RICE UNIVERSITY

Research on Dynamics and Thermodynamics near Quantum Critical Points

by

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ABSTRACT

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Quantum phase transition arises in general as second order phase transition at zero temperature, tuned by a non-thermal parameter such as pressure, doping or a magnetic field. The point in the phase diagram of the material in which different phases meet is called a quantum critical point (QCP). Physics around QCPs are of extensive current interest because the critical quantum fluctuations influence the physical properties in a wide temperature range (quantum criticality), and are believed to be responsible for many emergent physical properties such as non-Fermi liquids and unconventional superconductivity. In this research we explore dynamics and thermodynamics near QCPs via investigating three classes of models, which all have real material correspondence. Specifically first, we study local dynamics in a perturbed quantum critical Ising chain with $E_8$ symmetry, where we show the local dynamical spin susceptibility has a singular dependence on frequency, but differs
from the diffusion form. The nuclear magnetic resonance (NMR) relaxation rate at low temperatures depends exponentially on the inverse temperature, whose prefactor we also determine. We propose NMR experiments as a means to further test the applicability of the $E_8$ description for CoNb$_2$O$_6$. Second, we investigate the thermodynamic properties of itinerant ferromagnets near quantum critical points, described by the quantum Landau-Ginzburg theory. We provide a regularized perturbative renormalization group procedure to calculate the free energy. We further carry out numerical calculations on thermodynamic quantities, capturing not only the leading critical behaviors, but also the subleading and nonsingular contributions. We demonstrate various thermodynamic signatures of quantum criticality, including the entropy accumulation effect and the divergence of the specific heat coefficient. A detailed comparison to the recent experimental results on an itinerant ferromagnet Sr$_3$Ru$_2$O$_7$ is also presented. Third, we explore Ising-nematic and magnetic phases and their transitions in iso-electronically doped iron pnictides by carrying out a large-$N$ study of an effective low-energy Ginzburg-Landau model for these systems. We demonstrate that the magnetic and Ising orders transitions are concurrent at zero temperature, and both transitions are weakly first-order, which is consistent with RG-based prediction and experimental observations.
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Chapter 1

Introduction

1.1 Quantum phase transition

The classical phase transitions are driven by a competition between the energy of a system and the entropy of its thermal fluctuations. Therefore the classical phase transitions cannot happen at zero temperature since the entropy is zero. When tuning temperature the thermal fluctuations might drive the system to undergo classical phase transitions, which could be discontinuous (first order) or continuous (second order or higher) classified by the non-analyticity of free energy v.s. temperature. In the first-order phase transitions such as liquid-gas transition, the associated order parameter jumps at transition point and the correlation length, $\xi$, is finite. In the continuous phase transitions like paramagnetic-ferromagnetic transition, the order parameter goes to zero continuously as the system approaches the critical point ($T_c$). At the same time, the correlation length diverges as $\xi \sim \frac{[|T - T_c|/T_c]}{\nu}$, where $\nu$ is a critical exponent — the correlation length exponent.

In contrast to classical phase transitions which occur at finite temperature, quantum phase transitions, which are uniquely driven by quantum fluctuations, arise at zero temperature when ground state energy meets non-analyticity via tuning a non-
thermal parameter, \( \delta \), such as pressure, doping or a magnetic field \([1, 2]\). The point, \( \delta_c \), at which different phases meet at zero temperature is called a quantum critical point (QCP). Sometimes, the quantum phase transitions may involve sudden jumps of physical properties as we shall study in this thesis on the magnetic and Ising order quantum phase transitions in iso-electronically tuned iron pnictides (Chap. 4); such first order quantum phase transitions are analogous to first-order thermally driven phase transitions, like liquid-gas transition. What is more common and more interests is the continuous quantum phase transition, in which the change of the physical observables is more gradual.

Around QCPs the strong quantum fluctuations influence the physical properties in a wide temperature range (quantum critical regime). That regime of quantum criticality is believed to be responsible for many emergent physical properties such as non-Fermi liquids and unconventional superconductivity, and the key to explaining a wide variety of experiments. In quantum phase transitions the correlation length not only diverges in space as its classical counterpart but also diverges in (imaginary) time, \( \xi_t \sim |\delta - \delta_c|^{-\nu z} \) where \( \delta_c \) denotes the QCP, and \( z \) is the dynamical exponent \([2]\).

Fig. (1.1) is a typical phase diagram of a continuous quantum phase transition. The transition temperature is continuously suppressed until the QCP, \( \delta_c \), via tuning non-thermal control parameter \( \delta \) (pressure, magnetic field, or doping etc.). This implies strong interplay of thermal fluctuations and quantum fluctuations around the QCP. Qualitatively, from \( \xi_t \sim |\delta - \delta_c|^{-\nu z} \) we can have a characteristic energy scale
Figure 1.1: A typical phase diagram of quantum phase transition with $\delta$ and $\delta_c$ as tuning parameter and quantum critical point respectively. The blue regime denotes the ordered regime. The light-purple regime enclosed by two red dashed-dot lines is the typical quantum critical regime, the shaded regime enclosed by two purple dashed-dot lines around the classical transition line is the Ginzburg-Landau regime. The blue regime circled by black solid line is the ordered regime. All the dashed-dot lines shown in the figure are not transition line but just used to qualitatively illustrate crossover regimes. The broken line on the top is used to denote the cut off temperature, $T^*$, beyond which quantum criticality is negligible.

$\Delta \sim \hbar c/\xi_r$ with $c$ as the characteristic propagation velocity of the wavefunction in the system (e.g. velocity of spin wave in Heisenberg models). Then when $\Delta \gg k_B T$, i.e., $\hbar/\Delta \ll \hbar/(k_B T)$, it means the characteristic coherent time (correlation length) of the wavefunction in the system is much smaller than the thermal relaxation time (or thermal de Broglie length), implying the wavefunction of the system has a short correlation length scale with itself manifestly as a product form (short-range
entangled form). As a result, the thermal fluctuations will only excite non-critical modes, corresponding to the light-yellow regime of Fig. (1.1).

When in the opposite limit $\Delta \ll k_B T$, i.e., $\hbar/\Delta \gg \hbar/(k_B T)$, we meet the novel quantum critical regime, where the characteristic coherent time (or correlation length) of the wavefunction in the system is much larger than the thermal relaxation time (or thermal de Broglie length), as a result, the thermal fluctuations directly kick in the quantum-critical (long-range-entangled) state, leading to a complicated mixture of statics and dynamics. This complicated mixture of statics and dynamics can strongly affect the thermodynamical quantities and local/nonlocal dynamics in the system, bringing in interesting unconventional physics beyond the classical picture. For the aspects of thermodynamics, one can expect the entropy should be greatly enhanced due to the strong competition between thermal and quantum fluctuations, which can be probed by Grüneisen ratio defined as ratio of thermal expansion coefficient and specific heat [3]. Indeed it has been shown that the Grüneisen ratio diverges generically when the systems approaches QCPs in quantum critical regimes [4, 5], which is in strong contrast to the constant result of the classical systems. For the aspects of dynamics it has been shown that the mixture of statics and dynamics near QCPs can lead to bizarre local dynamics of local quantum criticality with the behavior of $\omega/T$ scaling [6].

Even more surprisingly, in contrast to the narrow Ginzburg-Landau regime near the classical transition line (Fig. (1.1)), the quantum critical regime is very robust that
it can persist in a broad regime when temperature increases far above the QCP until temperature is comparable with the characteristic coupling strength of the system, which is denoted as dashed line on the top of Fig. (1.1) with a cut-off temperature $T^*$. And this broad range of quantum criticality has been observed for a variety of systems — including unconventional copper-oxide and iron-pnictide superconductors [7], heavy Fermion systems [8], and one-dimensional systems [9].

The specific phase diagrams for real models or materials can be different from that shows in Fig. (1.1), e.g., the classical finite temperature transition line can collapse (no-phase transition at finite temperature) in one-dimensional transverse field Ising model; the quantum critical regime may contain more subtle structure in itinerant spin-density-wave systems; the quantum phase transitions can be weakly first order in the iso-electronically doped iron pnictides. Nevertheless, for these systems, they all have broad regimes of quantum criticality.

Despite of the great interests of quantum criticality, to exactly describe the thermodynamics or the low-frequency dynamics of quantum criticality at finite temperature ($\omega \ll k_B T / h$) still remains to be challenging. Even for the dynamics in the quantum systems of one spatial dimension, the analytical results are also limited [10,11]. In this thesis we shall take this challenge via trying to understand the quantum criticality in three systems. Specifically we will study the low-frequency and low-temperature spin dynamics in a perturbed quantum critical Ising chain with an $E_8$ symmetry (Chap. 2); the thermodynamics in itinerant spin-density-wave systems (Chap. 3); and
zero-temperature quantum phase transitions in iso-electronically-doped iron pnictides (Chap. 4). Before jumping to the details, following, we will give a brief introduction for the quantum phase transitions in these three systems in the following sections.

1.2 The quantum Ising chains

The one-dimensional-transverse-field Ising model (1DTFIM) is one of the most widely studied one-dimensional quantum systems [2,12], with the Hamiltonian

\[
H_I = -J \left( \sum_i \sigma_i^x \sigma_{i+1}^x + g \sum_i \sigma_i^z \right)
\]

(1.1)

where \( \sigma_i^x \) and \( \sigma_i^z \) are the Pauli matrices associated with the spin components \( S^\mu = \sigma^\mu / 2, (\mu = x, y, z) \), \( i \) marks site positions, and \( g \) is the the transverse field, in unit of the nearest-neighbor ferromagnetic exchange coupling \( J \) (here we take \( J > 0 \) for simplicity) between the longitudinal (\( z \)) components of the spins. In this simple quantum model due to the non-commutativity between different directions of the spin, the quantum fluctuations appear when the transverse field is turned on. At zero temperature when the transverse field is weak, namely, \( g \ll 1 \), the system stays in the order phase with two degenerate ground states of product from,

\[
\prod_i |\uparrow_i \rangle \text{ or } \prod_i |\downarrow_i \rangle
\]

(1.2)

with \( |\uparrow_i \rangle \) and \( |\downarrow_i \rangle \) as eigenstates of \( \sigma_i^z \) of eigenvalues of +1 and -1 respectively. However this degeneracy is unstable, any randomly small external perturbative field along \( z \) direction can break this degeneracy, as a result, the system will stay in a
unique ground state of either $\prod_i |\uparrow\rangle_i$ or $\prod_i |\downarrow\rangle_i$. And apparently this ground state breaks the $Z_2$ symmetry along z-direction of the Hamiltonian. On the opposite limit, when the transverse field is strong, namely, $g \gg 1$, the system stays in the "quantum disorder" regime with the form of the ground state in another product form,

$$\prod_i |\rightarrow\rangle_i = \prod_i \frac{1}{\sqrt{2}} (|\uparrow\rangle_i + |\downarrow\rangle_i)$$

(1.3)

with $\prod_i |\rightarrow\rangle_i$ as eigenstate of $\sigma^z_i$ of eigenvalue $+1$. Apparently this ground state at large transverse-field limit is invariant under the $Z_2$ operation of $\sigma_z$ coincident with the symmetry of the Hamiltonian. This indicates when the transverse field $g$ is tuned from a small value to a large one (or reverse), the ground state wavefunction can not transform analytically due to the different symmetry (different topology too) of the ground state wavefunction in these two different-limit regimes. As a result, the
ground state will meet the non-analytical point, $g_c$, when tuning the parameter $g$, which is just the quantum critical point. Thus at zero temperature it undergoes a quantum phase transition when the transverse field is tuned across its critical value $g = g_c = 1$ [12]. Near $g_c$, the correlation length diverges as $|g - g_c|^{-1}$, and the gap of the system closes as $|g - g_c|$ with critical exponent $\nu = 1$, and dynamical exponent $z = 1$. The divergence of the correlation length implies the existence of long-range entanglement of the ground state wavefunction which form will be a complicated linear-superposition of all possible product states in the huge $2^N$ Hilbert space with $N$ as the total number of sites. And apparently it can not be further simply written as the product forms in the two limits we discussed just now. This long range entangled state near the QCP of 1DTFIM strongly affects the physics nearby, leading to a rich phase diagram as it’s shown in Fig. (1.2) [2]. Fig. (1.2) shows that at finite temperature this model does not have phase transitions, therefore, there are only crossovers between different regimes. And this phase diagram has also been further confirmed by the experiments on the insulator of cobalt niobate CoNb$_2$O$_6$, a quasi-one-dimensional ferromagnet [9]. Very surprisingly the NMR experiments on local dynamics, via measuring the critical behavior of the local dynamics, show a broad regime of the quantum criticality, where the quantum critical regime can survive until $T \approx 0.4J$!

At the quantum critical point the 1DTFIM can be fully described by an exactly solvable two-dimensional conformal field theory (CFT) with central charge $1/2$ [13].
More surprisingly, when the 1DTFIM at its quantum critical point is subjected to a small longitudinal field $h$ coupled to $\sigma^z$, namely

$$H_Z = -J \left( \sum_i \sigma_i^z \sigma_{i+1}^z + \sum_i h \sigma_i^z \right),$$  \hspace{1cm} (1.4)

in the scaling limit it can be described by an integrable quantum field theory – Zamolodchikov’s celebrated $E_8$ model, describing a scattering theory of eight massive particles [14, 15]. Small $h$ manifestly shows the system stays close to the QCP of 1DTFIM, thus a natural question raises that how the statics and dynamics of the system behaves in this “quantum critical” regime (consider it on the $g - h$ plane). The statics behaviors have been detailedly studied in Ref. [16], however a study on its finite temperature dynamics is lacking. In Chap. 2 we will detailedly study its low-temperature and low-frequency dynamical behaviors ($k_B T, \hbar \omega \ll$ mass of the lightest particle), which can be directly compared with a delicate experiment of NMR relaxation rate on the material of CoNb$_2$O$_6$.

