiments on CePd$_{1-x}$Ni$_x$Al [187] have suggested that the frustration in this material is not large enough to yield a spin liquid, but instead leads to a ground state where some of the magnetic moments form long range AF order, while the others are completely screened by the Kondo effect. It will be instructive to explore whether related phases arise in other geometrically-frustrated heavy-fermion metals.

In conclusion, we have studied the global phase diagram in the prototypical
geometrically-frustrated Shastry-Sutherland Kondo lattice. Our work represents the first concrete calculation in which all four phases, with and without static Kondo screening and in the presence and absence of antiferromagnetic order, appear in a single zero-temperature phase diagram. Our results have elucidated the rich variety of quantum phases and their transitions in heavy-fermion metals, and provide new insights into the puzzling experimental observations recently made in geometrically frustrated heavy fermion metals such as Yb$_2$Pt$_2$Pb and CePd$_{1-x}$Ni$_x$.Al.
In this thesis we have studied a variety of QCPs relevant to experiments on heavy fermion metals and non Fermi liquid phases in general. We have used a combination of CT-QMC methods, NRG calculations, and sophisticated mean field theories to solve the representative models. We developed a method to access both relaxational regimes of dynamic correlation functions by relying on a scaling ansatz that is motivated by dynamic large $N$ calculations. We have shown that Binder cumulants can be used to systematically locate Kondo destroyed QCPs in CT-QMC calculations. Using these techniques, we have shown, Kondo destroyed quantum critical points give rise to local correlation functions that obey $\omega/T$ scaling, and a linear in temperature relaxation rate consistent with the fixed point being interacting. Our results are compatible with the experimental results on the heavy fermion metals YbRh$_2$Si$_2$ and CeCu$_{6-x}$Au$_x$.

We have shown that Kondo destroyed QCPs still exist when the impurity valence is not close to an integer. As a result of breaking particle hole symmetry we have shown in addition to a diverging local spin susceptibility, local charge fluctuations are also critical with a universal exponent. Our results are pertinent to the mixed valent quantum critical heavy fermion $\beta$-YbAlB$_4$. Lastly, we have also shown Kondo destroyed QCPs fall into three universality classes that we have dubbed B, M, and F.
We have developed the framework to study superconductivity in the vicinity of Kondo destroyed quantum critical points and introduced an effective two impurity Bose-Fermi Anderson model as a result. This approach allows us to study superconductivity in the absence of any Landau quasiparticle description. We have solved the effective model using CT-QMC and NRG to determine both the quantum critical and superconducting normal state properties. We have shown that the local pairing susceptibility is enhanced in the singlet channel in the vicinity of the QCP. We have then solved the full C-EDMFT equations of the periodic Anderson model, using the CT-QMC as the impurity solver and determined the resulting phase diagram. Studying pairing correlations across the QCP we have shown the Kondo breakdown quantum critical fluctuations enhances the lattice pairing susceptibility and represents a new unconventional pairing mechanism. Our results are pertinent to experiments on CeRhIn$_5$, as well as the theory of unconventional superconductivity.

In order to understand the role of quantum fluctuations, we have systematically studied the effect of magnetic frustration in the Shastry-Sutherland Kondo lattice. Pertinent to experiments on Yb$_2$Pt$_2$Pb and YbAl$_3$C$_3$, we studied the quantum phase transition between a valence bond solid and heavy Fermi liquid phase. Interestingly, we have found intermediate phases that exhibit partial Kondo screening. Lastly, we have quantitatively determined a global phase diagram of heavy fermion metals. Our work represents the first concrete calculation of the global phase diagram of heavy fermion metals, that had been proposed earlier on general theoretical grounds. Our results are relevant to understanding a number of existing experiments on Yb$_2$Pt$_2$Pb, YbAl$_3$C$_3$, and CePd$_{1-x}$Ni$_x$Al and are important to predicting properties that can be tested by future experiments.
Appendices
Appendix A: Appendix of Chapter 5

In the following appendix we discuss various details of the pseudogap Bose Fermi Kondo and Anderson models. We first show using a modified Schrieffer-Wolff transformation how the Bose-Fermi Anderson model can be mapped to the corresponding Kondo model. We then discuss in detail the calculation of the function $B(\tau)$ in equation (5.8) We provide a detailed list of the critical exponents obtained with NRG for various values of $r$ and $s$. We then discuss the RG flow diagrams of each type of universality class and then conclude with a discussion of breaking particle hole symmetry.

A.1 Schrieffer Wolf Transormation

In this section, using a modified Schrieffer-Wolf transformation [52] we show that the low energy description of the BFA and BFK models are equivalent over a wide range of parameters. We focus on the particle-hole symmetric case, $U = -2\epsilon_d$. First, we perform the Firsov-Lang (FL) transformation to eliminate the term linear in $\phi$, which can be done exactly. We choose a generator $S_{FL} = gS_z \sum_q \frac{1}{\omega_q} (\phi^\dagger_q - \phi_{-q})$ and
the transformed Hamiltonian $\tilde{H} = e^{S_{FL}}H e^{-S_{FL}}$ becomes

$$\tilde{H} = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^+ c_{k,\sigma} + \tilde{\epsilon}_d (n^\uparrow + n^\downarrow) + \tilde{U} n^\uparrow n^\downarrow + \sum_{k,\sigma} (V_k d_{k,\sigma}^+ c_{k,\sigma} + V_k^* c_{k,\sigma}^+ d_{\sigma}) + \sum_q \omega_q \phi_q^\dagger \phi_q, \quad (A.1)$$

where $\tilde{d}_{k,\sigma}^\dagger = d_{k,\sigma}^\dagger \exp(\frac{\sigma q}{2} \sum_q \frac{1}{\omega_q} (\phi_q^\dagger - \phi_q))$, $\sigma = \pm 1$ for $\uparrow/\downarrow$, $\tilde{U} = U + \frac{1}{2} g^2 \sum_q \frac{1}{\omega_q}$, and $\tilde{\epsilon}_d = -\tilde{U}$. It is important to note that $\tilde{n}_\sigma = n_\sigma$ and the transformation does not destroy particle-hole symmetry.

We now use a modified Schrieffer-Wolff (SW) [52] transformation to eliminate the hybridization term in Eq. (A.1). We only consider the Kondo limit, and for simplicity neglect the $k$ dependence on $V_k = V$. The generator $S_{SW}$ is the same as in the original SW transformation but with $U, \epsilon_d, d, d^\dagger$ replaced by $\tilde{U}, \tilde{\epsilon}_d, \tilde{d}, \tilde{d}^\dagger$, namely $S_{SW} = \sum_{k,\sigma} V (\frac{1-n^\sigma_{\epsilon_d}}{\epsilon_d - \epsilon_c} + \frac{n^\sigma_{\epsilon_d}}{\epsilon_d + \epsilon_c - \epsilon_u}) (\tilde{d}_{k,\sigma}^\dagger c_{k,\sigma} - c_{k,\sigma}^\dagger \tilde{d}_{\sigma})$. Writing the Hamiltonian in Eq. (A.1) as $\tilde{H} = H_0 + H_b + \tilde{H}_h$ where $H_0 = \tilde{\epsilon}_d (n^\uparrow + n^\downarrow) + \tilde{U} n^\uparrow n^\downarrow + \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^+ c_{k,\sigma}$, $H_b = \sum_q \omega_q \phi_q^\dagger \phi_q$ and $\tilde{H}_h = \sum_{k,\sigma} V (\tilde{d}_{k,\sigma}^\dagger c_{k,\sigma} + c_{k,\sigma}^\dagger \tilde{d}_{\sigma})$, we have $H' = e^{S_{SW}} \tilde{H} e^{-S_{SW}} \approx H_0 + H_b + [S_{SW}, H_0] + \frac{1}{2} [S_{SW}, \tilde{H}_h]$ and have used the fact that $[S_{SW}, H_0] + \tilde{H}_h = 0$.

Projecting out unoccupied and doubly occupied states we arrive at our final result

$$H' = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^+ c_{k,\sigma} + \sum_{q} \omega_q \phi_q^\dagger \phi_q + \sum_{k,k',\sigma} (\frac{1}{2} \tilde{W}_{k,k'} + \frac{1}{4} \tilde{J}_{k,k'}) c_{k,\sigma}^+ c_{k',\sigma}$$

$$- \sum_{k,k'} \tilde{J}_{k,k'} (\frac{1}{2} (s_{k,k'}^+ \tilde{S}^- + s_{k,k'}^- \tilde{S}^+) + s_{k,k'}^+ \tilde{S}^z) + s_{k,k'} \tilde{S}^z), \quad (A.2)$$

where $\tilde{W}_{k,k'} = V^2 (\frac{1}{\epsilon_k - \epsilon_d} + \frac{1}{\epsilon_{k'} - \epsilon_d})$ is a potential scattering term, $\tilde{J}_{k,k'} = V^2 (\frac{1}{\epsilon_k - \epsilon_d - U} + \frac{1}{\epsilon_{k'} - \epsilon_d - U} - \frac{1}{\epsilon_k - \epsilon_d} - \frac{1}{\epsilon_{k'} - \epsilon_d})$ is the Kondo coupling, $\tilde{S}^+ = S^+ \exp(g \sum_q \frac{1}{\omega_q} (\phi_q^\dagger - \phi_q))$, $\tilde{S}^- = S^- \exp(-g \sum_q \frac{1}{\omega_q} (\phi_q^\dagger - \phi_q))$, $\tilde{S}^z = \frac{1}{2} \sum_{\alpha,\beta} \tilde{d}_\alpha^\dagger \tilde{d}_\beta \tilde{s}_{\alpha,\beta}$ and $\tilde{s}_{k,k'} = \frac{1}{2} \sum_{\alpha,\beta} \tilde{c}_{k,\alpha}^\dagger \tilde{c}_{k',\beta} \tilde{s}_{\alpha,\beta}$, $\tilde{s}$ is a vector of Pauli spin matrices. The third term in equation (A.2) represents a potential scattering of the conduction electrons, and the last is the Kondo term, but with renormalized impurity spin flip operators due to the presence of the bosonic
bath. The Kondo coupling in Eq. (A.2), $\tilde{J}_{k,k'}$ differs from the standard Anderson to Kondo coupling, $J_{k,k'}$ by replacing $U$ and $\epsilon_d$ by $\tilde{U}$ and $\tilde{\epsilon}_d$.