1.3 Itinerant spin-density-wave transitions

We illustrate the itinerant spin-density-wave (SDW) transitions beginning with following simple one-band Hubbard model,

$$H = - \sum_{\langle ij \rangle, \sigma} t_{i-j} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i, \sigma} c_{i\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$  \hspace{1cm} (1.5)

where $i$ denotes site positions, $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are fermion creation and annihilation operators, $t_{i-j}$ is the hopping coefficient between nearest site, $\mu$ is the chemical potential,
\( \sigma = \{\uparrow, \downarrow\} \) is the spin index for spin up and down, \( U \) is the on-site repulsive Hubbard interaction, and \( n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \). Apparently when in the strong interaction limit, \( U \gg t \), the electrons in the system are highly localized, which usually becomes Mott insulator; when the system is in opposite limit, weak interaction limit, \( U \ll t \), the electrons are highly delocalized, which usually becomes metal. Therefore when tuning \( t \) or \( U \), the system can be tuned to the boarder of these two phases leading to a quantum phase transition — the metal-insulator transitions. In this section we shall briefly discuss the spin-density-wave transition in the weak-interaction limit. We then decompose the interaction term in Eq. (1.5) into the charge and SDW channels,

\[
U \sum_i n_{i\uparrow} n_{i\downarrow} = \frac{U}{4} \sum_i \left[ (n_{i\uparrow} + n_{i\downarrow})^2 - (n_{i\uparrow} - n_{i\downarrow})^2 \right]. \tag{1.6}
\]

For the moment of interests we neglect the charge fluctuations, and only keep the SDW fluctuations. Then following the conventional Hubbard-Stratonovich decoupling procedure, a conjugate bosonic field \( \hat{\phi} \) to the spin-density operator \( n_{i\uparrow} - n_{i\downarrow} \), corresponds to low-energy fluctuations fields of the SDW order parameters, can be introduced to decouple the interaction of SDW channel. In the weak interaction limit, only degrees of freedom around the magnetic ordering wave vector \( \hat{Q} \) are critical, where \( \hat{Q} = \vec{0} \) or \( (\pi, \cdots, \pi) \) for ferro- and antiferro- magnetic ordering, respectively. As a result, the electron modes far away from the part of the Fermi surface connected by \( \hat{Q} \) are essentially not affected by quantum criticality and remain as Fermi-liquid quasi-particles (backgrounds). After integrating out the fermionic degrees of freedom, we obtain an effective quantum Ginzburg-Landau-Wilson functional of the \( O(n) \) \( \hat{\phi}(\vec{q}, i\omega_l) \).
Figure 1.3: Typical phase diagram for the itinerant spin-density-wave quantum phase transitions

field ($\omega_l$ is the Matsubara frequency), which is an effective quantum $\phi^4$ model with additional quantum dissipation terms. This model has been systematically studied by Hertz, Millis, Moriya, etc. [17–22], and is also called as Hertz-Millis-Moriya model.

The effective action in terms of the order parameter fluctuations $\vec{\phi}$ can be written as:

$$S[\vec{\phi}] = \frac{1}{2} \sum_{q, i\omega_l} \chi_0^{-1}(q, i\omega_l) \vec{\phi}_q^T (q, i\omega_l) \cdot \vec{\phi}(-q, -i\omega_l) + u \int_0^\beta d\tau \int d\mathbf{r} \left[ \vec{\phi}_q^T (\mathbf{r}, \tau) \cdot \vec{\phi}(\mathbf{r}, \tau) \right]^2$$

(1.7)

where

$$\chi_0^{-1}(q, i\omega_l) = r_0 + (q\xi_0)^2 + \frac{|\omega_l|}{\Gamma_q}.$$  

(1.8)

Here $r_0$ is bare control parameter which may be a function of pressure or chemical doping. This differs from the classical $\phi^4$ model in the quantum Landau damping.
term $|\omega_l|/\Gamma_q$ with $\Gamma_q = \Gamma_0(q\xi_0)^{-2}$, which leads to an effective dimension $d + z$. The dynamical exponent $z$ takes the value of 2, 3 respectively for antiferro- and ferro- magnetic spin fluctuations. $\xi_0$ is a microscopic length in the order of $k_F^{-1}$ and $\Gamma_0$ is a microscopic energy scale in the order of Fermi energy $E_F$. $\{\omega_l\}$ are Bosonic Matsubara frequencies. For later convenience we further introduce reduced temperature $t \equiv T/\Gamma_0$.

Fig. (1.3) shows a typical phase diagram for the itinerant SDW quantum phase transitions. In Fig. (1.3), the control parameter $r$ is the renormalized control parameter consisting of bare control parameter $r_0$ and temperature-independent-renormalized part $r_u$. Similar to the classical $\phi^4$ model, when $r < 0$, the order parameter takes a finite value, corresponding to a magnetic ordered state; when $r > 0$, the order parameter vanishes, describing a quantum disordered state (a paramagnetic Fermi liquid state for metallic systems). In the quantum model, $r$ is tuned by pressure or chemical doping, e.g., $r = (p - p_c)/p_c$, rather than the temperature in classical phase transitions $r \sim (T - T_c)/T_c$. The quantum phase transition at $T = 0$ therefore characterizes a change in ground state tuned by non-thermal physical parameters regulating the strength of quantum fluctuations. Fig. (1.3) also shows the subtle structure inside the quantum critical regime, which details can be found in Refs. [18,19].

In Chap. 3 we shall detailedly investigate the thermodynamic properties of itinerant ferromagnets near quantum critical points, following a regularized perturbative renormalization group procedure of free energy of the quantum Ginzburg-Landau
We further carry out numerical calculations on thermodynamic quantities. We demonstrate various thermodynamic signatures of quantum criticality, including the entropy accumulation effect and the divergence of the specific heat coefficient. A detailed comparison to the recent experimental results on an itinerant ferromagnet Sr$_3$Ru$_2$O$_7$ [23, 24] is also presented.

1.4 Magnetic and spin-Ising phase transitions in iron pnictides

From the simple one band Hubbard model Eq. (1.5), in the strong-correlated limit of $U \gg t$, the system becomes an insulator dubbed as Mott insulator. Therefore a quantum phase transition must happen when $U/t$ reaches certain critical point, which can be sketched as follows. In this section we will focus on the new class of material, iron arsenides, which has been generally argued [25–28] that its bad metal behavior [29–32] can be attributed to a incipient-Mott picture, leading to the theoretical proposal for a quantum critical point (QCP) under iso-electronic phosphorous for arsenic doping in the parent iron arsenides [33]. The P doping can increase the in-

![Figure 1.4 : Sketchy quantum phase transition for metal-insulator transition.](image-url)
plane electronic kinetic energy and thus the coherent electronic spectral weight while leaving other model parameters little change \[34–38\], thereby it suppresses the finite temperature AF magnetic order and the associated Ising-nematic spin order to zero temperature \[33, 39\], and finally tuning the system across magnetic quantum phase transitions. Extensive experimental measurements in the P-doped CeFeAsO and BaFe\(_2\)As\(_2\) \[36, 40–42\] have provided strong evidence for such a QCP. The experiments on P-doped CeFeAs\(_{1-x}\)P\(_x\)O \[41\] shows the nematic-Ising order and AF magnetic order can be suppressed to near zero temperature at \(x\) near 0.4, which suggests existence of magnetic quantum phase transitions. The experiments of transportation \[42\] and NMR \[43\] on BaFe\(_2\)(As\(_{1-x}\)P\(_x\))\(_2\) indicate large area of non-Fermi liquid regime above superconductivity dome, which suggests a “hidden” magnetic QCP inside the superconductivity dome. A further London penetration depth on this material \[44\] indicates the AF quantum fluctuations near the suggestive QCP \[42, 43\] could strongly influence the transition temperature of SC even the QCP is “hidden” inside the SC dome. All of these observations imply important roles of magnetic- and Ising- phase transitions in iron pnictides, which is part of motivation of the research.

The undoped material can be described by either an \(S = 1\) or \(S = 2\) minimum spin model with nearest- and next-nearest-neighbor couplings \(J_1, J_2\) that depend on the competition between the on-site Hubbard interaction, crystal field splitting and the Hunds rule \[25\],

\[
H = \sum_{\langle i,j \rangle} J_1 \vec{S}_i \cdot \vec{S}_j + \sum_{\langle\langle i,j \rangle\rangle} J_2 \vec{S}_i \cdot \vec{S}_j
\]  

(1.9)
Figure 1.5: Classical ground state of the $J_1 - J_2$ model. Two interpenetrating Néel square lattices with staggered magnetizations of sublattices of $A$ and $B$.

where $\langle \cdots \rangle$ and $\langle \langle \cdots \rangle$ respectively denote the nearest neighbor and next nearest neighbor sites. The first-principal calculations [45] suggest that both $J_1$ and $J_2$ are large and antiferromagnetic, and Ref. [46] showed that $J_2 \sim 2J_1$. It is well-known that when $J_2 > J_1/2$, the classical ground state of model Eq. (1.9) has the symmetry of $O(3) \times O(3)$ consisting of two interpenetrating Néel lattices (the dotted squares in Fig. (1.5)) with independent staggered magnetizations (Néel vectors) $\vec{m}_A$ and $\vec{m}_B$, where the energy is independent of the angle $\phi$ between $\vec{m}_A$ and $\vec{m}_B$. However there is no generic symmetry in the model of Eq. (1.9) can protect the classical ground state. The quantum or thermal fluctuations can break the degeneracy in $\phi$, leading to the collinear order $\phi = (0, \pi)$ or $(\pi, 0)$ [47, 48]. Thus $\vec{m}_A \cdot \vec{m}_B = \pm 1$ becomes an
Ising order parameter in the model of Eq. (1.9).

Figure 1.6: Above figure shows iron pnictides phase diagram near a magnetic quantum critical point. The yellow dot denotes quantum critical point determined by the critical tuning parameter $w_c$. The purple solid line is the line of the thermally driven antiferromagnetic transition and the dashed line is a structural transition.

Upon P doping, the in-plane electronic kinetic energy will increase with little change in potential energy, resulting in an increase of spectral weight ($w$) (electronic itinerancy), which will suppress the magnetic and Ising orders until phase transitions [33, 39, 49]. The effect of non-zero $w$ can be treated order-by-order in terms of a Ginzburg-Landau action [26, 33]. With the presence of the damping rate, the effective dimension of the system is $d + z = 4$, at which the Ising coupling becomes marginal relevant. However, the RG calculation suggests, due to the marginal nature of the Ising coupling, the transitions are very weak first-order and essentially continuous at zero temperature [50]. Therefore we can get a sketchy phase diagram as it’s shown in Fig. 1.6 [39].
The finite temperature magnetic and nematic-Ising order phase transitions in this material have been studied via large N calculation in NLσM Ref. [51] and variational spin wave theory [52] without considering effects of dynamics. However, the transition nature when including coherent effects and SDW damping remains to be studied. Here we explore these phases and their transitions at zero temperature by carrying out a large-\(N\) study of the effective action, which details can be found in Chap. 4.
Chapter 2

Spin dynamics in a perturbed quantum critical Ising chain with an $E_8$ symmetry

The collective fluctuations of a quantum critical point (QCP) often lead to unusual properties. Even in equilibrium, the statics and dynamics are mixed at a QCP. This gives rise to dynamical scaling in many cases, while also making it difficult to calculate the fluctuation spectrum. The latter is especially so for the dynamics at nonzero temperatures ($T > 0$) in the “quantum relaxational” regime, which corresponds to small frequencies ($\omega \ll k_B T / \hbar$) or long times. Indeed, even for the canonical QCP of a transverse-field Ising model in one dimension, it has been challenging to calculate such real-frequency dynamics [10, 11].

In the one dimensional transverse field Ising model in the presence of a small longitudinal field. The transverse-field-induced QCP in the absence of a longitudinal field [12] has an emergent conformal invariance in the scaling limit [13]. When a small longitudinal field is turned on at the QCP, the excitation spectrum becomes discrete at low energies. The perturbed conformal field theory [14] provided evidence that the discrete spectrum corresponds to eight particles whose masses (of relativistic dispersions) have definite ratios, and the corresponding integrable quantum field theory has a celebrated $E_8$ symmetry. The first two particles correspond to bound
Figure 2.1: (Courtesy of Ref. [53]) Above figures show the inelastic neutron scattering experiments on the quasi-one-dimensional ferromagnet CoNb$_2$O$_6$, which corresponding critical transverse field is around 5.2T. The experimental results show that when the transverse field approaches the critical field, the mass ratio of the lightest and the second lightest particles approaches the golden ratio as it is predicted by Zamolodchikov [14]. The data for the second lightest mass is cut at around 5T due to experimental resolution limit.

states that are well below the continuum part of the spectrum [14]. Recently neutron scattering measurements have been carried out in a cobalt niobate CoNb$_2$O$_6$, whose Co$^{2+}$ are coupled in a quasi-1D way; the experiment identified two excitations whose energy ratios are close to the predicted value, the golden ratio as it is shown in the Fig. (2.1) [53].

We study the low-frequency dynamical spin structure factor at finite temperatures using the form factor method [15]. From theoretical perspective, our calculation provides an illustrative setting to determine the dynamics in the quantum-relaxational
regime. For the $E_8$ model, the dynamics at finite temperatures have not been systematically studied even thought its zero-temperature counterpart is known. From the perspective of the material CoNb$_2$O$_6$, our study determines the temperature dependence of the NMR relaxation rate. Our results suggest that NMR experiments at low temperatures provide a concrete and independent test on the the $E_8$ description for CoNb$_2$O$_6$. We note that a numerical analysis of a generalized transverse-field Ising chain suggests that the E8 description survives suitable generalizations of the interactions beyond the nearest-neighbor ferromagnetic coupling [54].

In Sec. 2.1 we introduce the celebrated Zamolodchikov $E_8$ model. In Sec. 2.2 we discuss local dynamics and NMR relaxation rate. In Sec. 2.3 we introduce the low-temperature form factor expansion series. In Sec. 2.4 we gives the leading contributions to the local spin dynamics of the $E_8$ model. In Sec. 2.5 we compares the analytical result with numerical results and have a short discussion. In Appendix. A.1 we gives general relation between $\chi_{yy}(x,t)$ and $\chi_{zz}(x,t)$ in one-dimensional-transverse-field Ising model with the presence of longitudinal field. In Appendix. A.2 we list expressions for the relevant form factors. In Appendices. A.3 and A.4 we give detailed calculation for the leading dynamical structure factor. In Appendix. A.5 we give detailed calculation for the local dynamical structure factor between one-particle and two-particle states. In Appendix. A.6 we give detailed calculation for the local dynamical structure between two-particle and two-particle states. In Appendix. A.7 we discuss contributions of disconnected parts in the form-factor expansion series.
2.1 Zamolodchikov $E_8$ model

Let’s start with the Hamiltonian

$$H_Z = -J \left( \sum_i \sigma_i^z \sigma_{i+1}^z + g \sum_i \sigma_i^x + h \sum_i \sigma_i^z \right)$$  \hspace{1cm} (2.1)

where $\sigma_i^x$ and $\sigma_i^z$ are the Pauli matrices associated with the spin components $S^\mu = \sigma^\mu/2, (\mu = x,y,z)$, $i$ marks site positions, and $g$ and $h$ are respectively the transverse and longitudinal fields in unit of the nearest-neighbor ferromagnetic exchange coupling $J$ among the longitudinal ($z$) components of the spins. In the absence of the longitudinal field ($h = 0$) the system undergoes a quantum phase transition when the transverse field is tuned across its critical value $g = g_c = 1$ [12]. As is well known, the QCP is described by a 1 + 1-dimensional conformal field theory (CFT) with a central charge $1/2$ [13]. More surprising is what happens when a small longitudinal field $h$ is introduced at the QCP $g = g_c$. Here, the model in the scaling limit can be described by an integrable quantum field theory. This $E_8$ model [14, 15] corresponds to the action

$$A_{E_8} = A_{c=1/2} + h \int \sigma(x) dx.$$ \hspace{1cm} (2.2)

Here, $A_{c=1/2}$ stands for the action of the two dimensional CFT with central charge $1/2$, $h$ has scaling dimension $15/8$, and $\sigma(x)$ is a primary field with scaling dimension $1/8$. This describes a scattering theory of eight massive particles, which we will denote by $a, b, c, d, e, f, g, h$ from the lightest to the heaviest. The mass of the lightest particle, $\Delta_a$, scales with the longitudinal field as $\Delta_a \approx 4.405 |h|^{8/15}$ [55]. The mass of the
second lightest particle $\Delta_b$ is equal to $\Delta_a$ multiplied by the golden ratio $(\sqrt{5} + 1)/2$. These two particles are clearly separated from the two-particle continuum, which appears at energies above $2\Delta_a$.

2.2 Local dynamics and NMR relaxation rate

We focus on the local dynamical structure factor (DSF) of the $E_8$ model in the low frequency and low temperature limit: $\omega \ll \Delta_a$ and $T \ll \Delta_a$ (hereafter we set $\hbar = 1$ and $k_B = 1$).

A useful means to probe the local DSF is via NMR. The NMR relaxation rate is given by [56]

$$\frac{1}{T_1^\alpha} = \frac{1}{2N} A^2 \sum'_\beta S_{\beta\beta}(\omega_0). \quad (2.3)$$

Here, $\alpha$ and $\beta$ label the principal axes, and the prime on the summation is over the principal axes perpendicular to the field orientation $\alpha$; $T_1^\alpha$ is the spin-lattice relaxation time, $N$ is the number of ions per unit cell, and $\omega_0$ is the nuclear resonance frequency which is much smaller than the typical electronic energy scales. In addition, $A$ describes the hyper-fine coupling between the spins of the nucleus and the electron; while this coupling depends on the wavevector $q$, this dependence is generically smooth and we will take it as a constant. We will consider the static field of the NMR setup to be the transverse field, $\alpha = x$, which can cause the rotation of the nuclear spin around $x$ axes leading to linear response along $y$ and $z$ directions, as it’s illustrated in the Fig. (2.2). Correspondingly, the local DSF of interest to NMR is
Figure 2.2: Above figure illustrates the NMR measurements. The red arrow in the figure denotes a local nuclear spin, where we only draw out one for simplicity. A pulse of $x$-direction magnetic field is applied to a local site, which frequency is tuned to resonant with splitting energy levels of Zeeman effect due to the coupling between the nuclear spin and the longitudinal magnetic field. This pulse can cause the transition of the nuclear spin from its ground state to an excited state. However the excited nuclear spin will relax to its ground state due to the hyperfine coupling between nuclear and electronic spins surrounded. The relaxation rate can be calculated following Fermi Golden rule, which result turns out to be Eq. (2.3) [56].

given by $S_{zz}(\omega_0) + S_{yy}(\omega_0)$. As shown in Appendix A.1, for the model we consider,

\[
C_{yy}(t) = (-1/4)\partial^2 C_{zz}(t)/\partial t^2,
\]

where the two spin correlator $C_{\beta\beta}(t) = \langle \sigma^\beta(t)\sigma^\beta(0) \rangle_T$, with $\beta = y, z$. This implies $S_{yy}(\omega) = \omega^2 S_{zz}(\omega)/4$ since $S_{\mu\nu}(\omega) = \int_{-\infty}^{\infty} C_{\mu\nu}(t)e^{i\omega t}dt$. Thus in the low-frequency regime of interest here, $S_{yy}(\omega)$ is negligible compared with $S_{zz}(\omega)$. In the following, we will therefore only consider $S_{zz}$.

We now turn to the calculation of $S_{zz}(\omega)$ through a systematic form factor expansion. Because the excitation spectrum has a gap, in the low temperature and low frequency limit we expect that the leading contributions will be from those associated with the few particle states of the lightest particles. Indeed, we will show below that the dominant contribution comes from the two 1-particle states of the lightest
particle, which we calculate analytically. This conclusion is confirmed by a numerical calculation for contributions that extend to higher orders.

2.3 The form factor series

Integrable field theory techniques made possible the analytic calculation of matrix elements of local observables in the asymptotic scattering state basis, called form factors. The asymptotic states are eigenstates of the energy and momentum operators. In terms of the rapidities \( \{ \theta_i \} \) of the particles, the energy and momentum eigenvalues of the eigenstate \( | \theta_1^{\alpha_1}, \cdots, \theta_n^{\alpha_n} \rangle \) (\( \{ \alpha_1, \cdots, \alpha_n \} \) denote different types of particles) are

\[
E = \sum_{i=1}^{n} \Delta_{\alpha_i} \cosh(\theta_i), \quad (2.5)
\]

\[
P = \sum_{i=1}^{n} \Delta_{\alpha_i} \sinh(\theta_i). \quad (2.6)
\]

We denote by \( F_n^\sigma(\theta_1, \cdots, \theta_n) \) the form factors of the primary field \( \sigma(x, t) \) in the \( E_8 \) model (c.f. Eq. (2.2)) between the vacuum and an \( n \)-particle asymptotic state,

\[
F_n^\sigma(\theta_1^{\alpha_1}, \cdots, \theta_n^{\alpha_n}) = \langle 0 | \sigma(0, 0) | \theta_1^{\alpha_1}, \cdots, \theta_n^{\alpha_n} \rangle. \quad (2.7)
\]

The few-particle form factors are explicitly known [16, 57, 58] and have been used to calculate the static spin-spin correlations of the \( E_8 \) model in the ground state [16, 57]. Here we study the finite-temperature dynamics by low-temperature expansion series for integrable field theory [59, 60].

The finite temperature two-point correlation function is given by

\[
C(t, x) = \text{Tr} \left[ \frac{e^{-H/T}}{Z} \mathcal{O}(t, x) \mathcal{O}^\dagger(0, 0) \right], \quad (2.8)
\]
where $Z = \text{Tr} e^{-H/T}$ is the partition function, and we are interested in the local observable operator $\mathcal{O}(t, x) = \sigma(t, x)$. The corresponding DSF is

$$S(\omega, q) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dt \, C(t, x)e^{i\omega t - iqx},$$

(2.9)

We insert the complete set of asymptotic states between the operators, yielding a double sum,

$$C(t, x) = \sum_{r,s} C_{r,s}(t, x),$$

where

$$C_{r,s}(t, x) = \sum_{\{\theta_j\}, \{\theta'_j\}} \int d\theta_1 \cdots d\theta_r \int d\theta'_1 \cdots d\theta'_s e^{-\beta E_r}
\times e^{-i(E_s - E_r)} e^{-i(P_s - P_r)x} \langle \theta_1^{a_1} \cdots \theta_r^{a_r} | \mathcal{O} | \theta'_1^{a'_1} \cdots \theta'_s^{a'_s} \rangle^2,$$

(2.10)

with $E_n = \sum_{i=1}^{n} \Delta_{\alpha_i} \cosh \theta_i$, $P_n = \sum_{i=1}^{n} \Delta_{\alpha_i} \sinh \theta_i$.

We use the same set of states to write the partition function as

$$Z = \sum_{n=0}^{\infty} Z_n,$$

where

$$Z_n = \sum_{\{\theta_j\}} \int d\theta_1 \cdots d\theta_n e^{-\beta E_n} \langle \theta_1^{a_1} \cdots \theta_n^{a_n} | \theta_1^{a_1} \cdots \theta_n^{a_n} \rangle.$$

(2.11)

In infinite volume all the $Z_n$'s contain singularities associated with the scalar product of two momentum eigenstates with identical rapidities. Similarly, for the observables we are calculating, $C_{r,s}$ also diverge due to the kinematical poles of the form factors whenever two rapidities in the two sets coincide, $\theta_i = \theta'_i$ [59]. However, the double sums can be re-organized such that the aforementioned singularities cancel each other [60],

$$C(t, x) = \sum_{r,s=0}^{\infty} D_{r,s}(t, x),$$

(2.12)
where

\[ D_{0,s} = C_{0,s} , \quad (2.13) \]

\[ D_{1,s} = C_{1,s} - Z_1 C_{0,s-1} , \quad (2.14) \]

\[ D_{2,s} = C_{2,s} - Z_1 C_{1,s-1} + (Z_1^2 - Z_2) C_{0,s-2} , \quad (2.15) \]

\[ \ldots \text{etc.} \]

The natural small parameter in the series (2.12) is \( e^{-\Delta_a/T} \). At low frequencies, the energy conserving Dirac-deltas in the Fourier transform Eq. (2.9) force the two states appearing in the form factors to have nearly equal energy, \( E_r = \omega + E_s \). The magnitude of the Boltzmann factor is then set by the sum of the masses in the "heavier" state, i.e.,

\[ D_{r,s} \sim \exp \left\{ -\frac{1}{T} \max \left[ \sum_{i=1}^{r} \Delta_i , \sum_{i=1}^{s} \Delta_i \right] \right\} . \quad (2.16) \]

Thus, in the regime of interest \( (T/\Delta_a \ll 1 \text{ and } \omega/\Delta_a \ll 1) \), the expansion series in Eq. (2.12) is a good perturbation series. In this regime, we can safely truncate the series beyond the terms up to the order of \( e^{-2\Delta_a/T} \). Simple counting implies that we only need \( D_{0,1}, D_{1,0}, D_{0,2}, D_{2,0}, D_{1,1}, D_{1,2}, D_{2,1}, D_{2,2} \) with highest particles, which we now determine. We also note that the series for the two-point correlator \( \text{per se} \) contain a \( \delta(\omega) \) piece, which are however absent in the connected correlation function of interest here (c.f. Appendix A.7).
2.4 Leading contributions of the local spin dynamics

$D_{0,1}$ is the channel between vacuum and one-particle asymptotic in state, and is equal to $C_{0,1}$ from Eq. (2.13). The corresponding contribution to DSF is

$$S_{0,1}(\omega, q) = 2\pi |F_1^\sigma|^2 \int d\theta \delta(q - \Delta_1 \sinh \theta) \delta(\omega - \Delta_1 \cosh \theta), \quad (2.17)$$

where $\Delta_1$ is the mass of a single particle state, and the one particle form factor $F_1^\sigma(\theta)$ is rapidity independent [16]. Since $\cosh \theta \geq 1$ always holds, for the parameter regime $\omega < \Delta_a$ the terms $S_{0,1}$ and $S_{1,0}$ do not contribute. Similarly, the $D_{0,r}$ and $D_{r,0}$ terms for general $r$ and $s$ also vanish.

The first non-trivial contribution is given by connected parts in $D_{1,1}$, i.e. the term coming from the 1-particle – 1-particle form factors, for which we obtain (c.f. Appendix A.3)

$$S_{1,1}(\omega, q) = \frac{|F_2^\sigma(\alpha + i\pi, 0)|^2 (e^{-\beta \Delta_1 \cosh \theta_+} + e^{-\beta \Delta_1 \cosh \theta_-})}{\Delta_1 \Delta_2 |\sinh \alpha|}, \quad (2.18)$$

where $\Delta_1$ and $\Delta_2$ are the masses of the 1-particle states, $\alpha = \arccosh[(\Delta_1^2 + \Delta_2^2 - (\omega^2 - q^2))/(2\Delta_1 \Delta_2)]$ and $\cosh \theta_\pm = [\omega(\Delta_1^2 - \Delta_2^2 + \omega^2 - q^2) \pm 2q\Delta_1 \Delta_2 \sinh \alpha]/[2\Delta_1(q^2 - \omega^2)]$, and from now on the symbols to denote types of particles in the form factor are dropped for convenience (Eq. (2.7)).

The corresponding local DSF is $S_{1,1}(\omega) = \int_{-\infty}^{\infty} S_{1,1}(q, \omega) dq$. Eq. (2.16) implies that, up to $e^{-2\Delta_a/T}$, we need only to consider the channels $a - a$, $b - b$ and $c - c$, as well as $a - b$, $a - c$, $b - c$. When $\Delta_1 = \Delta_2 = \Delta_i$ ($i = a, \ldots, h$),

$$S_{1,1}(\omega)|_{\Delta_1 = \Delta_2 = \Delta_i} = \int_{\omega}^{\infty} f(q, \omega)e^{-\frac{\Delta_i}{T}g(q, \omega)} dq \quad (2.19)$$
with \( f(q, \omega) = \frac{2}{\Delta T} |F^2_{\omega}(\alpha + i\pi, 0)|^2 / |\sinh \alpha| \) and \( g(q, \omega) = -\frac{\omega}{2\Delta} + \frac{q}{2\Delta} \sqrt{1 + \frac{4\Delta^2}{\Delta^2 - \omega^2}} \). We can expand the result for small \( \omega \). With the details given in Appendix A.4), we find the result to leading order:

\[
S_{1,1}(\omega)|_{\Delta_1=\Delta_2=\Delta_a} \approx \left\{ \begin{array}{ll}
\frac{2|F^2_{\omega}(\pi,0)|^2}{\Delta_a} e^{-\Delta_a/T} \left\{ -\ln \frac{\omega}{4T} - \gamma_E + \cdots \right\} & (\omega \ll T \ll \Delta_a) \\
\frac{2|F^2_{\omega}(i\pi,0)|^2}{\Delta_a} e^{-\Delta_a/T} \left\{ \sqrt{\frac{T}{\omega}} - \sqrt{\frac{\pi^2}{4}} \left( \frac{T}{\Delta_a} \right)^{3/2} + \cdots \right\} & (T \ll \omega \ll \Delta_a) 
\end{array} \right.
\]

(2.20)

where \( \gamma_E \) is the Euler constant. (The same form applies to the contributions by the other particles \( b, \cdots, h \), which are suppressed by their thermal factors.) In deriving this expression, we have replaced \( \alpha(\omega, q) \) by \( \alpha(\omega = 0, q = 0) \); this is because the dominant contribution comes from the minimum of the energy dispersion at small momentum, and is well supported by the numerical calculation carried out without this replacement (see below).