We will now discuss the opposite order of transformations, namely, $H'' = e^{S_{FL}}e^{S_{SW}}He^{-S_{SW}}e^{-S_{FL}}$. Applying the SW transformation, projecting out charge fluctuations and then applying the FL transformation arrives at equation (A.2), however with $\tilde{W}_{k,k'}$, $\tilde{J}_{k,k'}$ replaced by $W_{k,k'}$, $J_{k,k'}$. We see that applying first the SW transformation, which is not an exact transformation, completely ignores the bosonic baths’ influence on the charge degrees of freedom of the impurity. Whereas applying the FL transformation first, which is an exact transformation, correctly captures the bosonic baths’ influence on the Anderson model and it actually lowers the Kondo coupling. The non-commutativity of the two transformations affects the effective Kondo scale at the quantum critical point quantitatively, but it does not change the universal scaling behavior of the quantum critical properties because the critical value of the Kondo coupling is not universal.

A.2 Momentum Sum and the Regularization Scheme

In this section we will calculate, $B(\tau)$ [in equation (5.8)] in two different ways and obtain the same result in the infinite boson bandwidth limit. We begin by converting the momentum sum to an integral over energy, yielding

$$B(\tau) = \sum_q \frac{1}{\omega_q^2} \left( \frac{e^{\beta \omega_q (\beta - \tau)}}{e^{\beta \omega_q} - 1} + \frac{e^{\beta \omega_q \tau}}{e^{\beta \omega_q} - 1} \right) = \int_{-\Lambda}^{\Lambda} \frac{dE}{E^2} \frac{\rho(E) e^{E(\beta - \tau)}}{e^{\beta E} - 1}.$$  

Where we take a sub-ohmic density of states

$$\rho(\omega) = \sum_q [\delta(\omega - \omega_q) - \delta(\omega + \omega_q)] = K_0 \text{sgn}(\omega) |\omega|^\alpha e^{-|\omega|/\Lambda}, \quad (A.3)$$
for $-\infty < \omega < \infty$, $0 < \alpha < 1$ and $K_0 = 1/(\Lambda^{1+\alpha}\Gamma(\alpha + 1))$. Writing the integral over positive values of energy gives

$$\int_0^\infty dE \frac{E^\alpha}{E^2} \left( \frac{e^{-E(\tau + \frac{1}{\Lambda})}}{1 - e^{-\beta E}} - \frac{e^{E(\tau - \frac{1}{\Lambda})}}{1 - e^{\beta E}} \right).$$

### A.2.1 Method 1: Contour Integration

In order to compare our result to the well known result in the limit $\alpha \to 1$ [140], we introduce a soft cut off and the previous integral becomes (we also replace $\Lambda \to -\Lambda$ in the second term)

$$\int_0^\infty dE \frac{E^\alpha}{E^2} \left( \frac{e^{-E(\tau + \frac{1}{\Lambda})}}{1 - e^{-\beta E}} - \frac{e^{E(\tau + \frac{1}{\Lambda})}}{1 - e^{\beta E}} \right) = \int_0^\infty dEf(E)E^\alpha,$$

where $f(E) = \frac{1}{E^2}(\frac{e^{-E(\tau + \frac{1}{\Lambda})}}{1 - e^{-\beta E}} - \frac{e^{E(\tau + \frac{1}{\Lambda})}}{1 - e^{\beta E}})$. We now proceed to evaluate this integral using contour integration, with a regularization procedure by subtracting off the infrared singular piece of the integral at $z = 0$. Since we have a multi valued function we first make a branch cut on the positive real axis. Then the contour we want to consider is a small circle of radius $\epsilon$ around $z = 0$ ($\Gamma_\epsilon$) which is connected to a big circle at infinity ($\Gamma$) by a path above ($\gamma_1$) and below ($\gamma_2$) the branch cut. Thus we obtain

$$\oint dz f(z)z^\alpha = (\int_{\Gamma_\epsilon} + \int_{\gamma_1} + \int_{\gamma_2} + \int_{\Gamma}) dz f(z)z^\alpha,$$

the integral over $\Gamma$ is zero by Jordan’s Lemma. We know the contour integral is also equal to

$$\oint dz f(z)z^\alpha = 2\pi i \sum_{Residues} f(z)z^\alpha$$
which occur at all the matsubara frequencies except $\omega_0$. We now want to handle the branch cut. Using $z = xe^{i\theta}$ we have

$$z^\alpha = x^\alpha \text{ on } \gamma_1$$

$$= x^\alpha e^{i\alpha 2\pi} \text{ on } \gamma_2,$$

where $x$ is a real number, which then allows us to write

$$(\int_{\gamma_1} + \int_{\gamma_2}) dz f(z)z^\alpha = \int_{-\infty}^{\infty} dx f(x)x^\alpha + \int_{\infty}^{\epsilon} dx f(x)x^\alpha e^{i\alpha 2\pi}$$

$$= (1 - e^{i\alpha 2\pi}) \int_{\epsilon}^{\infty} dx f(x)x^\alpha$$

The integral over $\Gamma_\epsilon$, which we will denote by $D(\epsilon)$ is bounded by

$$|\int_{\Gamma_\epsilon} dz f(z)z^\alpha| \leq \frac{\epsilon^\alpha}{\epsilon^2}$$

which diverges as $\epsilon \to 0$. Therefore, we subtract off $D(\epsilon)$ to regularize the integral and then take the limit as $\epsilon \to 0$. To mathematically justify we can subtract off all of $D(\epsilon)$ we must study the function $f(z)z^\alpha$ in more detail. First we must note that $f(z)z^\alpha$ is not an analytic function in the entire complex plane, or in the region of the complex plane we are considering. However $f(E)$ is analytic in the region we are considering, $f(E)$ has a third order pole at $z = 0$, which allows us to expand $f(E)$ in a Laurent series as follows

$$f(z) = \frac{a_{-3}}{z^3} + \frac{a_{-2}}{z^2} + \frac{a_{-1}}{z} + \sum_{n=0}^{\infty} a_n z^n,$$
where \( a_{-3} \neq 0 \). We then parameterize the circle around \( z = 0 \) as \( z = e^{i\theta} \) and we have

\[
D(\epsilon) = \int_{\Gamma_\epsilon} dz f(z) z^\alpha = \lim_{\epsilon \to 0} -\int_0^{2\pi} d\theta (\epsilon e^{i\theta})^\alpha i\epsilon e^{i\theta} \left( -\frac{a_{-3}}{(\epsilon e^{i\theta})^3} + \frac{a_{-2}}{(\epsilon e^{i\theta})^2} + \frac{a_{-1}}{(\epsilon e^{i\theta})} + \sum_{n=0}^{\infty} a_n (\epsilon e^{i\theta})^n \right)
\]

\[
= \lim_{\epsilon \to 0} -\int_0^{2\pi} d\theta (\epsilon e^{i\theta})^\alpha \left( \frac{a_{-3}}{(\epsilon e^{i\theta})^3} + \frac{a_{-2}}{(\epsilon e^{i\theta})^2} \right)
\]

\[
= \lim_{\epsilon \to 0} -\epsilon^\alpha (\epsilon^{2\pi} - 1) \left( \frac{a_{-3}}{(\alpha - 2)\epsilon^2} + \frac{a_{-2}}{(\alpha - 1)\epsilon} \right)
\]

Now we can see that all of \( D(\epsilon) \) is completely singular and must be subtracted out, there is no finite piece that is removed in the subtraction. Subtracting \( D(\epsilon) \) and putting together our previous results we have

\[
B(\tau)/K_0 = \int_0^\infty dx f(x) x^\alpha = \frac{1}{(1 - e^{2\pi})} 2\pi i \sum_{\text{Residues}} f(z) z^\alpha.
\]

Using the fact that the residue of the Bose-Einstein distribution at \( z = \frac{2\pi i n}{\beta} \) is \( \frac{1}{\beta} \), and taking the limit \( \Lambda \to \infty \) we arrive at (after much simplification)

\[
B(\tau)/K_0 = 2 \left( \frac{2\pi i}{\beta} \right)^{\alpha - 1} \cos \left( \frac{\pi \alpha}{n} \right) \sum_{n=1}^{\infty} \frac{1}{n^{2-\alpha}} \cos \left( \frac{2\pi n\tau}{\beta} \right).
\]

(A.4)

As opposed to the \( \alpha = 1 \) result, at \( \tau = 0 \) and \( \Lambda \to \infty \) this is still convergent.

**A.2.2 Method 2: Using the Hurwitz Zeta function**

Let us first rewrite \( B(\tau) \) in integral form with a soft cut off in the infinite boson bandwidth limit (this is equivalent to what we have in the previous section in the limit \( \Lambda \to \infty \)),

\[
B(\tau) = K_0 \beta^{1-\alpha} \int_0^\infty dE E^{\alpha - 2} \left( \frac{e^{-E(\frac{\tau}{\beta} + \frac{1}{\beta})}}{1 - e^{-E}} + \frac{e^{-E(1 + \frac{1}{\beta} - \frac{\tau}{\beta})}}{1 - e^{-E}} \right).
\]
The contour representation of the Hurwitz Zeta function is [200]

\[
\zeta(s, z) = \frac{\Gamma(1 - s)}{2\pi i} \int_{C(\epsilon, \epsilon')} (-t)^s \frac{e^{-zt}}{t(1 - e^{-t})} \, dt + \frac{1}{\Gamma(s)} \int_{\epsilon}^{\infty} t^{s-1} \frac{e^{-zt}}{1 - e^{-t}} \, dt,
\]

where \( C(\epsilon, \epsilon') \) is a contour along the real axis from \( \epsilon' \) to \( \epsilon \), a counterclockwise circle of radius \( \epsilon \) about the origin, and then along the real axis from \( \epsilon \) to \( \epsilon' \) (see ref. [200]). In the limit \( \epsilon' \to \epsilon \to 0 \) the first term is singular for \( s \leq 1 \), and is the same pole that we regularized in the previous section, but here you can see the pole clearly isolated without really any work. Thus we regularize the infrared singularity by subtracting the first term above, and then take the limit \( \epsilon' \to \epsilon \to 0 \), this yields

\[
B(\tau) = \frac{\beta^{1-\alpha}}{\alpha(\alpha - 1)\Lambda^{\alpha+1}} \left[ \zeta(\alpha - 1, 1 + \frac{\tau}{\beta}) + \zeta(\alpha - 1, 1 + \frac{1}{\beta\Lambda} - \frac{\tau}{\beta}) \right]. \tag{A.5}
\]

A symmetric form of \( B(\tau) \) is obtain by using the functional relation

\[
\zeta(s, z + 1) = \zeta(s, z) - z^{-s}, \quad \text{and we have}
\]

\[
B(\tau) = \frac{1}{\alpha(\alpha - 1)\Lambda^2} \left[ (1 + \Lambda\tau)^{1-\alpha} + (\Lambda\beta)^{1-\alpha} \left\{ \zeta(\alpha - 1, 1 + \frac{1}{\beta\Lambda} + \frac{\tau}{\beta}) + \zeta(\alpha - 1, 1 + \frac{1}{\beta\Lambda} - \frac{\tau}{\beta}) \right\} \right],
\]

this form will be useful when obtaining the zero temperature limit and is identical to the result obtained by Weiss in reference [140]. The Hurwitz Zeta function, \( \zeta(s, z) \), for \( s < 0 \) and \( 0 < z \leq 1 \) can be written as [201]

\[
\zeta(s, z) = \frac{2\Gamma(1 - s)}{(2\pi)^{1-s}} \left[ \sin\left(\frac{\pi z}{2}\right) \sum_{n=1}^{\infty} \frac{\cos(2\pi n z)}{n^{1-s}} + \cos\left(\frac{\pi z}{2}\right) \sum_{n=1}^{\infty} \frac{\sin(2\pi n z)}{n^{1-s}} \right].
\]

Since we are considering the sub ohmic case we have \( 0 < \alpha < 1 \) and we always have \( 0 < \tau < \beta \) we can use the above form in the limit \( \Lambda \to \infty \) to obtain,

\[
B(\tau)/K_0 = 2 \left(\frac{2\pi}{\beta}\right)^{\alpha-1} \frac{\cos(\frac{\pi \alpha}{2})}{\sin(\pi\alpha)} \sum_{n=1}^{\infty} \frac{1}{n^{2-\alpha}} \cos\left(\frac{2\pi n \tau}{\beta}\right).
\]
which is identical to the result we obtained in the previous section.

Before proceeding we would like to observe the $\alpha$ dependence on the spin-spin interaction $\chi_0^{-1}(\tau)$. $B(\tau)$ is the second integral of $\chi_0^{-1}(\tau)$. Below we plot $\chi_0^{-1}(\tau)$ for four values of $\alpha$ at $\beta = 1500\Lambda$, it is clear the interaction falls of faster for large values of $\alpha$.

![Graph showing $\chi_0^{-1}(\tau)$ for $\alpha = \{0.2, 0.4, 0.6, 0.8\}$ at $\beta = 1500\Lambda$.](image)

Figure A.1: $\chi_0^{-1}(\tau)$ for $\alpha = \{0.2, 0.4, 0.6, 0.8\}$ at $\beta = 1500\Lambda$.

### A.3 Critical Exponents

Here we present a summary of the critical properties of the Bose-Fermi Kondo (BFK) model with pseudogap exponent $r$ and bosonic bath exponent $s$. All of our results are summarized in table A.1. On each line, an estimate of $g_u$—the value of $g$ that produces the highest temperature $T_u$ of entry into the quantum-critical regime for $J \simeq J_u \equiv J_c(g_u)$, is followed by the assignment of the critical many-body spectrum to
one of three categories (F, B, or M) described further below. The remaining columns of Table A.1 list critical exponents, $x$, $\beta$, and $1/\nu$ [defined in Eqs. (5.15), (5.18), and (5.16), respectively] are values calculated or inferred for the pair $(r, s)$ in question. For purposes of comparison, we also list $1/\nu_B(s)$, the reciprocal of the order-parameter exponent at a pure-bosonic QCP with the same $s$, as determined within the metallic BFK model. The exponent $x$ has been calculated for all but a small number of $(r, s)$ pairs, and in all cases its value is consistent with Eq. (5.17). The order-parameter exponent $\beta$ can generally be evaluated to higher accuracy than $\nu$ (because the latter depends on $T_L$ values obtained by interpolation of data collected at a discrete set of temperature points), and has also been calculated for almost all $(r, s)$ pairs. By contrast, we have explicitly computed $1/\nu$ for only about half the pairs. We have found all of the calculated exponents satisfy the hyper scaling relation [Eq. (5.21)], therefore we can confidently apply Eq. (5.21) to predict the value of $1/\nu$ in cases where it has not been computed directly. Finally, we note that wherever it has been calculated, $\delta$ [defined in Eq. (5.19), but not listed in Table A.1] obeys Eq. (5.22) to high precision.

### A.4 RG Flow Diagrams

In this section we provide a discussion of the RG structure of the Ising-anisotropic pseudogap BFK model in the different regions of the $r$-$s$ plane. It is important to recognize that the bare couplings $(g, J)$ entering Eq. (5.2) are insufficient to describe this RG structure. Since a coupling $g > 0$ breaks spin-rotation symmetry, SU(2) symmetry of the Kondo exchange need not be preserved under renormalization, and a minimal description involves keeping track of a triad of effective couplings ($g$, $J_z$, $J_\perp$).

The stable fixed points of the pseudogap BFK model are the Kondo fixed point at $g_K = 0$, $J_{z,K} = J_{\perp,K} = \infty$ and a line of localized fixed points at $g_L = \infty$, $J_{\perp,L} = 0$, $J_{z,L} = \infty$. 

<table>
<thead>
<tr>
<th>$r$</th>
<th>$s$</th>
<th>$g_u/D$ spectrum</th>
<th>$x$</th>
<th>$\beta$</th>
<th>$1/\nu$</th>
<th>$1/\nu_B(s)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.5</td>
<td>$&gt;10$ B</td>
<td>0.499</td>
<td>0.256</td>
<td>0.48</td>
<td>0.475</td>
</tr>
<tr>
<td></td>
<td>0.7</td>
<td>6–8 B</td>
<td>0.700</td>
<td>0.296</td>
<td>0.506</td>
<td>0.506</td>
</tr>
<tr>
<td></td>
<td>0.75</td>
<td>6–8 B</td>
<td>0.800</td>
<td>0.213</td>
<td>0.46</td>
<td>0.470</td>
</tr>
<tr>
<td></td>
<td>0.8</td>
<td>5.0(5) B</td>
<td>0.900</td>
<td>0.142</td>
<td>0.352</td>
<td>0.376</td>
</tr>
<tr>
<td></td>
<td>0.85</td>
<td>3.58(3) M</td>
<td>0.989</td>
<td>0.060</td>
<td>0.093</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>0.9</td>
<td>2.8(3) M</td>
<td>0.500</td>
<td>0.252</td>
<td>0.508</td>
<td>0.509</td>
</tr>
<tr>
<td></td>
<td>no bosons</td>
<td>-</td>
<td>0.499</td>
<td>0.256</td>
<td>0.508</td>
<td>0.509</td>
</tr>
<tr>
<td>0.2</td>
<td>0.5</td>
<td>5–10 B</td>
<td>0.394</td>
<td>0.347</td>
<td>0.504</td>
<td>0.512</td>
</tr>
<tr>
<td></td>
<td>0.65</td>
<td>3.40(5) M</td>
<td>0.313</td>
<td>0.382</td>
<td>0.479</td>
<td>0.506</td>
</tr>
<tr>
<td></td>
<td>0.7</td>
<td>2.98(3) M</td>
<td>0.328</td>
<td>0.412</td>
<td>0.443</td>
<td>0.493</td>
</tr>
<tr>
<td></td>
<td>0.75</td>
<td>2.63(3) M</td>
<td>0.380</td>
<td>0.365</td>
<td>0.398</td>
<td>0.470</td>
</tr>
<tr>
<td></td>
<td>0.8</td>
<td>2.30(5) M</td>
<td>0.313</td>
<td>0.365</td>
<td>0.270</td>
<td>0.470</td>
</tr>
<tr>
<td></td>
<td>0.9</td>
<td>1.4 M</td>
<td>0.900</td>
<td>0.189</td>
<td>0.265</td>
<td>0.376</td>
</tr>
<tr>
<td></td>
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<td>-</td>
<td>0.948</td>
<td>0.160</td>
<td>0.161</td>
<td>-</td>
</tr>
<tr>
<td>0.3</td>
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<td>0.500</td>
<td>0.582</td>
<td>0.427</td>
<td>0.475</td>
</tr>
<tr>
<td></td>
<td>0.6</td>
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<td>0.493</td>
<td>0.405</td>
<td>0.356</td>
<td>0.509</td>
</tr>
<tr>
<td></td>
<td>0.7</td>
<td>1.65(5) M</td>
<td>0.422</td>
<td>0.370</td>
<td>0.270</td>
<td>0.470</td>
</tr>
<tr>
<td></td>
<td>0.8</td>
<td>1.1 M</td>
<td>0.862</td>
<td>0.355</td>
<td>0.194</td>
<td>0.376</td>
</tr>
<tr>
<td></td>
<td>0.9</td>
<td>0 F</td>
<td>0.862</td>
<td>0.355</td>
<td>0.194</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>no bosons</td>
<td>-</td>
<td>0.862</td>
<td>0.355</td>
<td>0.194</td>
<td>-</td>
</tr>
<tr>
<td>0.4</td>
<td>0.5</td>
<td>1.15(5) M</td>
<td>0.500</td>
<td>0.930</td>
<td>0.269</td>
<td>0.475</td>
</tr>
<tr>
<td></td>
<td>0.6</td>
<td>0.84(2) M</td>
<td>0.600</td>
<td>0.853</td>
<td>0.233</td>
<td>0.509</td>
</tr>
<tr>
<td></td>
<td>0.7</td>
<td>0 F</td>
<td>0.688</td>
<td>0.914</td>
<td>0.171</td>
<td>0.506</td>
</tr>
<tr>
<td></td>
<td>0.8</td>
<td>0 F</td>
<td>0.688</td>
<td>0.914</td>
<td>0.171</td>
<td>0.470</td>
</tr>
<tr>
<td></td>
<td>0.9</td>
<td>0 F</td>
<td>0.688</td>
<td>0.914</td>
<td>0.171</td>
<td>0.376</td>
</tr>
<tr>
<td></td>
<td>no bosons</td>
<td>-</td>
<td>0.688</td>
<td>0.914</td>
<td>0.171</td>
<td>-</td>
</tr>
</tbody>
</table>