We observe that the finite-T local structure factor is logarithmically divergent as \( \omega \to 0 \). This divergence, however, differs from the diffusion form \([61]\) of inverse square may not be too surprising given that the total \( S_z \) is not conserved here. When \( \Delta_1 \neq \Delta_2 \), the denominator in the integrand of Eq. (2.18) does not have any singularity so there will be no divergence.

Next, we consider \( D_{1,2} + D_{2,1} \), the terms with a one-particle and a two-particle state. Up to the order \( O(e^{-2\Delta_a/T}) \), we focus on the case when all three particles are the lightest \( a \) particle (other possible channels \( aa - b \) and \( aa - c \) are similar), which
Figure 2.3: The NMR relaxation rate as a function of temperature. The frequency is chosen to be $\omega/\Delta_a = 0.001$. The temperature dependence is well described by $\Delta_a S(T) = 631e^{-\Delta_a/T}$. The inset picture shows that channels other than $a-a$ give negligible contributions.

we find to be (Appendix A.5),

$$S_{(1,2)+(2,1)}(\omega, q) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\theta e^{-\beta \Delta_a \cosh \theta} \sqrt{(f(\tilde{\omega}, \tilde{q}, \theta) - 1)^2 - 1}$$

$$\cdot F_3^\sigma (\theta + i\pi, \ln x_+, \ln x_-) F_3^\sigma (\theta + i\pi, \ln x_-, \ln x_+) \, , \quad (2.21)$$

where

$$x_\pm = \frac{1}{2}(\tilde{\omega} + \cosh \theta + \tilde{q} + \sinh \theta) \left( 1 \pm 2\sqrt{1 - 2/f(\tilde{\omega}, \tilde{q}, \theta)} \right) \, , \quad (2.22)$$

and $f(\tilde{\omega}, \tilde{q}, \theta) = [(\tilde{\omega} + \cosh \theta)^2 - (\tilde{q} + \sinh \theta)^2]/2$ with $\tilde{\omega} = \omega/\Delta_a$ and $\tilde{q} = q/\Delta_a$. Our analysis (Appendix A.5) shows no contributions from the range $\tilde{\omega} > \tilde{q} \geq 0$, where $\cosh \theta \sim 1/\tilde{\omega} \gg 1$. In the range $\tilde{\omega} \leq \tilde{q}$, we have $\cosh \theta \gtrsim 2 - \tilde{\omega}$, indicating there exists a small region of $\tilde{q}$ where $\cosh \theta$ is slightly smaller than 2. This contribution is expected to be small, and we confirm this by including the channels $D_{1,2} + D_{2,1}$ in
our numerical calculation shown below.

For connected parts in $D_{2,2}$, a similar Jacobian will appear as in the calculation of the equal mass case of Eq. (2.19), and we will encounter the same logarithmic divergence in the frequency dependence. We find that singular terms beyond the logarithmic divergence are absent (c.f. Appendix A.6). This contribution is therefore suppressed by the thermal weight $e^{-2\Delta_a/T}$. Low-frequency divergences are also expected to come from the $D_{nn}$ terms (at $n > 2$) with particles of the same mass in the two asymptotic states of the form factors. The fact that $D_{22}$ with the same particle does not contain singularities stronger than $\log \omega$ is a strong indication that none of the higher terms in the series will give a stronger (e.g. power-law) singularity. We conjecture that the $D_{nn}$ terms at $n > 2$ contain a similar logarithmic singularity in the frequency dependence, which are then also negligible compared to $D_{11}$ due to the stronger thermal suppression factor.

2.5 Numerical analysis and discussions

**Numerical analysis** — Fig. 2.3 shows the results and fit for the NMR relaxation rate as a function of temperature in the temperature range $\Delta_a/T \in [10, 100]$ at fixed low frequency $\omega/\Delta_a = 0.001$ in the typical temperature range of the NMR experiments ($\omega/\Delta_a \ll T/\Delta_a$). The fitting function $\Delta_a S(T) = 631e^{-\Delta_a/T}$ indicates that the behavior of relaxation rate at low frequency and low temperature region is dominated by the $a - a$ channel, as it’s clearly shown in the inset of Fig. 2.3. The
prefactor 631 compares well with the analytical expression associated with $S_{1,1}$ of the lightest $a$-particle: since $2|F^q_2(\alpha(\omega = 0) + i\pi, 0)|^2_{\Delta_1=\Delta_2=\Delta_a} \approx 130$.

We also study the frequency dependence of the local DSF at fixed temperatures for $T, \omega \ll \Delta_a$. Fig. 2.4 shows the result at fixed temperature $T/\Delta_a = 0.05$ with $\omega/\Delta_a$ changing from 0.001 to 0.01. It is well fitted as $10^7 \Delta_a S(\omega) = -5.28 - 2.48 \ln(\omega/\Delta_a)$, which is in accordance with the asymptotic form Eq. (2.20). When comparing our results with experiments on real material of lattice spins, the prefactor should be modified as $\sigma_{\text{lattice}}(x) = 0.783(3)\sigma(x)$ [16,62].

Discussion.— We conclude that the temperature dependence of the NMR relaxation rate is given by

$$\frac{1}{T_1} \approx \frac{b}{2N} A^2 e^{-\Delta_a/T}; \quad \Delta_a \approx 4.405 |\hbar|^{8/15} \tag{2.23}$$

with the prefactor $b \approx \ln(4T/\omega_0) - \gamma_E$. 
We next consider the implications of our results for CoNb$_2$O$_6$. The neutron scattering experiments provided evidence for the two lightest particles of the $E_8$ spectrum in CoNb$_2$O$_6$ [53]. This has been understood by considering the effect of the inter-chain coupling in the three-dimensionally ordered state as inducing a longitudinal field [53, 63]. In order to further test the $E_8$ description, measuring the temperature dependence of the spin dynamics would be invaluable. Our study here provides a concrete prediction of the temperature-dependence of the NMR relaxation rate in the $E_8$ model. We therefore propose that the NMR relaxation rate provides the desired further test of the applicability of the $E_8$ model to CoNb$_2$O$_6$. During the final stage of writing the present manuscript, an NMR experiment in CoNb$_2$O$_6$ has been reported in the higher-temperature quantum critical regime [9]; measurements of the NMR relaxation rate at the lower-temperature $E_8$ regime should therefore be feasible.
Chapter 3

Thermodynamics near quantum critical point in itinerant spin-density-wave systems

One class of QCPs which has been under extensive theoretical and experimental studies is the itinerant magnetic QCP identified in many transition metal oxides and intermetallic heavy fermion compounds. In these studies, thermodynamics has been playing an important role in elucidating the quantum critical properties. It has been shown that the entropy has a more singular dependence on the non-thermal tuning parameter than on the temperature. As a result, the Grüneisen ratio, the ratio between the thermal expansion and the specific heat, diverges at a generic QCP. For QCPs tuned by a magnetic field, the equivalent divergent quantity is the magnetocaloric effect (or magnetic Grüneisen ratio [3,64]). In addition, the Grüneisen ratio changes sign at the transition point, which implies that the entropy reaches a maximum value near QCP. [4] These thermodynamic signatures have been serving as a sensitive probe to identify and classify QCPs, which indeed have been confirmed by experiments on a class of quantum critical materials. [8,24,65] The entropy accumulation also implies that the quantum critical state is susceptible to an ordered state which can reduce the entropy, such as a superconducting state or the symmetry broken state in Sr$_3$Ru$_2$O$_7$, arising as a dome-structure near the presumed QCPs.
These thermodynamic signatures have been derived from the hyperscaling analysis to QCPs [4]. Specifically, if we assume the system’s critical behavior is governed by correlation lengths $\xi$ and $\xi_r$ (cf. Sec.1.1 in Chap.1), then the critical free energy density, $F_{cr} = F - F_{reg}$, can be written into following single-variable scaling form (hyperscaling),

$$\frac{F_{cr}}{V} = -\rho_0 r^{\nu(d+z)} \tilde{f} \left( \frac{T}{T_0 r^{\nu z}} \right) = -\rho_0 \left( \frac{T}{T_0} \right)^{(d+z)/z} f \left( \frac{r}{(T/T_0)^{1/(\nu z)}} \right)$$

(3.1)

where $\rho_0$ and $T_0$ are non-universal constants, while $\tilde{f}(x)$ and $f(x)$ are universal scaling forms. Here, we extend the studies to itinerant magnetic systems, where the hyperscaling relation in general fails. There are some theoretical efforts to develop a proper theory for understanding the itinerant magnetic systems [17–19, 66]. Here we accepted the approach developed by Hertz [17] and Millis [18,19]. In Hertz-Millis approach, the order parameter fluctuations in itinerant magnetic systems have been described by a quantum Landau-Ginzburg theory (QLGT) in terms of paramagnons or spin density waves. [17–19] This is equivalent to an $O(n) \phi^4$ with the effective dimension $d + z$, where $d$ is the spatial dimension and $z$ is the dynamical exponent [Cf. Eq. (3.2)]. This model has been treated by many theoretical methods, including the self-consistent renormalization (SCR) [20, 21] and the perturbative renormalization group (RG) method. It has been shown [22] that when the effective dimension is larger than the upper critical dimension 4, the quartic coupling term $u\phi^4$ [Cf. Eq. (3.4)] is dangerously irrelevant which leads to the failure of the hyperscaling relation. Although we can write down the free energy in terms of a renormalized Gaussian
model, \( u \) contributes to the free energy as corrections to the renormalized control parameter. We notice that in previous perturbative RG approaches, the regularization for the quartic term is not well prescribed, such that there exists a more singular term \( F \sim uT^{(d+z-2)/z} \) to the free energy as corrections to the zero-point fluctuations. Here, we provide a complete account of the perturbative RG procedure to regularize this singular contribution, and we show that it stems from the unphysical renormalization of the zero-point fluctuations and can be systemically canceled out order by order in regularized RG procedure. As a result, we find that the leading contributions to the free energy are given by a renormalized Gaussian model with the zero-point fluctuations subtracted. With this formalism, we carry out numerical calculations on the free energy and various thermodynamic quantities. Our results are exact in the sense that they not only captures the most singular contributions from the critical degrees of freedom, as obtained from the asymptotic analysis, but also contain the subleading and/or non-singular contributions. This is essential in comparison with experimental data for realistic materials.

Some of our results, especially for a 3-dimensional (3D) antiferromagnetic QCP were briefly reported in Ref. [22]. Here, we focus on itinerant ferromagnetic systems, in particular, targeting to understand the quantum critical behaviors of \( \text{Sr}_3\text{Ru}_2\text{O}_7 \). It has been shown [24,67] that this bilayer ruthenate metal is close to the quantum critical end point (QCEP) of a metamagnetic transition, tuned by both the magnetic field and pressure. The most interesting feature of this compound is that a novel
phase develops at the QCEP. While some ingenious pictures such as Pomeranchuk instability and electron nematicity have been proposed, the nature of this order remains unknown. To understand the quantum critical properties associated with this QCEP therefore provides a key to elucidate this order, and in general, how matters reorganize into new phases near QCPs. However, it remains unclear that whether conventional theory on itinerant magnetic QCPs applies to this materials. We therefore compare the thermodynamic properties obtained from both the 3D and the 2D ferromagnetic theoretical models with the experimental results. We find that while the generic features of the experimental results, such as the entropy accumulation effect and the divergence of the specific heat coefficient, are compatible with the thermodynamic signatures of quantum criticality, the detailed critical exponents are not well fitted by either the 3D or the 2D itinerant ferromagnet model. This implies that Sr$_3$Ru$_2$O$_7$ demands a theoretical description beyond the conventional itinerant magnetic criticality.

In Sec. 3.1, we present the quantum Landau-Ginzburg theory for itinerant magnets. In Sec. 3.2, we show the deficit of conventional Gaussian universality, i.e., the singularity from the zero-point fluctuations, and provide a regularized RG procedure to remedy the deficit. In Sec. 3.3, we present detailed numerical results of entropy and the specific heat, illustrating the generic thermodynamic signatures of itinerant magnetic QCPs. In Sec. 3.4, we compare numerical results with experimental results. Some of the technical details are relegated to the appendices. In Appendix B.3 we
provide complete RG equations to the linear order in $u$. In Appendix B.4 we give out explicit expressions for running parameter in quantum Landau-Ginzburg model. In Appendix B.5 we show the cancellation of singular contribution to linear order in $u$. In Appendix B.6, based on our recipe we re-calculate scaling behaviors in the Fermi-liquid regime (FLR) and the quantum critical regime (QCR) for two and three dimensional ferromagnetic systems.

3.1 The quantum Landau-Ginzburg model

As developed by Hertz [17] and refined by Millis [18,19], quantum phase transitions in itinerant magnetic systems are described in terms of $T = 0$ spin-density wave (SDW) transitions and are formulated as the QLGT in terms of a $\phi^4$ model with additional quantum dissipation terms. In this picture, the effective action in terms of the order parameter fluctuations $\vec{\phi}$ can be written as:

$$S[\vec{\phi}] = S^{(0)}[\vec{\phi}] + S^{(2)}[\vec{\phi}] + S^{(4)}[\vec{\phi}],$$

$$S^{(0)}[\vec{\phi}] = 0,$$

$$S^{(2)}[\vec{\phi}] = \frac{1}{2} \sum_{\mathbf{q},i\omega_l} \chi_0^{-1}(\mathbf{q},i\omega_l) \vec{\phi}^T (\mathbf{q},i\omega_l) \cdot \vec{\phi}(-\mathbf{q},-i\omega_l),$$

$$S^{(4)}[\vec{\phi}] = u \int_0^\beta d\tau \int d\mathbf{r} \left[ \vec{\phi}^T (\mathbf{r},\tau) \cdot \vec{\phi}(\mathbf{r},\tau) \right]^2,$$

where

$$\chi_0^{-1}(\mathbf{q},i\omega_l) = r_0 + (q\xi_0)^2 + \frac{|\omega_l|}{\Gamma_q}.$$
Here $r_0$ is bare control parameter which may be a function of pressure or chemical doping. This differs from the classical $\phi^4$ model in the quantum Landau damping term $|\omega_l|/\Gamma_q$ with $\Gamma_q = \Gamma_0(q\xi_0)^{z-2}$, which leads to an effective dimension $d+z$. The dynamical exponent $z$ takes the value of 2, 3 respectively for antiferro- and ferromagnetic spin fluctuations. $\xi_0$ is a microscopic length at the order of $k_F^{-1}$ and $\Gamma_0$ is a microscopic energy scale in the order of Fermi energy $E_F$. $\omega_l$ is a Bosonic Matsubara frequency. For later convenience we further introduce reduced temperature $t \equiv T/\Gamma_0$.

A typical phase diagram for this model is shown in Fig. 3.1(a). Similar to the classical $\phi^4$ model, when $r < 0$, the order parameter takes a finite value, corresponding to a magnetic ordered state; when $r > 0$ ($r$ here is control parameter), the order parameter vanishes, describing a quantum disordered state (a paramagnetic Fermi liquid state for metallic systems). In the quantum model, $r$ is tuned by pressure or chemical doping, e.g., $r = (p - p_c)/p_c$, rather than the temperature in classical phase transitions $r \sim (T - T_c)/T_c$. The quantum phase transition at $T = 0$ therefore characterizes a change in the ground state tuned by non-thermal physical parameters regulating the strength of quantum fluctuations.

The metamagnetic transition, as postulated for Sr$_3$Ru$_2$O$_7$, describes a rapid increase in the magnetization of a materials with a small change in an externally applied magnetic field, and is a first-order phase transition. With the additional tuning of pressure, the transition temperature can be reduced to zero, yielding a quantum critical end-point (QCEP), which is a continuous transition point. The effective di-
mension of this material is larger than upper critical dimension, thus the dominant fluctuation is Gaussian fluctuation. Therefore a mean field theory can be formulated to qualitatively describe the system’s behavior near QCEP. The minimum form of mean field theory including coupling between order parameter and magnetic field is

\[ F[\phi] = \frac{1}{2} r\phi^2 + \frac{1}{4} u\phi^4 + \frac{1}{6} v\phi^6 + H\phi \]  

(3.6)

where all temporal and spatial degrees of freedom are suppressed. In the above theory \( u < 0 \) for the existence of first order transition, and \( v > 0 \) for guaranteeing the stability of the system. At critical end-point the linear, quadratic and cubic-order fluctuations around the minimum of free energy vanish, leaving us irrelevant quartic fluctuations dominant. By fixing \( r, u, v \) at the same values of critical end point and tuning the magnetic field away from the critical magnetic field of the critical end-point, we find that the system regains Gaussian fluctuations around the new minimum with its coefficient (mass) now proportional to \( (H - H_c)^{2/3} \). The above static-mean-field-level analysis qualitatively tells us how the mass depends on magnetic field near the QCEP. We then directly incorporate this mean-field result into above QLGT near the QCEP, by substituting the effective tuning parameter as \( r \sim (H - H_c)^{2/3} \) (Ref. [68]), where \( H \) is strength of the external magnetic field and \( H_c \) is the critical value. In this scenario, the QCP is always approached from the quantum disordered regime, for both \( H > H_c \) and \( H < H_c \), which is illustrated in Fig. 3.1(b).
Figure 3.1: (a) A schematic phase diagram for systems exhibiting itinerant magnetic quantum phase transitions. With the tuning of a control parameter $r$, the system changes from a magnetic ordered state ($r < 0$) to a paramagnetic Fermi liquid state ($r > 0$) at $T = 0$. In the ordered side, there is a line of finite temperature transition which ends at the QCP ($r = 0$). Two characteristic directions approaching the QCP, for which the results are presented in this chapter, are also illustrated: 1) from the quantum disordered (paramagnetic Fermi liquid) regime, by setting $t \ll r^\nu z$ and tuning $r \to 0$; 2) from the quantum critical regime, by setting $r = 0$ and tuning $T \to 0$. (b) shows a schematic phase diagram for a quantum critical end-point of a metamagnetic transition, with Fermi liquid regimes on both sides of the QCP.

### 3.2 A regularized RG procedure for the free energy calculation

The free energy can be calculated from the action, for instance, by a perturbative expansion in orders of $u$. To the linear order, it can be written as

\[
F = F_G + F_u + O(u^2),
\]

\[
F_G = \frac{nT}{2V} \sum_{\omega_n \neq 0} \ln \chi_{0}^{-1}(i\omega_n, \mathbf{q})
\]

\[
= -n \int_{0}^{\Lambda} \frac{d^{d}q}{(2\pi)^{d}} \int_{0}^{\Gamma_q} \frac{d\varepsilon}{2\pi} \coth \frac{\varepsilon}{2T} \tan^{-1} \frac{\varepsilon}{\Gamma_q} \frac{\varepsilon}{r_0 + (q\xi_0)^2},
\]

\[
F_u = un(n + 2)f^2,
\]
with $I = \sum_{i\omega, q} \chi_0(i\omega_l, q) = -\frac{2}{n} (\partial F_G/\partial r_0)$. Here $F_G$ is the contribution from the Gaussian term $S^{(2)}$, and $F$ in Eq. (3.7) is referred to free energy density.

However, such plain expansion in general does not capture correctly the singular behaviors near the critical point. Instead, the perturbative renormalization group method has been introduced to treat this model. The details can be found in, e.g., Ref. [18]. We reproduce some of the results here in Appendix B.3 for easiness of discussions, with some corrected signs and prefactors from previous references. The procedures of the RG approach can be summarized as follows. One takes a scale transformation, $\Lambda \rightarrow \Lambda/b$ with $b > 1$, and integrates out the high-energy/short-wavelength degrees of freedom between $(\Lambda/b, \Lambda)$ to obtain an effective action at the new scale. In general, the new action has the form as the original action but is in terms of renormalized parameters. A set of RG equations describe how the renormalized parameters change with the scale transformation [Cf. Eq.(B.60,B.61,B.62)], from which, the fixed points, in particular, the critical points, can be identified at $b \rightarrow \infty$.

Different physical quantities including the free energy can also be calculated from the RG procedure. In practice, one stops RG flow at $r(b = b_0) = 1$, and integrates out the degrees of the freedom for $b$ from 1 to $b_0$ to obtain the singular contributions from quantum fluctuations to the free energy [Cf. Eq. (B.98)]. The degrees of freedom for $b$ within $(b_0, \infty)$ are classical in nature and can be trivially determined.

In this chapter, we focus our discussions on cases where the effective dimension $d + z$ is larger than the upper critical dimension 4. This is relevant to most realistic itinerant
magnets, i.e., $d > 1$ for ferromagnets with $z = 3$, and $d > 2$ for antiferromagnets with $z = 2$. In this case, the quartic coupling $u(b) \sim ub^{4-(d+z)}$ always decreases with the RG flow, and vanishes at the critical point. Therefore, the quartic coupling is deemed as an irrelevant parameter, and we are left with a Gaussian (quadratic) term with the renormalized control parameter. Various physical quantities can be subsequently determined from the resulting renormalized Gaussian action, where $u$ is present in the correction term for the renormalized control parameter $r(t)$. In the Fermi liquid regime (FLR) or quantum critical regime (QCR), the correlation length is determined respectively as $[18,19,21]$

$$
\xi^{-2} \sim r(t) = r + Au^{(d+z-2)/2}(t/r^{z/2})^2 (FLR), \quad \xi^{-2} \sim r(t) = r + cut^{(d+z-2)/z} (QCR),
$$

(3.10)

where $A$ and $c$ are non-universal constants depending on parameters of specific materials [See Appendix B.4 for details]. In the FLR where $t \ll r^{z/2}$, $u$-dependent correction is much smaller than the control parameter $r$, which determines the correlation length. However, in the QCR where $t \gg r^{z/2}$, the correction term $ut^{(d+z-2)/z}$ becomes dominant and determines the correlation length instead, i.e., $u$ is dangerously irrelevant. The scaling functions for generic physical quantities should be expressed in terms of two variables $f(r/t^{2/z}, ut^{(d+z-2)/z}/r)$. Fig. 3.2 shows the Feynman diagrams for the free energy to the linear order in $u$ (the cross symbol in the figure represent dangerously irrelevant coupling $u$).

Various thermodynamic quantities can be calculated from the free energy. From
Figure 3.2: Feynman diagrams for the bare free energy of the QLGT to the linear order in $u$ in bare loop-perturbative expansion. The cross symbol is used to denote the bare coupling $u$. $F_G$ here is bare Gaussian free energy, and the two-loop diagram represents bare two-loop contribution $F_u$.

The renormalized Gaussian action, it takes the same form as Eq. (3.8), but replacing the bare control parameter $r_0$ with the renormalized one $r(t)$ [see details in Appendix B.3]. It can be written as

$$F_G^R = F_G^{(1)} + F_G^{(2)},$$

$$F_G^{(1)} = -n \int_0^\Lambda \frac{d^d q}{(2\pi)^d} \int_0^{\Gamma_q} \frac{d\varepsilon}{2\pi} \left( \coth \frac{\varepsilon}{2T} - 1 \right) \tan^{-1} \frac{\varepsilon/\Gamma_q}{r(t) + (q/\Lambda)^2},$$  \hspace{1cm} (3.11)

$$F_G^{(2)} = -n \int_0^\Lambda \frac{d^d q}{(2\pi)^d} \int_0^{\Gamma_q} \frac{d\varepsilon}{2\pi} \tan^{-1} \frac{\varepsilon/\Gamma_q}{r(t) + (q/\Lambda)^2},$$  \hspace{1cm} (3.12)

where we have explicitly separated the contributions into two terms. When $T \to 0$, it can be easily verified that $F_G^{(1)} \to 0$ and $F_G^{(2)} \to const$. The latter can also be viewed as the zero-point fluctuation contributions to the free energy at the Gaussian level. The renormalized Gaussian free energy is illustrated by the single closed loop in Fig. 3.2.

For $F_G^{(1)}$, it is found that the $u$-dependent terms are always subleading in the free energy, while the leading contribution satisfies the hyperscaling relation. In terms of
the scaling functions, we can write the results as

$$F_G^{(1)} = t^{ \frac{d+z}{z}} \int \left( \frac{r}{t^{2/z}} \right) \approx t^{ \frac{d+z}{z}} f'_F \left( \frac{r}{t^{2/z}} \right) \sim \begin{cases} t^2 r^{(d-z)/2} & t \ll r^{2z/2} (FL) \\ t^{(d+z)/z} & t \gg r^{2z/2} (QC) \end{cases} \quad (3.13)$$

For $F_G^{(2)}$, we notice that its temperature dependence only comes from the correction term in the renormalized control parameter $r(t)$, and find that

$$F_G^{(2)} \sim \begin{cases} \text{const.} + ut^2 r^{(d-z-2)/2} & t \ll r^{2z/2} (FL) \\ \text{const.} + ut^{(d+z-2)/z} & t \gg r^{2z/2} (QC) \end{cases} \quad (3.14)$$

The detailed calculations are presented in Appendix B.5. Here, we demonstrate that the above results can be easily obtained from the relation:

$$F_G^{(2)}[r(t)] \approx F_G^{(2)}(r) + \left. \frac{\partial F_G^{(2)}[r(t)]}{\partial r} \right|_{r(t)=r} [r(t) - r], \quad (3.15)$$

where the first term is the zero-point fluctuation term in the bare Gaussian action (a constant), and the second term comes from the renormalization correction to the control parameter. In the quantum critical regime, we find that $ut^{(d+z-2)/z}$ is in fact more singular than the leading terms in $F_G^{(1)}$. Similarly, in the Fermi liquid regime, although the temperature dependence $t^2$ is the same as in $F_G^{(1)}$, the prefactor $r^{(d-z-2)/2}$ is more singular when $r \to 0$. Most literatures have neglected the singular contribution from $F_G^{(2)}$ without explicit explanation.

The only papers which have discussed this contribution are Refs. (69), (70) following SCR calculation, which is finally cured in Ref. [70] in the framework of SCR. Here beyond the framework of SCR we shall show that the unphysical singular term
in $F_G^2$ is naturally canceled by the singular term from two-loop RG calculation [c.f. Appendix B.5]. With this "natural" cancelation we present a recipe for this theory in Eq. (3.20).

We discuss the origin and provide a remedy for this singular term. We can trace the emergence of this singularity to two aspects, the correction to the renormalized control parameter from the dangerously irrelevant quartic coupling, and its subsequent correction to the zero-point fluctuation of the free energy. The former is determined by the quantum to classical crossover $r(b_0) = 1$, or the length scale is compatible with the correlation length $b(\Lambda \xi) \sim 1$. Such corrections are accumulated as long as the RG starts to flow, i.e., it stems from the high-energy or ultraviolet physics [see details at the end of Appendix B.5]. In this energy range, there is also a residual contribution to the free energy from the two-loop diagram $F_u$ [Cf. Fig. (3.1)], as shown in Appendix B.5. In other words, a complete RG procedure should include all contributions in each order of $u$: to the linear order, it is therefore necessary to consider the renormalization of $F_u$ as well. As shown in Appendix B.3, the RG equation for the free energy by including the renormalization of $F_u$ can be written as

$$\frac{dF(b)}{d\ln b} = (d + z)F(b) - \left(\frac{1}{2}nNT^* f^{(0)}(b) - 2n(n + 2)(NT^*)^2 u(b)h(b)f^{(2)}(b)\right)$$
from which we obtain the free energy

\[ F = F_{RG}^G(t, r(t)) + F_{RG}^u(t, r(t)), \]

\[ F_{RG}^G(t, r(t)) = \frac{1}{2} nNT^* \int_{\ln b}^{\ln b} e^{-(d+z)x} f^{(0)}(te^{xx}, r(e^{x})e^{x/\nu})dx, \tag{3.16} \]

\[ F_{RG}^u(t, r(t)) = -2n(n + 2)(NT^*)^2 u \int_{\ln b}^{\ln b} e^{(4-2(d+z)x)h(te^{xx}, r(e^{x})e^{x/\nu})f^{(2)}(te^{xx}, r(e^{x})e^{x/\nu})dx, \tag{3.17} \]

where \( f^{(0)}, f^{(2)}, \) and \( h \) are given in Eqs.(B.64,B.65,B.91) respectively, \( b \to \infty, \) and \( T^* \) is a microscopic energy scale which is expected to be of the order of \( \Gamma_0. \) Here we set \( T^* = \Gamma_0. \) A two-loop diagram is used to illustrate \( F_{RG}^u \) in Fig. 3.2.

\( F_{RG}^G(t, r(t)) \) has been evaluated earlier, where we show that it contains a regular contribution \( F_{G}^{(1)} \) and a singular contribution \( F_{G}^{(2)} \). We evaluate \( F_{RG}^u \) in Appendix B.5, and find that the leading contribution is, e.g., in the quantum critical regime

\[ F_{RG}^u \sim -ut^{(d+z-2)/z}, \tag{3.18} \]

which is in the same form as the singular term in \( F_{G}^{(2)} \) but with an opposite sign, i.e., it exactly cancels out the singularity [c.f. Appendix B.5]. We therefore reach the conclusion that the leading contributions to the free energy to the linear order in \( u \) is given by \( F_{G}^{(1)}. \) This is the renormalized Gaussian contribution with the zero-point fluctuation subtracted.