Table A.1: As defined in chapter 5, $g_u$ is the value of the bosonic coupling $g$ that yields the highest temperature of entry into the quantum-critical regime. In the fourth column, “F”, “B”, and “M” refer to three different types of universality classes: Fermionic, Bosonic, and Mixed, as defined and discussed in chapter 5. Exponents $x$, $\beta$, and $\nu$ are as defined in Eqs. (5.15), (5.18), and (5.16), respectively, while $1/\nu_B(s)$ is the reciprocal of the order-parameter exponent at a pure-bosonic QCP with the same $s$, as calculated in the metallic $(r = 0)$ BFK model. All values of $1/\nu_B$ and those values of $1/\nu$ followed by an asterisk were obtained from the corresponding value of $\beta$ using hyperscaling [Eq. (5.21)] under the assumption that $x = s$. Any exponent followed by “§” has been set to that for the pure-fermionic pseudogap Kondo model (see the line labeled “no bosons” for each value of $r$) since $g_u = 0$ indicates that the bosonic bath plays no part in the criticality. A number in parentheses represents the uncertainty in the last digit, equal to 1 where omitted.
Figure A.2: The schematic RG flow diagrams for the pseudogap BFK model projected onto the plane spanned by the impurity-boson coupling $g$ and the spin-flip exchange scattering $J_\perp$, valid for bath exponents $(r, s)$ such that the quantum criticality is of the (a) B or M, and (b) F types. We have not shown in these diagrams a third axis describing the longitudinal exchange coupling $J_z$. The dashed line marks the boundary between the Kondo and localized phases. Arrows show the direction of RG flow of the effective couplings between fixed points represented by circles: free moment (FM, at $J_z = 0$), Kondo (K, at $J_z = \infty$), localized (L, a line of fixed points spanning $0 \leq J_z \leq \infty$), fermionic critical (FC, at $J_z = J_\perp$), and Bose-Fermi critical (BFC, at $J_z = \infty$ in region B but at finite $J_z > J_\perp$ in region M). Very similar RG flow diagrams can be constructed for the pseudogap BFA model.

and (at least for $r = 0$; see Ref. [132]) $J_{z,L} \propto (g - g_c)^{-\beta}$ where $g$ is the bare bosonic coupling and $\beta$ is the order-parameter exponent. The QCP of the pseudogap Kondo model is located at $g_F = 0$ and $J_{z,F} = J_{\perp,F} = J_c(g = 0)$, where $\rho_0 J_c \to r$ for $r \to 0$.

Within a perturbative RG treatment of the model valid for $r = 0$ and $0 < 1 - s \ll 1$, it has been shown [130] that the Bose-Fermi QCP is located at $K_0 g^* = O(1)$, $J_z^* = \infty$, and $\rho_0 J_\perp^* \simeq \sqrt{1 - s} \ll 1$, with the NRG having confirmed the result $J_z^* = \infty$ over a wider range of $s$ values [132]. What remains to be established is the manner in which $(g^*, J_z^*, J_\perp^*)$ evolves with increasing $r$ and/or $s$ to reach $(0, J_c(0), J_c(0))$ upon entry into the region F of the $r$-$s$ plane. Since region F is bounded by the line $x_F(r) = s$, 
and the exponent $x_F(r)$ is very well described [91] by $x_F = 1 - |\rho_0 J_c(0)|^2 = 1 - |\rho_0 J^*_\perp|^2$, one is led to conclude that for a given value of $s$ satisfying $0 < 1 - s \ll 1$, the relation $\rho_0 J^*_\perp \simeq \sqrt{1 - s}$ holds true both at $r = 0$ (on the left-most edge of region B in Fig. 5.13) and at the border between regions M and F. This observation, when combined with the asymptotic spectral decomposition (BF critical) = (B critical) $\otimes$ (F strong-coupling) that holds throughout region B, naturally leads to the conjecture that upon increasing $r$ from 0 to the point of entry into region F, (1) $J^*_\perp$ remains constant (or very nearly so); (2) $K_0 g^*$ decreases monotonically from a value of order unity to reach zero; and (3) $J^*_z$ is infinite throughout region B, and decreases monotonically to $J_c(r)$ on crossing region M. In region M the existence of finite exchange couplings satisfying $J^*_z > J^*_\perp$ is consistent with the observation of broken SU(2) spin symmetry in the asymptotic low-energy critical spectrum. By contrast, the value $J^*_z = \infty$ in region B ensures that the spectrum appears to be SU(2) invariant at energy scales much below $J^*_\perp$.

Support for this picture comes from Table A.1, which shows a clear trend with increasing $r$ at fixed $s$ (or with increasing $s$ at fixed $r$) in the value $g_u$ of the bosonic coupling that brings the model into its quantum-critical regime at the highest temperature. Throughout region B in Fig. 5.13, $g_u$ and the corresponding Kondo coupling $J_u = J_c(g_u)$ are very large in order to achieve rapid flow to $J^*_z = \infty$ and the large fixed-point value of $K_0 g^*$. While region M is crossed, $g_u$ and $J_u$ decrease in line with $g^*$ and $J^*_z$. In region F, the value $g_u = 0$ shows that the critical point can be reached without any coupling of the impurity to the bosons, meaning that $g^*$ is necessarily zero and that $J^*_z = J^*_\perp = J_u$.

Thus, based on the preceding considerations we propose the schematic RG flow diagrams shown projected onto the $g-J_{\perp}$ plane in Fig. A.2. In regions B and M, a QCP labeled BFC in Fig. A.2(a) lies on the separatrix between the basins of attraction.
of the Kondo and localized fixed points (K and L, respectively). RG flow along the separatrix is toward BFC, and on the small-\(g\) side, away from the fermionic pseudogap critical point FC. With increasing \(r\) at fixed \(s\) (or increasing \(s\) at fixed \(r\)), BFC moves to smaller values of \(g\), and merges with FC at the boundary between regions M and F. Throughout the latter region of the \(r\)-\(s\) plane, the RG structure is as shown in Fig. A.2(b), with flow along the separatrix toward FC.

A.5 Effect of Particle-Hole Asymmetry

Up until this point, we have focused exclusively on conditions of strict particle-hole \((p-h)\) symmetry, i.e., \(U = -2\epsilon_d\) for the BFA model, which maps to a BFK model with potential scattering \(W = 0\). In this section, we consider the effects of breaking this symmetry, supporting our arguments with NRG results for the critical spectrum and for the critical exponent \(x\) entering Eq. (5.15), as obtained in a preliminary study of the BFK model with \(W \neq 0\).

Under the conditions of \(p-h\) symmetry defined in the previous paragraph, the pseudogap Kondo and Anderson models exhibit a Kondo-destruction QCP only over the range of band exponents \(0 < r < \frac{1}{2}\); for \(r \geq \frac{1}{2}\), the Kondo phase disappears and over the entire parameter space the system approaches the FM fixed point at low temperatures. In these models, it is known that away from \(p-h\) symmetry, a strong-coupling or Kondo phase is present for all \(r > 0\), and that for \(0 < r < 1\) this phase is separated from the free-moment phase by an interacting QCP. For exponents \(0 < r < r^* \approx 0.375\), \(p-h\) asymmetry is irrelevant at the QCP and the quantum criticality is identical to that at \(p-h\) symmetry, whereas for \(r^* < r < 1\), quantum criticality away from \(p-h\) symmetry is governed by a distinct asymmetric QCP [90].

Combining these well-established properties of the pure-fermionic pseudogap models with the results presented in Sec. 5.5 allows informed speculation about the effects
of p-h asymmetry in the pseudogap BFA and BFK models. We expect the persistence of a region of B type criticality in which the critical spectrum has the product form \((\text{BF critical}) = (\text{B critical}) \otimes (\text{F strong-coupling})\), with p-h asymmetry affecting the fermionic strong-coupling spectrum but not the critical properties studied in this work, all of which are determined solely by the bosonic spectrum. For \(r = 0\), p-h asymmetry should be marginal (as it is in the metallic Anderson and Kondo models), giving rise to a line of QCPs sharing the same critical properties. For \(r > 0\), by contrast, p-h asymmetry should be relevant, with the fermionic spectrum being that of the asymmetric strong-coupling fixed point. These conjectures are consistent with preliminary NRG studies of the cases \((r, s) = (0, 0.7)\) and \((0.1, 0.7)\).

In the presence of p-h asymmetry, we also expect a region in which the dynamical spin response arising from the fermions is more singular than that from the bosonic bath. This region of what we will dub F'-type criticality is likely to span the range of exponents \(0 < r < 1\) and \(\frac{1}{2} < r < 1\) in which \(s > x'_F(r)\). Here, \(x'_F(r)\) is the value of the exponent \(x\) in Eq. (5.15) at the asymmetric pseudogap QCP. For \(0 < r < r^*\), \(x'_F = x_F\) (Ref. [91]) so F' criticality should be identical to F-type. For \(r^* < r < 1\), by contrast, \(x'_F > x_F\) (Ref. [91]), and the F' critical exponents should belong to the universality class of the asymmetric pseudogap QCP. We have found an example of F' criticality for \((r, s) = (0.4, 0.9)\).

Lastly, it seems probable that the B and F' regions will be separated by one in which the critical spectrum does not have a simple direct product form. At p-h symmetry, the M-type region covers the range \(1 - 2r < s < x_F(r)\). As discussed in Sec. 5.5.1, the lower bound on the range of \(s\) seems to be defined by the equality of the frequency exponents of the bare bosonic propagator and the fermionic particle-hole bubble. Since p-h asymmetry is irrelevant at the FM fixed point, [90] there seems to be no reason to expect the boundary to be affected by this breaking of symmetry. On the
other hand, the upper bound \( s = x_F(r) \) seems likely to be replaced by \( s = x'_F(r) \), the condition discussed in the previous paragraph for entry into a region of \( F' \) criticality.
Appendix B: Derivation of the CT-QMC

B.1 Introduction

In the following appendix we derive the CT-QMC approach [87] for the two impurity Bose-Fermi Anderson model in the limit of infinite impurity separation. We consider two Anderson impurities, hybridized with a band of conduction electrons and the $z$-component of each spin is coupled to a bosonic bath. The results can easily be simplified to a single impurity, with or without a bosonic bath, and can also be generalized to include inter impurity interactions as well as an additional bosonic bath that (commutes with the original bath). Therefore, this appendix, serves as the derivation of the CT-QMC used throughout the thesis.
B.2 Model

The two impurity Anderson model, with an Ising coupling of the impurity spin to a bosonic bath is defined as

\[ H = \sum_{\tilde{k},\sigma} \epsilon_{\tilde{k}} \hat{c}_{\tilde{k},\sigma}^\dagger \hat{c}_{\tilde{k},\sigma} + \sum_{\tilde{k},i,\sigma} (e^{i\tilde{k} \cdot \tilde{r}_i} V_{\tilde{k},i,\sigma}^\dagger c_{\tilde{k},\sigma} + e^{-i\tilde{k} \cdot \tilde{r}_i} V_{\tilde{k},i,\sigma}^* d_{i,\sigma}) \]

\[ + \sum_{i,\sigma} \epsilon_d d_{i,\sigma}^\dagger d_{i,\sigma} + \sum_{i=1,2} U n_{i\uparrow} n_{i\downarrow} \]

\[ + \sum_q \omega_q \phi_q^\dagger \phi_q + g (P_1 S_1^z + P_2 S_2^z) \sum_q (\phi_q^\dagger + \phi_q^\top), \]  \hspace{1cm} (B.1)

where \( S_i^z = \frac{1}{2} (n_{i\uparrow} - n_{i\downarrow}) \) and we consider two choices for \( P \), \( P_1 = P_2 = +1 \) (FM) or \( P_1 = -P_2 = +1 \) (AFM) for a ferromagnetic or anti-ferromagnetic interaction respectively between spin one and two generated by the bosonic bath. Choosing the origin of the coordinate system to be located half way between the impurities we get \( \tilde{r}_1 = +\tilde{R}/2 \) and \( \tilde{r}_2 = -\tilde{R}/2 \), we will eventually take the limit \( R \to \infty \). For convenience we rewrite the Hamiltonian as follows,

\[ H = H_0 + H_{\text{loc}} + H_2 + H_B \]  \hspace{1cm} (B.2)

where \( H_0 = H_0^c + H_0^\phi = \sum_{\tilde{k},\sigma} \epsilon_{\tilde{k}} \hat{c}_{\tilde{k},\sigma}^\dagger \hat{c}_{\tilde{k},\sigma} + \sum_q \omega_q \phi_q^\dagger \phi_q \), \( H_{\text{loc}} = \sum_{i,\sigma} \epsilon_d d_{i,\sigma}^\dagger d_{i,\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} \) and \( H_B = g (P_1 S_1^z + P_2 S_2^z) \sum_q (\phi_q^\dagger + \phi_q^\top) \). Anticipating an expansion in \( V \) we write \( H_2 = H_{\text{mix}} + H_{\text{mix}}^\dagger = \sum_{\tilde{k},i,\sigma} (e^{i\tilde{k} \cdot \tilde{r}_i} V_{\tilde{k},i,\sigma}^\dagger c_{\tilde{k},\sigma} + e^{-i\tilde{k} \cdot \tilde{r}_i} V_{\tilde{k},i,\sigma}^* d_{i,\sigma}) \). We now have to make the Hamiltonian amenable to a continuous time quantum Monte Carlo (CT-QMC) approach. First we will perform a Firsov-Lang transformation to eliminate \( H_B \). We perform time dependent perturbation theory in the hybridization. Then we trace out the fermionic and bosonic bath. Lastly we trace over the impurity degrees using a matrix representation of the \( d \) operators.
B.3 Firsov-Lang Transformation

We choose a generator

\[ S = g(P_1 S_1^z + P_2 S_2^z) \sum_q \frac{1}{\omega_q} (\phi_q^\dagger - \phi_{-q}) \],

(B.3)

note \( S \) is anti-hermitian \( S^\dagger = -S \). We apply a canonical transformation to \( H' = e^S H e^{-S} = H + [S, H] + \frac{1}{2!}[S, [S, H]] + \ldots \) Performing this transformation to all orders yields

\[ H' = H_0 + \tilde{H}_{loc} + \sum_{\tilde{k}, i, \sigma} (e^{i\tilde{k} \cdot \tilde{r}_i} V_{\tilde{k}, i, \sigma} c_{\tilde{k}, \sigma} e^{\frac{g \sigma P_i}{2}} \Phi_{\tilde{k}, \sigma} + e^{-i\tilde{k} \cdot \tilde{r}_i} V_{\tilde{k}, i, \sigma} c_{\tilde{k}, \sigma} e^{-\frac{g \sigma P_i}{2}} \Phi_{\tilde{k}, \sigma}), \]

(B.4)

where we have defined \( \tilde{H}_{loc} = H_{loc} - \sum_q \frac{1}{\omega_q} (g(P_1 S_1^z + P_2 S_2^z))^2 \) and \( \Phi = \sum_q \frac{1}{\omega_q} (\phi_q^\dagger - \phi_{-q}) = -\Phi^\dagger \).

B.4 CT-QMC

We will now describe the CT-QMC approach to calculating the partition function for the Hamiltonian \( H' \), we first write \( H' = H_0 + \tilde{H}_{loc} + \tilde{H}_2 \) where \( \tilde{H}_2 = \sum_i H_{mix}^{i} e^{\frac{g \sigma P_i}{2}} \) and \( (H_{mix}^{i})^\dagger e^{-\frac{g \sigma P_i}{2}} \) and we now proceed to expand in \( \tilde{H}_2 \). To calculate the partition function \( Z \), we go to the interaction picture and perform time dependent perturbation theory in \( \tilde{H}_2 \), which yields

\[ Z = \sum_{n=0}^\infty \frac{1}{(2n)!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_2 \ldots e^{-\beta (H_0 + \tilde{H}_{loc})} \tilde{H}_2(\tau_2) \ldots \tilde{H}_2(\tau_1)). \]

(B.5)

We will now make a series of simplifications, first is that there must be an equal number of creation and annihilation impurity operators which leaves \((2n)!/(n!n!)\) terms, the same argument holds for each spin species \( \sigma \) as well as impurity channel
or 2), which leaves \((2n!/(n!n!))\Pi_{\sigma}[n!/\Pi_{\sigma}n!]\Pi_{i}[n_{\sigma i}!/\Pi_{\sigma i}(n_{\sigma i}!)^2] = (2n!\Pi_{\sigma i} 1/(n_{\sigma i}!)^2)\) terms left, where \(n = \sum_{\sigma,i} n_{\sigma i}^2\). This yields

\[
Z = \sum_{\{n_{\sigma i}^2\}} \prod_{i,\sigma} \frac{1}{(n_{\sigma i}^2)!^2} \left( \int_0^\beta d\tau_{1i,\sigma} \cdots \int_0^\beta d\tau_{n_{\sigma i}^2,i,\sigma} \right) \left( \int_0^\beta d\tau_{1i,\sigma} \cdots \int_0^\beta d\tau_{n_{\sigma i}^2,i,\sigma} \right) \\
\times Tr_{c,d}(e^{-\beta(H_0^c+H_{\text{loc}})}T_{\tau}H_{\text{mix}}(\tau_{n}^c) \cdots H_{\text{mix}}(\tau_{1}^c)) \\
\times Tr_{\phi}(e^{-\beta H_0^\phi} e^{s_2\sum \sigma_2 \sigma_2 \Phi(\tau_{2n})} \cdots e^{s_1\sum \sigma_1 \sigma_1 \Phi(\tau_{1})}).
\] (B.6)

Tracing over the bosonic bath yields

\[
w_B(\{\tau_{2n}\}) = Tr_{\phi}(e^{-\beta H_0^\phi} e^{s_2\sum \sigma_2 \sigma_2 \Phi(\tau_{2n})} \cdots e^{s_1\sum \sigma_1 \sigma_1 \Phi(\tau_{1})}) \\
= Z_0^\phi \exp \left[ -\left( \frac{g}{2} \right)^2 \left\{ nB(0) + \sum_{i<j} s_is_j\sigma_i\sigma_jP_iP_jB(\tau_j - \tau_i) \right\} \right] \] (B.7)

where \(Z_0^\phi = Tr_{\phi}(e^{-\beta H_0^\phi}) = \prod_q (1 - e^{-\beta\omega_q})^{-1}\) and \(B(\tau)\) is given below, in terms of the non-interacting bosonic greens function

\[
B(\tau) = \sum_q \frac{e^{\omega_q(\beta - \tau)} + e^{\omega_q\tau}}{\omega_q^2(e^{\beta\omega_q} - 1)} = \sum_q \frac{1}{\omega_q^2} G(\omega_q, \tau). \] (B.8)

Tracing out all the conduction electron degrees of freedom we arrive at our final result.

\[
Z = Z_0 \sum_{\{n_{\sigma i}^2\}} \prod_{i,\sigma} \frac{1}{(n_{\sigma i}^2)!^2} \left( \int_0^\beta d\tau_{1i,\sigma} \cdots \int_0^\beta d\tau_{n_{\sigma i}^2,i,\sigma} \right) \left( \int_0^\beta d\tau_{1i,\sigma} \cdots \int_0^\beta d\tau_{n_{\sigma i}^2,i,\sigma} \right) \\
\times Tr_{d_1,d_2} \left\{ e^{-\beta H_{\text{loc}}} T_{\tau} \prod_{\sigma} d_1^\dagger (\tau_{n_{\sigma}^2}^{\sigma,1,1}) d_1^\sigma (\tau_{n_{\sigma}^2}^{\sigma,1,1}) \cdots d_1^\sigma (\tau_{1}^{\sigma,1,1}) d_1^\dagger (\tau_{1}^{\sigma,1,1}) \right\} \\
\times \prod_{\sigma} d_2^\sigma (\tau_{n_{\sigma}^2}^{\sigma,2,2}) d_2^\dagger (\tau_{n_{\sigma}^2}^{\sigma,2,2}) \cdots d_2^\sigma (\tau_{1}^{\sigma,2,2}) d_2^\dagger (\tau_{1}^{\sigma,2,2}) \right\}) \\
\times \prod_{\sigma} \det [(M_{\sigma 12}^{\sigma})^{-1}] s_\sigma \\
\times w_B(\{\tau_{2n}\}).
\] (B.9)
Where $Z_0 = Z_0^\phi Z_0^c$, $Z_0^c = Tr_c(e^{-\beta H_0}) = \prod_{p,\sigma} (1 + e^{-\beta \epsilon_p})$ is the partition function of the non-interacting fermion bath, and the matrix $M_{12}^{-1}$ is the hybridization matrix that is a function of both sets of time points $\{\tau_1^\sigma\}$ and $\{\tau_2^\sigma\}$ for a particular spin $\sigma$ and $s_\sigma$ denotes the sign of permutation to permute the $c$ operators from their time order sequence to the factorized form corresponding to the determinant of the $M$ matrix.