The above calculation implies that in the renormalization procedure, we have absorbed an unphysical contribution to the zero-point fluctuations. In the perturbative expansions in terms of the bare parameters, the zero-point fluctuation part of the free
energy can also be expanded as

\[
F_{ZP} = F_{ZP}^{(0)}(r_0) + u F_{ZP}^{(1)}(r_0) + O(u^2)
\]

\[
F_{ZP}^{(m)}(r_0) = c_0^m + c_1^m r_0 + c_2^m r_0^2 + \ldots
\]

(3.19)

The zero-point fluctuation does not contribute to thermodynamics, as it is independent of the temperature. In the RG procedure, as the control parameter acquires a temperature-dependent correction, the renormalized zero-point fluctuation term becomes temperature dependent, for instance, the singular term \( c_1^0 r(T) \) as in \( F_G^{(2)} \).

However, we observe that in a complete RG procedure, by examining all terms in the same order of \( u \), these singular terms can cancel out each other [c.f. Appendix B.5]. We have shown in Appendix B.3 that this is valid in the linear order in \( u \) and we expect this cancellation to follow order by order. In other words, the regularized calculation to the free energy should be on \( F(t, r(t)) - F(0, r(t)) \), with the zero-point fluctuation term subtracted.

To the linear order in \( u \), we therefore find that the free energy is given by \( F_G^{(1)} \), i.e.,

\[
F/V \approx F_G^{(1)} = -n \int_0^\Lambda \frac{d^d q}{(2\pi)^d} \int_0^{\Gamma_q} \frac{d\varepsilon}{2\pi} \left( \coth \frac{\varepsilon}{2T} - 1 \right) \tan^{-1} \frac{\varepsilon/\Gamma_q}{r(t) + (q/\Lambda)^2}
\]

(3.20)

which we evaluate in the next section.
3.3 Results of thermodynamic quantities for the quantum critical itinerant ferromagnets

We proceed to calculate the thermodynamic properties of itinerant ferromagnets near quantum phase transitions based on the regularized RG procedure. We focus on the entropy and the specific heat coefficient, which we intend to compare with experimental results. Other thermodynamical quantities, such as thermal expansion (magnetization), and the Grüneisen ratio (magnetocaloric effect) can also be easily calculated from the free energy.

As discussed above, the regularized contribution to the free energy can be determined from $F_G^{(1)}$ [Cf. Eq.(3.20)]. This renormalized Gaussian model has been calculated in Ref. [22], and its scaling behavior has been analyzed by analytic methods. In Appendix B.6, we repeat these calculations for the itinerant ferromagnets. In particular, we provide the exact expressions for the universal constants, which have never been published.

However, when we compare with the experimental results for realistic materials, especially when physical parameters slightly deviate from the scaling region, we need not only to capture the leading and/or scaling behaviors, but also the subleading and/or non-singular contributions. We therefore perform an exact numerical calculation on the free energy given by Eq. (3.20). In Appendix B.5, we also show that this is equivalent to the Gaussian part from the RG procedure $F^{RG}(r(t), t) - F^{RG}(r(t), 0)$, where $F^{RG}$ is given in Eq. (B.99). In practice, we firstly input a set of initial values of
temperatures and bare control parameters, then for each pair of initial temperature
and bare parameter, we determine the renormalized control parameter \( r(t) \) which is
a functional integral of \( r(b) \) from Eqs.(A2) and (A6). We iterate this equation until
the self-consistency is achieved (to a precision of \( 10^{-16} \)). Subsequently, we input the
obtained renormalized control parameter \( r(t) \) into \( F_{\text{RG}}(r(t), t) - F_{\text{RG}}(r(t), 0) \) (which
is just Eq. (3.20)) to calculate the free energy, and various thermodynamic quantities.

Our results for the entropy for 2D and 3D itinerant ferromagnets are shown in
Figs. (3.3,3.4) respectively. We choose two characteristic directions approaching the
QCP, by setting a small temperature (e.g. \( t = 1/100 \)) and varying \( r \to 0 \) from
the Fermi liquid regime, and by setting \( r = 0 \) and varying \( T \to 0 \) in the quantum
critical regime. The results for these two directions are respectively shown in the
left and the right panels. We also set the component \( n = 2, u = 1/200(2DFM), \) and
\( u = 1/100(3DFM) \). For each figure, we also provide the fitting curves from the scaling
functions.

For the 2D itinerant ferromagnet case[Fig.(3.3)], we find that in the Fermi liquid
regime, the scaling form \( S/t = a + b(r_0 + c)^{-1/2} \) fits the data pretty well in the
range \( r_0 = (0.1, 0.9) \), where \( a \) captures the background FL contribution and \( c \) is
the constant piece of the correction to the bare control parameter from \( u \). Here the
exponent \(-1/2\) is universal, as given by \( r^{(d-z)/2} \), while \( a, b, \) and \( c \) are non-universal as
they depend on specific parameters. In the quantum critical regime, the scaling form
\( S/t = a' + c't^{-1/3} \) fits well the numerical results in small \( T \) region while noticeable
deviations are observed as \( t \to 1 \). For the 3D itinerant ferromagnet case[Fig.(3.4)], we find that similarly the leading behaviors of \( S/t \) near the QCP are given by the scaling forms \( S/t = a + b \ln[1+1/(r_0+c)] \) and \( S/t = a' + b' \ln(1/t) \), in the FL and QC regimes, respectively. When the next order correction to the scaling function is included in the fitting for both systems, we find that it fits better with numerical data through the whole range of temperature. The agreement between the numerical results and the fitting formulas indicate that the leading contributions to the free energy in the 3D and 2D ferromagnets follow the scaling relations. This is partly due to the fact that the background FL contributions, \( S/t = a \), are subleading compared to those from critical degrees of freedom, which however is not valid for 3D antiferromagnets.

The above results are consistent with the generic thermodynamic features of quantum criticality obtained from the hyperscaling analysis, e.g., the entropy accumulation effect: the entropy reaches a maximal value near \( r = 0 \) for a given temperature. For \( d \leq z \), we also expect \( S/T \) and \( C_v/T \) to be divergent. The exponent associated with this divergence serves as a classification of QCPs. These signatures can therefore be employed to probe and classify QCPs in itinerant magnetic systems, which we proceed for a specific material \( \text{Sr}_3\text{Ru}_2\text{O}_7 \).

### 3.4 Comparison to the experimental data of \( \text{Sr}_3\text{Ru}_2\text{O}_7 \)

In this section, we explore whether \( \text{Sr}_3\text{Ru}_2\text{O}_7 \) can be described by a quantum critical itinerant ferromagnet. We will introduce some experimental facts on this material.
Figure 3.3: Entropy near the 2D itinerant ferromagnetic QCP. The left panel shows it as a function of the bare control parameter at a fixed temperature $t = 1/100$ in Fermi liquid regime. The fitting result is $S/t = -0.209 + 0.466(r_0 + 0.037)^{-1/2}$. The right panel shows it as a function of temperature in quantum critical regime with $r_0 = 0$. The fitting result without critical correction is $S/t = -0.4546 + 0.5192 t^{-1/3}$ (red), and the fitting result with critical correction is $S/t = -0.64007 + 0.609t^{-1/3} + 0.126t$ (green). All results are based on $u = 1/200$

We then show experimental data on thermodynamic properties, and argue that they are consistent with the thermodynamic signatures of quantum criticality. We perform two types of analysis on the data, to firstly fit them with the scaling behaviors of itinerant ferromagnets in different regimes, and further directly compare them with our numerical results.

3.4.1 Metamagnetic transition and quantum critical end point in Sr$_3$Ru$_2$O$_7$

Sr$_3$Ru$_2$O$_7$ is a bilayer perovskite strontium ruthenate among the family Sr$_{n+1}$Ru$_n$O$_{3n+1}$. It is found to be a paramagnetic metal on the verge of ferromagnetism. Under a strong
Figure 3.4: Entropy near the 3D itinerant ferromagnetic QCP. The left panel shows it as a function of the control parameter at a fixed temperature $t = 1/100$ in the Fermi liquid regime. The fitting curves are $S/t = 0.034 + 0.031 \ln(1/(r_0 - 0.044))$ (red) and $S/t = 0.001 + 0.052 \ln(1 + 1/(r_0 + 0.013))(green)$ which come from RG results Eq. (B.135) and Eq. (B.134) respectively. We notice that the later fitting formula, which is able to capture the correction to the shift of the control parameter, provides a better overall fitting to the scaling behavior than the previous one. The right panel shows the entropy as a function of temperature in the quantum critical regime, with $r_0 = 0$ and varying $T$. The fitting result with the leading critical term is $S/t = 0.002 + 0.041 \ln(1/t)(red)$, and the fitting result with also the subleading contribution is $S/t = -0.005 + 0.043 \ln(1/t) + 0.019t^{4/3}(green)$. All results are shown for $u = 1/100$

magnetic field along $c$–axis, a first order metamagnetic phase transition appears at about 7.9 T. Fine tuning by tilting the field angle or applying a hydrostatic pressure reveals physical properties consistent with the quantum criticality of an end-point of the metamagnetic transition, such as the non-Fermi liquid forms of the resistivity and enhanced specific heat coefficient. The most convincing evidence comes from the entropy measurement which shows the entropy accumulation effect [24], a generic thermodynamic signature of quantum criticality. Another interesting feature of this
materials, as mentioned earlier, is that, around the critical magnetic field 7.9T, the system goes through a second order phase transition at low temperatures (1.2K for H=7.9T) into a new phase. Therefore, Sr_{n+1}Ru_{n}O_{3n+1} is believed to be an important prototype system to study the conventional formalism of quantum criticality in metals. Here, the intriguing question is therefore whether Sr_{3}Ru_{2}O_{7}, as a ferromagnet, can be explained by conventional QCP formalisms on itinerant magnets. In addition, although it is a 3D material, the anisotropy in in-plane and c-axis resistivity indicates it is a quasi-2D system. We try to address these issues from the thermodynamics, by comparing the experimental data to theoretical results of conventional 3D and 2D quantum critical itinerant ferromagnets.

For this purpose, we provide comparisons in two characteristic regimes, one is for data in low-field (from 5T to 7.1T) Fermi liquid regime at T=250mK (the range of data in high-field Fermi liquid regime does not cover one decade data), the other is for data as a function of temperature at critical field (T= 7.9T) in quantum critical regime (the QCP here is a metamagnetic QCP). However the strong magnetic field and 1st-order phase transition means one more coupling term $H\phi$ needs to be added to quantum Landau-Ginzburg model discussed in Sec.II. RG calculation [71] at this situation shows the magnetic field is a relevant parameter, meanwhile the control parameter $r$ will be rescaled by a power low of distance away from critical magnetic field [68]

$$r = \alpha((H - H_c)/H_c)^{2/3},$$  (3.21)
where $H_c$ is critical field, and $\alpha$ is a non-universal parameter which can be treated as a free fitting parameter. For convenience of comparison/fitting, we also adopt the dimensionless parameters, such as $t = T/T^*$, and $r$, which is more revealing to the scaling relation Eq. (3.21).

### 3.4.2 Scaling analysis on the experimental data in the Fermi Liquid Regime

![Graph of experimental data and fittings](image)

**Figure 3.5**: Left panel shows fittings for experimental data (green) of entropy as a function of magnetic field in Fermi liquid regime in terms of 2D (blue) and 3D (red) FM, and free (black) at 250 mK. The fitting results are $S/T = -0.072 + 0.095(7.9 - H)^{-1/3}$ for 2DFM and $S/T = 0.023 + 0.027 \ln(7.9 - H)$ for 3DFM, and $S/T = -0.031 + 0.054(7.9 - H)^{-0.666}$ for free fitting. Right picture shows 2D (blue), 3D (red) FM, and free (black) fittings and free fitting for experimental data (green) of specific heat as a function of magnetic field at 250 mK. The fitting results are $C_v/T = -0.071 + 0.0938(7.9 - H)^{-1/3}$ for 2DFM, $C_v/T = 0.0226 + 0.0268 \ln(7.9 - H)$ for 3DFM, and $C_v/T = -0.018 + 0.041(7.9 - H)^{-0.973}$ for free fittings.

Fig. (3.5) shows the experimental data in the Fermi liquid regime, $H < H_c \approx 7.9T$, at a fixed temperature $T=250$ mK. It can be observed that the entropy increases as $H_c$
is approached. This is in accordance with the entropy accumulation effect associated with generic QCPs. Similar results are also observed in the high-field side $H > H_c$. From $S/T \approx C_V/T$, the FL behavior such as $C_V \sim T$ is well satisfied.

We firstly fit the experimental data with the scaling behavior of itinerant ferromagnetic QCPs, i.e., $S/T = a + b(H_c - H)^{-1/3}$ for 2DFM and $S/T = a' + b' \ln(H_c - H)$ for 3DFM. The fitting curves and the values of the fitting parameters are also shown in Fig. Fig. (3.5). In experiments, the specific heat is measured directly and thus more reliable while the entropy is integrated by interpolation from specific heat data. We also show and provide the fitting to the specific heat data. We find that neither the 2DFM nor the 3DFM forms provide an accurate description of the asymptotic divergent behavior of $S/T$ and $C_V/T$. If we allow the exponent $c$ in $(H_c - H)^c$ to be a free fitting parameter, we find that the best fit yields $c \approx -0.973$. But overall, the 2D form provides a better fit to the experimental data in this regime.

3.4.3 Scaling analysis on the experimental data in the quantum critical regime

We further show the experimental data and theoretical fittings in the quantum critical regime, for a fixed $H = 7.9T \approx H_c$ in Fig. (3.6). While $S \to 0$ when $T \to 0$ as required by the third law of thermodynamics, $S/T$ and $C_V/T$ show divergent behaviors as $T \to 0$. This is in accordance with the quantum critical behaviors in itinerant magnets for $d \leq z$. However, this divergent behavior is cut off at $T \approx 1.25K$ by the emergence
of a novel ordered phase. We fit the $T > 1.25K$ data with the scaling forms of itinerant ferromagnet QCPs, $S/T = a + bT^{-1/3}$ for 2DFM and $S/T = a' + b/\ln(1/T)$. We find that the experimental is better fitted by the $\log(1/T)$ divergence, i.e., given by the 3DFM. From the constant piece $a$ and $a'$, we can also determined the characteristic high-energy cutoff $T^* \approx 50K$, which is consistent with that obtained from the spin susceptibility and NMR measurements [23, 72].
3.4.4 Comparison between the theoretical and experimental results

In the above scaling analysis, we have fixed the critical exponent and kept the prefactors as free fitting parameters. In general, these fitting parameters are determined by the non-universal constants in the theoretical model, for example, the quartic coupling $u$ and coefficient $\alpha$ in $r = \alpha(H/H_c - 1)^{2/3}$. Sometimes, the ratios between certain prefactors may become universal. We therefore calculate the thermodynamic quantities with the chosen non-universal parameters and compare the results directly to the experimental data. Such a calculation can also capture the subleading contributions beyond the leading scaling behavior, and therefore allows a truthful examination whether the experimental data can be fitted by the conventional itinerant QCPs. In this procedure since $u$ and $\alpha$ are non-universal we can only compare power law behavior, as a result, there is a gap between numerical results and experimental data. And this gap may either be a constant if the numerical data has the same behavior as experimental data, or non-constant if the numerical data does not. In practice at both of these two situations we move the numerical results by hand to try to maximum overlap with experimental data.