In order to calculate $M_{12}^{-1}$ let us consider starting from the path integral representation for the partition function, and integrating out the conduction electrons would yield

$$Z = \int D[d^\dagger, d] \exp \left(-S_{loc} - \int_0^\beta d\tau d\tau' \sum_{i,j=1,2} d_i^\dagger(\tau') \Delta_{i,j}(\tau - \tau') d_j(\tau) \right) \quad (B.10)$$

where $\Delta(\tau)$ is the Fourier transform of $\Gamma_{i,j}(\omega)$ given below

$$\Gamma_{i,j}(\omega) = -\text{Im} \left( \frac{\sum_k |V_{k,i}|^2}{\omega + i0^+ - \epsilon_k} \frac{\sum_k |V_{k,j}|^2 e^{-ik\cdot R}}{\omega + i0^+ - \epsilon_k} \right) \quad (B.11)$$

Assuming momentum independent hybridization and a spherically symmetric dispersion for the bath electrons we can integrate out the angular dependence in $\vec{k}$,

$$\Gamma_{ab}(\omega) = \left( \begin{array}{cc} \Gamma_0 & 2\pi V^2 \sum_k \int_0^\pi d\theta \sin \theta \exp(-ikR \cos \theta) \\ 2\pi V^2 \sum_k \int_0^\pi d\theta \sin \theta \exp(+ikR \cos \theta) & \Gamma_0 \end{array} \right) \quad (B.12)$$

where we have defined the hybridization $\Gamma_0 = \pi \rho_0 V^2$. In the limit of infinite separa-
tion we diagonalize the hybridization matrix due to

$$\lim_{R \to \infty} \frac{\sin(kR)}{kR} = 0$$  \hspace{1cm} (B.13)

therefore we obtain two decoupled Anderson impurities

$$\Gamma_{ab}(\omega) = \begin{pmatrix} \Gamma_0 & 0 \\ 0 & \Gamma_0 \end{pmatrix}. \hspace{1cm} (B.14)$$

We can now obtain $\Delta_{ab}(\tau)$ by Fourier transform, $\Delta_{ab}(\tau) = \int \frac{d\omega}{\pi} \frac{e^{-\omega \tau}}{e^{-\beta \omega} + 1} \Gamma_{ab}(\omega)$ for $\tau > 0$ and $\Delta(\tau) = -\int \frac{d\omega}{\pi} \frac{e^{-\omega (\tau - \beta \tau)}}{e^{-\beta \omega} + 1} \Gamma_{ab}(\omega)$ for $\tau < 0$. These results allow us to determine the fermionic weight

$$\det(M_{12}^{-1}) = \det(M_1^{-1}) \det(M_2^{-1}) \hspace{1cm} (B.15)$$

where

$$\det(M_a^{-1}(i,j)) = \det(\Delta_a(\tau_i^{e,a} - \tau_j^{e,a})) \hspace{1cm} (B.16)$$

$a = 1, 2$. We have reduced the problem to two independent Anderson impurities that are only coupled via the sub ohmic bosonic bath. Since the one impurity Anderson model doesn’t have a sign problem our algorithm will also be free of any sign problem.

### B.4.1 Matrix Approach

We now have to solve the following Hamiltonian to determine the energy eigenvalues and eigenstates.

$$\tilde{H}_{loc} = \sum_{i,\sigma} \epsilon_d d_i^{\dagger} d_i, \sigma + \sum_{i=1,2} U n_{i\uparrow} n_{i\downarrow} - \sum_q \frac{1}{\omega_q} \left( g(P_1 S_1^z + P_2 S_2^z) \right)^2, \hspace{1cm} (B.17)$$
After solving the local Hamiltonian, we are now in a position to evaluate the local trace $Tr_d(\ldots)$, we insert the identity for the local basis states, $\sum_n |n\rangle\langle n|$ and the trace becomes a product of matrices of the form

$$\langle n|O(\tau)|m\rangle = e^{\tau(E_n - E_m)}\langle n|O|m\rangle$$

except for the largest time point $\tau_M$ in this case the matrix is of the form

$$\langle n|e^{-\beta H_{loc}}O(\tau_M)|m\rangle = e^{(\tau_M - \beta)E_n - \tau_M E_m}\langle n|O|m\rangle.$$ 

### B.5 Monte Carlo updates

We have three kinds of Monte Carlo updates, insertion/removal of a pair of creation and annihilation operators and shift of an operator end point [87]. In order for the algorithm to be ergodic we must include insertion/removal updates but shift updates help the sampling efficiency and since they are numerically cheaper then inserting or removing a segment they help to speed up the simulation. We denote the local weight $w_d$, the Fermionic weight $w_F$ and the Bosonic weight $w_B$.

#### B.5.1 Insertion/Removal

The detailed balance condition for the insertion/removal of a pair of creation and annihilation operators in the impurity-$p$ channel and the spin-$\sigma$ channel is

$$\frac{p(\{O\}_{2n}) \rightarrow p(\{\tilde{O}\}_{2n+2})}{p(\{O\}_{2n+2}) \rightarrow p(\{O\}_{2n})} = \frac{\beta^2}{(k_{p\sigma} + 1)^2} \frac{w_d(\{\tilde{\tau}_{n+2}\})}{w_d(\{\tau_n\})} \frac{w_F^{p\sigma}(\{\tilde{\tau}_{n+2}\})}{w_F(\{\tau_n\})} s_{p\sigma}.$$ 

(B.18)

Where $s_{\sigma}$ denotes the sign of permutation to permute the $d$ operators from their time order sequence to the factorized form corresponding to the determinant of the $M$
matrix.

B.5.2 Shift

Choosing an endpoint at random we then attempt to shift the endpoint. The detailed balance condition for shifting a segment endpoint is

$$\frac{p(\{O\}_{2n}) \rightarrow p(\{\tilde{O}\}_{2n})}{p(\{\tilde{O}\}_{2n}) \rightarrow p(\{O\}_{2n})} = \frac{w_d(\{\tilde{\tau}_n\}) w_F^{\sigma}(\{\tilde{\tau}_n\}) w_B(\{\tilde{\tau}_n\}) s_{\rho \sigma}}{w_d(\{\tau_n\}) w_F^{\sigma}(\{\tau_n\}) w_B(\{\tau_n\}) s_{\rho \sigma}}.$$  \hspace{1cm} (B.19)

B.5.3 Block approach to the local trace

It is very numerically costly to recompute the product of all the $d$ operators every Monte Carlo step and therefore we proceed as follows [87]: we divide the imaginary time axis into $n_B = \sqrt{\langle k \rangle}$ blocks, where $\langle k \rangle$ is the average perturbation order. Each block is of length $\tau_B = \beta / n_B$, and store the product of all the $d$ operators that have time arguments that will fall within each block, i.e. consider some operator $d_{n \sigma}^\dagger(\tau)$, if $(j - 1)\tau_B < \tau < j\tau_B$ then this operator falls within block $j$. At each Monte Carlo move we only need to recompute the product of operators that fall within a changed block which at most is two blocks and each block has roughly $\sqrt{\langle k \rangle}$ operators per block, therefore this approach speeds up the local trace to a computation of order $O(\sqrt{\langle k \rangle})$.

B.6 Measurements

In the following we would like to measure both static and dynamic quantities. First we will describe dynamics and then proceed to statics.
B.6.1 Dynamics

Single particle Greens function $G_{p,\sigma}(\tau)$

In order to measure the single particle greens function $G_{a,\sigma}(\tau, \beta) = \langle T_\tau d_{a\sigma}(\tau) d_{a\sigma}^\dagger \rangle$ we perform a Monte Carlo average of the weight of a Greens function configuration. This can be calculated by removing two $c$ operators that connect a pair of $d$ operators via a hybridization line, this yields \[ (-1)^{i+j} \frac{\det \tilde{M}_{a,\sigma}^{-1}}{\det M_{a,\sigma}^{-1}}, \]
where $\tilde{M}_{a,\sigma}^{-1}$ denotes the matrix $M_{a,\sigma}^{-1}$ with the row $i$ and column $j$ removed. Using fast-update matrix formulas [87] we have $(-1)^{i+j} \det \tilde{M}_{a,\sigma}^{-1} = \det(M_{a,\sigma}^{-1})M_{a,\sigma}(j, i)$, combining this with the T-matrix identity we obtain,

\[ G_{a,\sigma}(\tau) = \langle \frac{1}{\beta} \sum_{i,j} M_{a,\sigma}(j, i) \delta^-(\tau, \tau_i^{a,\sigma} - \tau_j^{a,\sigma}) \rangle. \]

Where $\langle \cdots \rangle$ denotes a Monte Carlo average and $\delta^-(\tau, \tau') = \text{sgn}(\tau')\delta(\tau - \tau' - \Theta(\tau' - \beta))$.

Pairing Susceptibility

To calculate the pairing susceptibility we calculate the four point correlation function as described in [202], and then take the limit to a two point function. We define the creation of $p$-wave and $d$-wave pair as

\[ \Delta^\dagger_p = \frac{1}{\sqrt{2}} \left( d_{1\uparrow}^\dagger d_{2\uparrow}^\dagger + d_{1\downarrow}^\dagger d_{2\downarrow}^\dagger \right) \]
\[ \Delta^\dagger_d = \frac{1}{\sqrt{2}} \left( d_{1\uparrow}^\dagger d_{2\downarrow}^\dagger - d_{1\downarrow}^\dagger d_{2\uparrow}^\dagger \right) \]

(B.20)
and we measure

\[ \chi_p(\tau) = \langle T_\tau \Delta_\tau \Delta_p \rangle \]
\[ \chi_d(\tau) = \langle T_\tau \Delta_\tau \Delta_d \rangle. \]  \tag{B.21} 

To do this we measure four point functions which have four time arguments but are really only a function of three differences due to time translational invariance, i.e. \( \chi(\tau_a, \tau_b, \tau_c, \tau_d) = \chi(\tau_{ab}, \tau_{cd}, \tau_{ad}) \), where \( \tau_{ab} = \tau_a - \tau_b \). To measure the p-wave susceptibility we calculate

\[ \chi_{12\uparrow\uparrow}(\tau_{ab}, \tau_{cd}, \tau_{ad}) = \langle T_\tau d_{1\uparrow}(\tau_a)d_{1\uparrow}^\dagger(\tau_b)d_{2\uparrow}(\tau_c)d_{2\uparrow}^\dagger(\tau_d) \rangle \]
\[ = \frac{1}{\beta} \langle \sum_{\alpha,\beta,\gamma,\delta} M_{\beta\alpha}^{(1\uparrow)(1\uparrow)} M_{\gamma\delta}^{(2\uparrow)(2\uparrow)} \delta^-(\tau_{ab}, \tau^{e\alpha}_\delta - \tau^{s\epsilon}_\beta)\delta^-(\tau_{cd}, \tau^{e\gamma}_\delta - \tau^{s\epsilon}_\delta)\delta(\tau_{ad}, \tau^{e\alpha}_\delta - \tau^{s\epsilon}_\delta) \rangle_{MC} \]

\[ \chi_{12\downarrow\downarrow}(\tau_{ab}, \tau_{cd}, \tau_{ad}) = \langle T_\tau d_{1\downarrow}(\tau_a)d_{1\downarrow}^\dagger(\tau_b)d_{2\downarrow}(\tau_c)d_{2\downarrow}^\dagger(\tau_d) \rangle \]
\[ = \frac{1}{\beta} \langle \sum_{\alpha,\beta,\gamma,\delta} M_{\beta\alpha}^{(1\downarrow)(1\downarrow)} M_{\gamma\delta}^{(2\downarrow)(2\downarrow)} \delta^-(\tau_{ab}, \tau^{e\alpha}_\delta - \tau^{s\epsilon}_\beta)\delta^-(\tau_{cd}, \tau^{e\gamma}_\delta - \tau^{s\epsilon}_\delta)\delta(\tau_{ad}, \tau^{e\alpha}_\delta - \tau^{s\epsilon}_\delta) \rangle_{MC} \]

To measure the d-wave susceptibility we calculate

\[ \chi_{12\uparrow\downarrow}(\tau_{ab}, \tau_{cd}, \tau_{ad}) = \langle T_\tau d_{1\uparrow}(\tau_a)d_{1\downarrow}^\dagger(\tau_b)d_{2\downarrow}(\tau_c)d_{2\uparrow}^\dagger(\tau_d) \rangle \]
\[ = \frac{1}{\beta} \langle \sum_{\alpha,\beta,\gamma,\delta} M_{\beta\alpha}^{(1\uparrow)(1\downarrow)} M_{\gamma\delta}^{(2\downarrow)(2\uparrow)} \delta^-(\tau_{ab}, \tau^{e\alpha}_\delta - \tau^{s\epsilon}_\beta)\delta^-(\tau_{cd}, \tau^{e\gamma}_\delta - \tau^{s\epsilon}_\delta)\delta(\tau_{ad}, \tau^{e\alpha}_\delta - \tau^{s\epsilon}_\delta) \rangle_{MC} \]

\[ \chi_{21\uparrow\downarrow}(\tau_{ab}, \tau_{cd}, \tau_{ad}) = \langle T_\tau d_{2\uparrow}(\tau_a)d_{2\downarrow}^\dagger(\tau_b)d_{1\downarrow}(\tau_c)d_{1\uparrow}^\dagger(\tau_d) \rangle \]
\[ = \frac{1}{\beta} \langle \sum_{\alpha,\beta,\gamma,\delta} M_{\beta\alpha}^{(2\uparrow)(2\downarrow)} M_{\gamma\delta}^{(1\downarrow)(1\uparrow)} \delta^-(\tau_{ab}, \tau^{e\alpha}_\delta - \tau^{s\epsilon}_\beta)\delta^-(\tau_{cd}, \tau^{e\gamma}_\delta - \tau^{s\epsilon}_\delta)\delta(\tau_{ad}, \tau^{e\alpha}_\delta - \tau^{s\epsilon}_\delta) \rangle_{MC} \]

Putting this all together we obtain the dynamic pairing susceptibility

\[ \chi_p(\tau) = \frac{1}{2} \left( \chi_{12\uparrow\uparrow}(\tau, \tau, \tau) + \chi_{12\downarrow\downarrow}(\tau, \tau, \tau) \right) \]
\[ \chi_d(\tau) = \frac{1}{2} \left( \chi_{12\uparrow\downarrow}(\tau, \tau, \tau) + \chi_{21\uparrow\downarrow}(\tau, \tau, \tau) \right). \]  \tag{B.24}
Local Spin Susceptibility $\chi(\tau)$

In order to calculate the spin susceptibility we compute the weight of a spin-spin correlator configuration. In the following we will compute various spin-spin correlation functions, we will mainly be interested in the symmetric and staggered spin susceptibilities defined as $\chi^z_s(\tau) = \langle T\tau \hat{S}^z_s(\tau) \hat{S}^z_s(\tau) \rangle$ and $\chi^z_a(\tau) = \langle T\tau \hat{S}^z_a(\tau) \hat{S}^z_a(\tau) \rangle$ where we have defined the total spin and staggered spin $S^z_{s/a} = (S^z_1 \pm S^z_2)/2$. For the following discussion we will focus on $\chi^z_p(\tau) = \langle T\tau \hat{S}^z_p(\tau) \hat{S}^z_p(\tau) \rangle$, where the spin operators are defined in terms of the local $d$ operators, $\hat{S}^i_p = \sum_{\alpha, \beta} d^\dagger_{p\alpha} \sigma^i d_{p\beta}$, where $p$ denotes parity and $\sigma^i$ is the Pauli spin matrix. The spin correlators are calculated from a collection of time segments $\{\tau_n\} = \{\tau^1_{n_1}, \tau^1_{n_1}, \tau^2_{n_2}, \tau^2_{n_2}\}$ as

$$\chi^i_p(\tau) = \frac{\text{Tr}_d[e^{-\beta H_{\text{loc}} T\tau} \hat{S}^i_p(\tau) \hat{S}^i_p(\tau) \prod_{\sigma} d_{\sigma}(\tau^e_{n\sigma}) d^\dagger_{\sigma}(\tau^s_{n\sigma}) \ldots d_{\sigma}(\tau^e_{1\sigma}) d^\dagger_{\sigma}(\tau^s_{1\sigma})]}{\text{Tr}_d[e^{-\beta H_{\text{loc}} T\tau} \prod_{\sigma} d_{\sigma}(\tau^e_{n\sigma}) d^\dagger_{\sigma}(\tau^s_{n\sigma}) \ldots d_{\sigma}(\tau^e_{1\sigma}) d^\dagger_{\sigma}(\tau^s_{1\sigma})]} \quad (B.25)$$

where $\langle \cdots \rangle$ denotes a Monte Carlo average and for the ease of notation we have used $\sigma$ to denote the pair $\sigma = \{1/2, \uparrow / \downarrow\}$.

Local Spin Eigenvalue

We can also determine the eigenvalue of the spin as a function of time for a given Monte Carlo configuration from

$$S^i_p(\tau) = \frac{\text{Tr}_d[e^{-\beta H_{\text{loc}} T\tau} \hat{S}^i_p(\tau) \prod_{\sigma} d_{\sigma}(\tau^e_{n\sigma}) d^\dagger_{\sigma}(\tau^s_{n\sigma}) \ldots d_{\sigma}(\tau^e_{1\sigma}) d^\dagger_{\sigma}(\tau^s_{1\sigma})]}{\text{Tr}_d[e^{-\beta H_{\text{loc}} T\tau} \prod_{\sigma} d_{\sigma}(\tau^e_{n\sigma}) d^\dagger_{\sigma}(\tau^s_{n\sigma}) \ldots d_{\sigma}(\tau^e_{1\sigma}) d^\dagger_{\sigma}(\tau^s_{1\sigma})]} \quad (B.26)$$

we can use this to measure the local magnetization defined later.
B.6.2 Statics

Static Susceptibility

We measure the static susceptibility from the dynamic

$$\chi_i^s(\beta) = \int_0^\beta d\tau \chi_i^s(\tau).$$  \hspace{1cm} (B.27)

Local Occupation

We also measure $\tau = 0$ quantities such as the local occupation, $\hat{n} = \sum_{p,\alpha} \hat{n}_{p,\alpha}$, from

$$n = \left\langle \frac{\text{Tr}_d[\hat{n} e^{-\beta H_{\text{loc}}} T_{\tau} \prod_\sigma d_\sigma(\tau_e^{n,\sigma}) d_\sigma^\dagger(\tau_s^{n,\sigma}) \ldots d_\sigma(\tau_e^{1,\sigma}) d_\sigma^\dagger(\tau_s^{1,\sigma})]}{\text{Tr}_d[e^{-\beta H_{\text{loc}}} T_{\tau} \prod_\sigma d_\sigma(\tau_e^{n,\sigma}) d_\sigma^\dagger(\tau_s^{n,\sigma}) \ldots d_\sigma(\tau_e^{1,\sigma}) d_\sigma^\dagger(\tau_s^{1,\sigma})]} \right\rangle,$$  \hspace{1cm} (B.28)

where $\langle \cdots \rangle$ is a Monte Carlo average. We also measure various other static quantities at $\tau = 0$.