We start from the Fermi liquid regime. We adopt $T^* \sim 50K$ from the scaling analysis and in agreement with other measurements. For $T=250\text{mK}$, we therefore choose the dimensionless temperature $t = 1/200$ in our calculation. As the quartic coupling $u$ gives negligible subleading corrections, the coefficient $\alpha$ is therefore the only free parameter in our calculation, for which we vary to find the best fit to the
experimental data. In Fig. (3.7) we show our numerical results as compared to the experimental data.

We observe that while the comparison for the entropy is satisfactory, there are noticeable deviations in the specific heat. This is similar to the above scaling analysis that the leading critical behavior in the Fermi liquid regime can not be well fitted into either the 2DFM or the 3DFM conventional ferromagnetic QCPs.

We proceed to calculate the thermodynamic quantities in the quantum critical regime. The comparison is shown in Fig. (3.8). As the leading temperature dependence is better fitted in the form log(1/T), our numerical results for 3DFM therefore are in better agreement with the experimental data, while the 2DFM results deviate
Figure 3.8: Left picture shows direct comparison among numerical data of 2D (blue) and 3D (red) FM, and experimental data (green) of entropy as a function of temperature in quantum critical regime at critical field $H = 7.9$T. Right picture shows direct comparison among numerical data of 2D (blue) and 3D (red) FM, and experimental data (green) of specific heat as a function of temperature in quantum critical regime at critical field $H = 7.9$T.

All of above analysis show that neither 3D or 2D itinerant ferromagnetic formalisms can fully account for the quantum critical behaviors in all regimes of Sr$_3$Ru$_2$O$_7$. One possible reason is the emergence of a novel ordered phase, which might change the scaling behaviors of QLGT for itinerant magnetism.
Chapter 4

Quantum phase transitions in iso-electronically tuned iron pnictides

Iron based materials not only show high temperature superconductivity [73], but also feature a rich phase diagram. For the parent iron arsenides, the ground state has a collinear \((\pi, 0)\) magnetic order [74]. Because superconductivity occurs at the border of such an antiferromagnetic (AF) order, a natural question is whether quantum criticality plays a role in the phase diagram. It was theoretically proposed early on that tuning the parent iron pnictides by an isoelectronic P-for-As doping induces a quantum critical point (QCP), where both the \((\pi, 0)\) AF order and an Ising-nematic spin order are suppressed [33]. This proposal was made within a strong-coupling approach, which attributes the bad-metal behavior of iron arsenides [29, 30, 75, 76] to correlation effects that are on the verge of localizing electrons [25–27, 77]. The P doping increases the in-plane electronic kinetic energy and thus the coherent electronic spectral weight while leaving other model parameters little changed [34, 35], thereby weakening the magnetic order and the associated Ising-nematic spin order [33, 39].

Such a QCP has since been observed by measurements in the P-doped CeFeAsO [40,41] and BaFe\(_2\)As\(_2\) [42–44,78]. Neutron scattering in the former has shown that the tetragonal-to-orthorhombic structural distortion vanishes at the same doping \((x_c \approx\)
0.4) where the AF order goes away [40], providing evidence for the simultaneous suppression of the AF and Ising-nematic spin orders. In the P-doped BaFe$_2$As$_2$, a large non-Fermi liquid regime has been shown in the phase diagram [42–44, 78]. Static structural order is also suppressed around the same P-doping concentration ($x_c \approx 0.33$) where the AF order goes away, although there may be an additional channel of electronic anisotropy [79]; While there is evidence for a QCP “hidden” inside the superconducting dome [44] quantum criticality has now been observed and studied in the normal state where superconductivity is suppressed by a high field [78]. The accumulated experimental evidences for a QCP in the P-doped parent iron arsenides motivate further theoretical analyses on the underlying quantum phase transitions.

Here, we study the zero-temperature phase transitions in a continuum model introduced earlier [33,39]. This effective field theory contains antiferromagnetic (vector) and Ising-nematic (scalar) order parameters appropriate for a $J_1$-$J_2$ model of local moments on a square lattice [25, 48, 51, 80]. It also incorporates a damping term caused by coupling of the local moments to the coherent itinerant electrons. Since it is important to establish the nature of quantum criticality in the absence of superconductivity [41,78], we will focus on the transitions in the normal state and will in particularly not consider the effect of superconductivity [81]. Using a large-$N$ approach [82,83], we demonstrate that the magnetic and Ising transitions are concurrent at zero temperature both for the case of a square lattice and in the presence of inter-
layer coupling. Moreover, the transitions in the presence of damping are essentially continuous, leading to quantum criticality over a wide dynamical range.

The structure of this chapter is organized as follows. In Sec. 4.1 we introduce the effective quantum Ginzburg-Landau action to describe the iso-electronically doped procedure. In Sec. 4.2 we set up the large N formalism and derive its variational equations. In Sec. 4.3 we give detailed discussions on the consequences of the large N formalism and its variational equations. Appendix C.1 shows the basic procedure to get the large N action. Appendices C.2 and C.3 give out the detailed calculations for the saddle-point equations, and show how to get a close form for the free energy to the leading order in $O(1/N)$. Appendix C.4 gives saddle-point equations in the ordered regime. Appendix C.5 gives detailed discussions on the nature of the Ising and magnetic phase transitions for $d2\times2$ systems. Appendix C.6 shows the two transitions at extreme anisotropy case for $d2\times2$ systems. Appendix C.7 gives detailed calculations and discussions for the two transitions in $d3\times2$ systems.

4.1 The model

The proximity of a bad metal to a Mott transition can be measured by the parameter $w$, the percentage of the single-electron spectral weight in the coherent itinerant part [25, 26, 49]. To the zero-th order in $w$, all the single-electron excitations are incoherent; integrating them out leads to an effective model of local moments with
couplings $J_1$ and $J_2$:

$$H = \sum_{\langle i,j \rangle} J_1 \vec{S}_i \cdot \vec{S}_j + \sum_{\langle\langle i,j \rangle\rangle} J_2 \vec{S}_i \cdot \vec{S}_j$$  \hspace{1cm} (4.1)$$

where $\langle \cdots \rangle$ and $\langle\langle \cdots \rangle\rangle$ respectively denote the nearest neighbor and next nearest neighbor sites. Sec. 1.4 has given a brief discussions for the Hamiltonian of Eq. (4.1).

Following the discussions, upon P doping, the in-plane electronic kinetic energy will increase with little change in potential energy, resulting in an increase of spectral weight $w$. To non-vanishing orders in $w$, the coherent itinerant electrons provide Landau damping. This leads to the following minimum quantum Ginzburg-Landau action [26,33,39]:

$$S = S_2 + S_4$$  \hspace{1cm} (4.2)$$

with

$$S_2 = \sum_{\vec{q}, i\omega_l} \left\{ \chi_0^{-1}(\vec{q}, i\omega_l) \left[ |\vec{m}_A(\vec{q}, i\omega_l)|^2 + |\vec{m}_B(\vec{q}, i\omega_l)|^2 \right] + 2v (q_x^2 - q_y^2) \vec{m}_A(\vec{q}, i\omega_l) \cdot \vec{m}_B(-\vec{q}, -i\omega_l) \right\}$$

$$S_4 = \int_0^\beta d\tau \int d\vec{r} \left\{ u_1 \left( |\vec{m}_A|^4 + |\vec{m}_B|^4 \right) + u_2 |\vec{m}_A|^2 |\vec{m}_B|^2 - u_I (\vec{m}_A \cdot \vec{m}_B)^2 \right\}$$  \hspace{1cm} (4.3)$$

where $\vec{m}_{A/B}(\vec{r}, \tau) = (m_{A/B}^1, m_{A/B}^2, m_{A/B}^3)$ are the $O(3)$-vector fields of sublattices $A$ and $B$, and

$$\chi_0^{-1}(\vec{q}, i\omega_l) = r + \omega_l^2 + c q^2 + \gamma |\omega_l|$$  \hspace{1cm} (4.4)$$

where $c$ is the square of the spin-wave velocity. The parameter $v$ leads to an anisotropic distribution of the spin spectral weight in the momentum space, which is described
by the ellipticity
\[ \epsilon \equiv \sqrt{(c - v)/(c + v)}, \] (4.5)
which goes from full isotropy \( \epsilon = 1 \) \((v = 0)\) to extreme anisotropy \( \epsilon = 0 \) \((v = c)\). For latter convenience, we also introduce the parameter
\[ a_c \equiv c/\sqrt{c^2 - v^2} = (\epsilon + 1/\epsilon)/2. \] (4.6)

In addition, \( \gamma \) is the damping rate, with \( \omega_l \) denoting Matsubara frequencies. Finally, \( r = r_0 + wA_{\mathbf{Q}} \), where the bare mass \( r_0 \) is negative, reflecting the ground-state order in the absence of damping, and \( A_{\mathbf{Q}} > 0 \) is a quasiparticle susceptibility at \( \mathbf{Q} = (\pi, 0) \) or \((0, \pi)\) [33]. When \( J_1 \ll J_2 \), we have \( u_1, u_2 \ll u_1 \). A biquadratic coupling [84, 85] can also be incorporated, which primarily renormalizes \( u_I \). When the damping is present, the effective dimensionality of the fluctuations with respect to the underlying \( O(3) \) transition is \( d + z = 4 \). From a renormalization-group (RG) perspective, because \( -u_I \) is negative, it is marginally relevant w.r.t the underlying QCP of \( O(3) \) transitions at \( d + z = 4 \) [33, 50]. So unlike the thermally-driven transitions or the case of zero-temperature transition in the absence of damping (where \( u_I \) is relevant), it is expected that any splitting between the magnetic and Ising transitions would be small, leading to a qualitative phase diagram shown in Fig. 1.6(b) [33, 39].

Given the extensive experimental observations of a similar phase diagram, here we theoretically study the phase transitions beyond the qualitative RG-based considerations. Our focus here is on the zero-temperature limit, and we place a particular focus on the effect of damping. We note that the effect of damping on the transitions
and dynamics at non-zero temperatures was studied before [52].

### 4.2 Large-\(N\) approach

generalize the spin symmetry of the model from \(O(3)\) to \(O(N)\), with \(\vec{m}_{A/B}\) now taking \(N\) components. The quartic couplings (rescaled by a \(1/N\) factor) are decomposed in terms of Hubbard-Stratonovich fields \(i\lambda_A, i\lambda_B,\) and \(\Delta_I\) [c.f. Appendix C.1]. To the leading order in \(1/N\), \(i\lambda_A = \langle m_A^2 \rangle\) and \(i\lambda_B = \langle m_B^2 \rangle\) contribute to the renormalization of the mass (quadratic coefficient), and \(\Delta_I = \langle \vec{m}_A \cdot \vec{m}_B \rangle\) is the Ising order parameter. We carry out our analysis from the ordered side, and set \(\vec{m}_{A/B} = (\sqrt{N}\sigma_{A/B}, \vec{\pi}_{A/B})\) with \(\sigma_{A/B}\) and \(\vec{\pi}_{A/B}\) as the static order and fluctuation fields of sublattices \(A\) and \(B\) respectively. To the order of \(O(1/N)\) we can integrate out \(\vec{\pi}_{A/B}\), which yields an effective free energy density:

\[
\begin{align*}
  f &= \frac{\Delta_I^2}{u_I} - \frac{(m^2 - r)^2}{2u_1 + u_2} + 2 \left( m^2 - |\Delta_I| \right) \sigma^2 + \frac{\gamma^2 a_c}{16c\pi^2} \left\{ \left( x - \frac{1}{6} \right) \ln x + \left( y - \frac{1}{6} \right) \ln y \right. \\
  &\quad - (x + y) \left[ \frac{1}{3} + \ln \left( 1 + 4\frac{c\Lambda_c^2}{\gamma^2} \right) \right] - \frac{1}{6} (1 - 4y)^{3/2} \ln \frac{1 + (1 - 4y)^{1/2}}{1 - (1 - 4y)^{1/2}} \\
  &\quad - \frac{1}{6} (1 - 4x)^{3/2} \ln \frac{1 + (1 - 4x)^{1/2}}{1 - (1 - 4x)^{1/2}} + \frac{4\sqrt{c}\Lambda_c}{\gamma} (x + y) \tan^{-1} \left( \frac{2\sqrt{c}\Lambda_c}{\gamma} \right) \right\} \\
\end{align*}
\]

where \(\Lambda_c\) is a cutoff wave vector, and \(m^2 = \langle \vec{m}_A^2 \rangle = \langle \vec{m}_B^2 \rangle\). Taking \(\sigma_A = \sigma_B = \sigma\) and \(\sigma_A = -\sigma_B = \sigma\) correspond to \(Q = (0, \pi)\) and \((\pi, 0)\) AF orders, respectively. We have introduced the notations

\[
x = \frac{(m^2 + \Delta_I)}{\gamma^2}, \quad y = \frac{(m^2 - \Delta_I)}{\gamma^2}
\]

(4.8)
with the physical requirement $m^2 \geq |\Delta_I|$, which guarantees the free energy to be real. We note that the free energy of Eq. (4.7) is analytic when $\gamma \to 0$. From these, we have variational equations w.r.t $\sigma$, $m^2$ and $\Delta_I$,

$$\frac{\partial f}{\partial \sigma} = \frac{\partial f}{\partial \Delta_I} = \frac{\partial f}{\partial m^2} = 0$$

(4.9)

which correspond to [c.f. Appendix C.2]

$$(m^2 - |\Delta_I|) \sigma = 0$$

(4.10)

$$\frac{\Delta_I}{u_I} = \frac{m^2 - r}{2u_1 + u_2} - 2\sigma^2 - G_1$$

(4.11)

$$\frac{\Delta_I}{u_I} = -\frac{m^2 - r}{2u_1 + u_2} + G_2$$

(4.12)

The details about $G_1$ and $G_2$ are relegated to Appendix C.3. Several limits provide a check on our approach. From Eqs. (4.11,4.12), setting $u_I = 0$ will lead to $\Delta_I = 0$; this is consistent with the Ising order being driven by the interaction $u_I$. In the absence of coupling to coherent itinerant fermions i.e., setting $\gamma^2/|\Delta_I| = 0$ and $\nu = 0$, we have a nonzero Ising order at zero temperature, which is what happens for the pure $J_1 - J_2$ model [47,48].