Local Magnetization and Binder Analysis

In order to study the quantum critical properties of the model we must be able to determine where the critical point occurs, for this we use the Binder ratio. First we measure the local magnetization,

$$M^i_p = \frac{1}{\beta} \int_0^\beta d\tau S^i_p(\tau)$$  \hspace{1cm} (B.29)

and calculate their Monte Carlo average $\langle M^i_p \rangle$ where $S^i_p(\tau)$ is given by Eq. (B.26) and the integral is evaluated numerically. We then calculate the Binder cumulants,

$$U^i_p(\beta) = \frac{\langle (\delta M^i_p)^4 \rangle}{\langle (\delta M^i_p)^2 \rangle^2},$$  \hspace{1cm} (B.30)
where $\delta M^i_p = M^i_p - \langle M^i_p \rangle$. We obtain error bars for the Binder ratio from a Jackknife error analysis.

**Reduced Density Matrix**

We also calculate the reduced density matrix of the impurity after the bath degrees of freedom have been traced out $\rho(\beta) = \frac{1}{Z} e^{-S_{\text{loc}}}$, where $S_{\text{loc}}$ is the effective local action after the conduction electrons have been traced out.

$$
\rho_{ij}(\beta) = \frac{\langle \langle i | e^{-\beta H_{\text{loc}}} T \prod_{\sigma} d_\sigma (\tau_{n^e,\sigma}^{\tau_1} d_\sigma \tau_{_n^e,\sigma}^{\tau_1} \cdots d_\sigma (\tau_{n^e,\sigma}^{\tau_1} d_\sigma \tau_{_n^e,\sigma}^{\tau_1} | j \rangle \rangle}{\langle \langle i | e^{-\beta H_{\text{loc}}} T \prod_{\sigma} d_\sigma (\tau_{n^e,\sigma}^{\tau_1} d_\sigma \tau_{_n^e,\sigma}^{\tau_1} \cdots d_\sigma (\tau_{n^e,\sigma}^{\tau_1} d_\sigma \tau_{_n^e,\sigma}^{\tau_1} | j \rangle \rangle}}. \quad (B.31)
$$
Appendix C: Appendix of Chapter 9

In this appendix we present more of the finer details related to the results of chapter 9. We first discuss the variety of intermediate symmetry broken phases, and discuss the effects of particular choices of model parameters on the overall phase diagram. We then discuss the band structure and corresponding Fermi surfaces in the VBS and HFL phases. To conclude, we present the magnetic phase diagram in the absence of the conduction band, that results from the fermionic mean field theory we have discussed in chapter 9.

C.1 Intermediate Phases and the Effect of Model Parameters

Here we present the full Large-N phase diagram for the metallic SS Kondo lattice, focusing in particular on the intermediate phases sketched in Fig. 2 of the main text. We consider tight binding parameters $t_1 = t_2 = 1$, and a conduction electron filling $n_c = 0.5$. We find a series of intermediate states that break the lattice symmetry within the unit cell. In particular we find four intermediate states labelled with
different colors in Fig. C.1: blue (1), green (2), red (3) and grey (4).

We first consider the blue region (1), which is the most physically relevant intermediate phase because it occurs in the transition region between the SSL-VBS and HFL phases. Here, we find a phase with partial Kondo screening defined as $b_A = b_D > 0$, $b_B = b_C = 0$, with $Q_{x-y} \gg Q_{x+y} > 0$. The local moments on sublattices A and D are screened by the Kondo effect, whereas those on the B and C sub-lattices are locked into a VBS singlet. Turning next to the green region (2), we find a square plaquette RVB phase with Kondo screening, defined by $b_A = b_D > b_B = b_C > 0$, $Q_{x-y} > Q_{x+y} > 0$, $Q_{x1} = Q_{y1} = Q_{x3} = Q_{y2}$ and $Q_{x2} = Q_{y3} = Q_{x4} = Q_{y4}$. In this phase, plaquette valence bonds form on each square plaquette that contains a $J_2$ bond. The red region (3) describes a phase where the RVB parameters are in a “kite” phase, and the local moments are screened. It is defined by $b_A = b_D > b_B = b_C$, $Q_{x+y} \neq Q_{x-y}$, $Q_{x1} = Q_{y1}$, $Q_{x2} = Q_{y3}$, $Q_{x3} = Q_{y2}$, and $Q_{x4} = Q_{y4}$. Lastly, we come to the grey region (4), which corresponds to a spin-Peierls phase with partial Kondo screening. Here, $b_A = b_B \neq 0$, $b_C = b_D = 0$ with $Q_{x3} \neq 0$; all the other parameters vanish.

We now turn the effect of changing model parameters on the global phase diagram. We first consider choosing a different value of $x = 0.75$ (see the main text for the definition of $x$) while keeping $t_1/t_2 = 1$ and $n_c = 0.5$. This choice of $x$ is still in the quantum antiferromagnetic phase (see below, Fig. C.6). Separately, we consider keeping $x = 0.70$ but setting $t_2 = 0$, with $t_1/J_1 = 4.0$ and $n_c = 0.5$; this allows us to study the effect of the conduction-electron band dispersion (cf. Figs. C.4 and C.5). Interestingly, for both cases we find the line of transitions between AF$_S$ and HFL collapse to a point. Therefore, whether the transition between AF$_S$ and HFL is a line or a single point is a question that needs to be addressed beyond the mean field level, for example within an extended dynamical mean field approach. The key point,
Figure C.1: Full large-N phase diagram of the SS Kondo lattice, for $t_2 = t_1$ and $n_c = 0.5$. The phases are described in the text.

Figure C.2: Phase diagram of the SS Kondo lattice incorporating magnetic order using $x = 0.75$, while keeping $t_2 = t_1$ (a) and for $x = 0.70$ with $t_2 = 0$. In both cases, the conduction electron filling, $n_c = 0.5$, is unchanged from before. The thin (thick) lines represent first order (continuous) transitions.

however, is that the overall profile of the global phase diagram is robust against these changes of parameters.

To explore further the robustness of our results against the change of the conduction-electron dispersion, we also discuss the effect of an additional tight binding parameter $t_3$, which connects every next nearest neighbor that is not connected via $t_2$. Just like
Figure C.3: (a) Fermi surface corresponding to the band structure in Fig. 3(b) of the main text, in the VBS phase. Here, $J_2/J_1 = 2$, $J_K/t_1 = 2.1$. Since the spinon bands are gapped, this corresponds to the band structure of the conduction electron dispersion alone, defined on the SSL with $t_1/t_2 = 1$ and $n_c = 0.5$; (b) Fermi surface corresponding to the band structure in Fig. 3(c) of the main text, in the HFL phase. The bare parameters are the same as in (a). Note that the Fermi volume does not change from (a) to (b), due to the even number of spins per unit cell as described in the main text.

Tuning $t_2/t_1$ away from 1, any finite $t_3$ will introduce a curvature to the region of the flat band; this flat portion existed for $t_2/t_1 = 1$ (and $t_3 = 0$), along the $k_x = k_y$ direction in the Brillouin zone and away from the Fermi energy, as shown in Fig. 3(b) in the main text. We find that tuning the ratio of $t_3/t_1$ can change the degree to which the intermediate PKS phases occur. The region of the intermediate phases that break the lattice symmetry within the unit cell narrows for increasing $t_3/t_1$, and can even be completely eliminated for a large $t_3/t_1$ ratio. Again, the overall profile of the global phase diagram is robust against the change of $t_3/t_1$.

We close this subsection by showing the Fermi surfaces of the SSL-VBS and HFL phases, both for the case $t_2 = t_1$ and $n_c = 0.5$ (Figs. C.3(a) and (b), respectively) and for $t_2 = 0$ and $n_c = 0.5$ (Figs. C.4 and C.5, respectively).
Figure C.4: (a) Band structure in the VBS phase when the diagonal hopping vanishes, \( t_2/t_1 = 0 \), and for \( J_2/J_1 = 1.6 \), \( J_K/t_1 = 0 \) and \( n_c = 0.5 \). The parameter \( t_1 = 1.0 \) sets the unit of energy. The blue lines are the gapped spinon bands. The Fermi energy is at \( \epsilon_k/t_1 = 0 \); (b) The corresponding Fermi surface.

Figure C.5: (a) Band structure in the HFL phase, for parameters as in Fig. C.4. The fermi energy is also at \( \epsilon_k/t_1 = 0 \); (b) The corresponding Fermi surface.

C.2 Magnetic Phase Diagram

Finally, we discuss the Heisenberg model in the absence of any Kondo coupling in our approach, when both the RVB correlations and Néel order are incorporated and the self consistent solutions with the lowest free energy are determined. The region for the candidate quantum Néel phase, as described in the main text, is also considered as a self consistent solution. The resulting phase diagram is shown in Fig. C.6, where both the P-VBS and SSL-VBS phases have been described in the main text. The
classical Néel state (Classical AFM) is defined as $M_A = M_D = -M_B = -M_C > 0$, with all the other parameters equal to zero. We find the candidate quantum Néel phase, with $M_A = M_D = -M_B = -M_C > 0$ and $Q_{xi} = Q_{yi} \neq 0, i = 1 - 4$ to be a self consistent solution only in the range $0.67 \leq x < 0.8125$. This is shown as the magenta region in Fig. C.6, where the boundary of the region at a finite ratio of $J_2/J_1$ marks the transition to the SSL-VBS phase. For a judicious choice of $x$ in the range $0.6 < x < 0.67$ we find the transition from the classical AFM phase to the SSL-VBS has an intermediate P-VBS phase similar to what is found in exact diagonalization studies (see reference [20] in the main text). We remark that for $x = 0.5$, which treats Neel and VBS order on equal footing, we find the location of the transition from the classical AFM phase to the SSL-VBS to be $(J_2/J_1)_c = 1.35$ which is close to the value obtained from a variety of other methods (see reference [21] in the main text).

![Figure C.6](image)

**Figure C.6:** The phase diagram of the Heisenberg model in the slave-fermion approach. The parameter $x$ and the phases are described in the main text.
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