It follows from these equations that [c.f. Appendix C.2] the vanishing of the Ising order implies a vanishing magnetic order. The converse can also be shown explicitly in the limits of $\Delta_I/\gamma^2, m^2/\gamma^2 \ll 1$, and is numerically confirmed for the generic cases (see below).
4.3 Nature of the magnetic and Ising transitions at zero temperature

We are now in position to address the concurrent magnetic and Ising transitions at $T = 0$. The RG arguments we outlined earlier suggest that there will be a jump of the order parameters across the transitions, but the jump will be smaller as the damping parameter $\gamma$ increases. To see how the damping affects the transition, we first consider the parameter regime where analytical insights can be gained in our large-$N$ approach. When $\gamma$ is sufficiently large so that $x, y \ll 1$, Eq. (4.12) simplifies to be

$$A(\eta) = a\eta - \eta \ln \eta = \mu(w)$$  \hspace{1cm} (4.13)

with $\eta = |\Delta_I|/\gamma^2$, and

$$a = -\frac{4\pi^2 \Gamma(a_I-a_0)}{a_c} - \ln 2 - 1/2,$$  \hspace{1cm} (4.14)

$$\mu(w) = \frac{4\pi^2}{a_c} r(w) \frac{\Gamma}{a_0 c_{\Delta_I}^2} + \frac{\tan^{-1}(2/\Gamma)}{\Gamma} - \frac{1}{4} \ln(1 + \frac{4}{\Gamma^2}),$$  \hspace{1cm} (4.15)

where $\Gamma = \frac{\gamma}{c^{1/2}a_c}$ is the normalized damping rate, while $a_0 = \frac{\Lambda c^{3/2}}{2u_1 + u_2}$ and $a_I = \frac{\Lambda c^{3/2}}{u_I}$ relate to the normalized interactions. As described in detail in the Appendix C.5, it follows from this equation that the transition is first order, with the jump of the order parameter decreasing as the damping rate $\Gamma$ is increased. The jump is exponentially suppressed when $\Gamma$ becomes large.

To study the transition more quantitatively, we have solved the large-$N$ equations numerically. Fig. 4.1 shows how the Ising and magnetic order parameters change...
Figure 4.1: The evolution of the Ising order parameter $\Delta_I$ (a) and the collinear AF order parameter $\sigma$ (b) vs. the control parameter at different damping rates ($\Gamma = \gamma/(c^{1/2}A_c)$) at a relatively strong anisotropy $a_c = 2$ (corresponding to an ellipticity $\varepsilon \approx 0.27$), with fixed values of the normalized interactions $a_I$ and $a_0$. The transitions are very weakly first order, with jumps in the order parameters (insets) that are very small and decrease with damping.

when tuning $w$, where, for comparison, we assume $r$ can still be tuned even at $\gamma = 0$.

The jump of the order parameter is seen to be very small, even for the case of a
very large anisotropy: $a_c = 2$ here corresponds to an ellipticity of $\epsilon \approx 0.27$, which is already considerably stronger than what is typically observed in the inelastic neutron scattering experiments, which is about $\epsilon \approx 0.6 – 0.9$ [52, 86]. When the anisotropy becomes extremely large, the system effectively becomes one-dimensional, and the effective dimensionality $d+z$ becomes 3; the quartic coupling $-u_I$ will become relevant (as opposed to being marginal) w.r.t. the underlying O(3) QCP, and we expect a stronger degree of first-orderness. Indeed, as shown in Fig. C.2 in the Appendix C.6 for an extreme value of anisotropy $a_c = 20$ (corresponding to $\epsilon = 0.025$), the order-parameter jump becomes larger.

4.4 Effect of the third-dimensional coupling

Iron pnictides have a finite Néel temperature, which results from an interlayer exchange coupling. In order to understand the role of this coupling on the quantum phase transition, we have studied the effective field theory in three-dimensional space. The details of the model are described in the Appendix C.7, and the results for the case with the spin-wave velocity on the third dimension being equal to the in-plane velocity at $v = 0$ are shown in Figs. (C.3,C.4). The AF and Ising transitions are still concurrent, and become genuinely continuous. Again, this is consistent with the RG considerations: given that the effective dimensionality in this case is $d+z = 5$, the quartic coupling $-u_I$ becomes irrelevant w.r.t. the underlying O(3) transition and will therefore not destabilize the continuous nature of the transitions.
In the more general case, with a varying third-dimensional coupling, it is more
difficult to solve the large-$N$ equations. However, the RG considerations imply that,
even in this case, the quantum transitions will be asymptotically continuous.

4.5 Discussion

Our results imply that the model for the isoelectronically doped iron pnictides yield
quantum phase transitions of the AF and Ising-nematic orders that are concurrent,
and essentially second order. This conclusion is consistent with the experimental
observations of essentially continuous quantum phase transitions in the normal states
of P-doped BaFe$_2$As$_2$ [78] and CeFeAsO [41].

In addition, the extremely small jump of the order parameters across the quantum
transitions in the 2D case is also important for understanding experimental observa-
tions. It implies that quantum criticality occurs over a wide dynamical range, with
two-dimensional characters. The logarithmic divergence of the effective mass expected
from such 2D quantum critical fluctuations [33, 39] has received considerable experi-
mental support in the P-doped BaFe$_2$As$_2$. It fits well the P-doping dependence of the
effective mass as extracted from the de Haas-van Alphen (dHvA) measurements [87],
as well as that of the square root of the $T^2$-coefficient of the electrical resistivity [78].
In turn, the latter provides further motivation to study the coupling between the
collective fluctuations and charge carriers.

Finally, our results also imply that there will be a wide dynamical range both
in temperature and frequency to observe the quantum fluctuations, not only in the staggered magnetizations but also in the Ising-nematic spin channel. Initial indications for the latter have come from inelastic neutron scattering measurements in the electron-doped BaFe$_2$As$_2$ detwinned by uniaxial strain [88]. It would be very instructive to measure such effects in the P-doped BaFe$_2$As$_2$. 
Chapter 5

Summary

To summarize, for the longitudinal-field-perturbed critical quantum Ising chain with $E_8$ symmetry, we have determined its local dynamical spin structure factor at temperatures and frequencies that are small compared to the mass of the lightest $E_8$ particle. The frequency dependence shows a logarithmic singularity. Our calculations yield a concrete prediction for the temperature dependence of the NMR relaxation rate, which we have suggested as a means to further test the $E_8$ description of the spin dynamics in CoNb$_2$O$_6$.

We have investigated the thermodynamic signatures of quantum criticality in itinerant magnetic systems, with a focus on itinerant magnets. By general RG study on quantum Landau-Ginzburg model we point out a generic deficit in the conventional Gaussian universality of this model which indicates this theory at Gaussian level is incomplete. We give out a general recipe by a proper regularization on the Gaussian free energy by including contributions beyond Gaussian level. Based on this, we have carried out numerical calculations to evaluate the free energy and several thermodynamic quantities of interest. We show that the leading scaling behaviors of thermodynamic quantities for this theory near QCP are consistent with traditional predictions. Our results reveal that the thermodynamic signatures of quantum criti-
cality, such as the entropy accumulation, predicted earlier by a hyperscaling relation, are also robust features for itinerant ferromagnets, where the hyperscaling relation does not hold.

We also make a detailed comparison between numerical results of entropy and specific heat on itinerant ferromagnetic models and experimental results on Sr$_3$Ru$_2$O$_7$ to investigate its relevance to conventional spin-density-wave formalism for metals. We have found that the entropy accumulation, the divergence of the specific heat coefficient are indeed in accordance with the quantum critical scenario. As we have argued, these signatures are unique to quantum critical points, and we conclude that indeed there exists a quantum phase transition in this material. However, in the detailed comparison in both the Fermi liquid and quantum critical regimes, we find that the experimental data cannot be fitted exactly by either a 3D or a 2D conventional itinerant magnet formalism. In the Fermi liquid regime, we find that the 2D formalism has a relatively better fit. This is in agreement with the prediction from other experiments that it is a quasi-2D system, for instance, the large anisotropy of the resistivity along the plane and the c-axis, $\rho_c/\rho_{ab} \approx 100$. However, in the quantum critical regime, we find that the specific heat coefficient is better fitted by a log$(1/T)$ form, which agrees with the 3D ferromagnet. We notice that this is also the form for 2D antiferromagnet with the dynamic exponent $z = 2$. One possibility is that additional mechanism such as the impurity scattering and the novel ordered phase could change the dynamics from the conventional Landau-damping for a ferromagnet.
This, of course, relies on further studies to elucidate the nature of the emergent new phase. The deviation from the conventional itinerant magnet formalism, as illustrated in this study, indicates that new physics beyond itinerant magnetic scheme is required to account for this novel metamagnetic material.

Last, we studied zero-temperature magnetic and Ising transitions in a model for isoelectronically-tuned iron pnictides using a large-N approach. We demonstrated that the magnetic and Ising orders transitions are concurrent at zero temperature. We also showed that the transitions in the presence of damping are essentially continuous; the jumps in the order parameters are extremely small. Our results imply that quantum criticality occurs over a wide dynamical range, thereby providing a systematic understanding of the RG-based considerations and experimental observations. Our approach can be used for further studies of the quantum critical properties in P-doped parent iron arsenides.
Appendix A

Appendix for spin dynamics in a perturbed quantum critical Ising chain with an $E_8$ symmetry

A.1 Derivaiton of $\chi_{yy}(x,t)$

The general Hamiltonian of one dimensional transverse field Ising model with a longitudinal field can be expressed as

$$H = -J \left( \sum_i \sigma_i^z \sigma_{i+1}^z + g \sum_i \sigma_i^x + h \sum_i \sigma_i^z \right) \quad (A.1)$$

where $J$, $g$ and $h$ has the same meaning as Chap.2. Denote $C(i,j,t,T) = \langle \sigma_i^z(t) \sigma_j^z(0) \rangle_T$, where $\langle \cdots \rangle_T$ is used to denote thermal average. Then

$$\frac{\partial C(i,j,t,T)}{\partial t} = -Jg \langle e^{iHt} [\sigma_i^z(0), \sigma_i^z(0)] e^{-iHt} \sigma_j^z(0) \rangle = -2Jg \langle \sigma_i^y(0) \sigma_j^z(-t) \rangle_T \quad (A.2)$$

and

$$\frac{\partial^2 C(i,j,t,T)}{\partial t^2} = (-Jg)^2 \frac{\partial \langle \sigma_i^y(0) \sigma_j^z(-t) \rangle_T}{\partial t} = -4 (Jg)^2 \langle \sigma_i^y(t) \sigma_j^y(0) \rangle_T \quad (A.3)$$

Recall the definition of linear response $\chi_{ij,T}^{\alpha\alpha}$, $\alpha = x, y, z$,

$$\chi_{ij,T}^{\alpha\alpha} = -i\theta(t) \langle [\sigma_i^\alpha(t), \sigma_j^\alpha(0)] \rangle_T \quad (A.4)$$

We have

$$\chi_{yy}^{yy}(x,t) = -\frac{1}{4(gJ)^2} \frac{\partial^2 \chi_{zz}^{zz}(x,t)}{\partial t^2} \quad (A.5)$$
Then
\[ \chi_{yy}^T(\omega) = \frac{\omega^2}{4(gJ)^2} \chi_{zz}^T(\omega) \]  \hspace{1cm} (A.6)

There, the low frequency response \( \chi_{yy}^T(\omega) \) is subleading.

### A.2 Relevant form factors

The main text considered two- and three-particle form factors of the \( E_8 \) model. The relevant two-particle form factors are known in the literature \([16,57]\). Here, for completeness, we present their detailed expressions, where \( n \) in \( F_n^\sigma \) is explicitly written as types of particles it contains.

\[ F_{aa}^\sigma (\theta_1, \theta_2) = \left\{ c_{11}^0 + c_{11}^1 \cosh (\theta_1 - \theta_2) \right\} \left\{ -i \sinh \left( \frac{\theta_1 - \theta_2}{2} \right) \right\} \cdot \]
\[ \frac{T_{2/3} (\theta_1 - \theta_2) T_{2/5} (\theta_1 - \theta_2) T_{1/15} (\theta_1 - \theta_2)}{P_{2/3} (\theta_1 - \theta_2) P_{2/5} (\theta_1 - \theta_2) P_{1/15} (\theta_1 - \theta_2)} \]  \hspace{1cm} (A.7)

\[ F_{bb}^\sigma (\theta_1, \theta_2) = \left\{ c_{22}^0 + c_{22}^1 \cosh (\theta_1 - \theta_2) + c_{22}^2 \cosh^2 (\theta_1 - \theta_2) + c_{22}^3 \cosh^3 (\theta_1 - \theta_2) \right\} \cdot \]
\[ \left\{ -i \sinh \left( \frac{\theta_1 - \theta_2}{2} \right) \right\} \frac{T_{3/5} (\theta_1 - \theta_2) T_{2/3} (\theta_1 - \theta_2) T_{3/15} (\theta_1 - \theta_2) T_{5/15} (\theta_1 - \theta_2) T_{2/3} (\theta_1 - \theta_2) T_{3/15} (\theta_1 - \theta_2) T_{5/15} (\theta_1 - \theta_2)}{P_{3/5} (\theta_1 - \theta_2) P_{2/3} (\theta_1 - \theta_2) P_{3/15} (\theta_1 - \theta_2) P_{5/15} (\theta_1 - \theta_2) P_{2/3} (\theta_1 - \theta_2) P_{3/15} (\theta_1 - \theta_2) P_{5/15} (\theta_1 - \theta_2)} \]  \hspace{1cm} (A.8)
\[ F_{cc}^\sigma (\theta_1, \theta_2) = (c_{33}^0 + c_{33}^1 \cosh (\theta_1 - \theta_2) + c_{33}^2 \cosh^2 (\theta_1 - \theta_2) + c_{33}^3 \cosh^3 (\theta_1 - \theta_2)) \cdot \left\{ -i \sinh \left( \frac{\theta_1 - \theta_2}{2} \right) \right\} T_{11/30} (\theta_1 - \theta_2) \left[ T_{2/3} (\theta_1 - \theta_2) \right]^3 T_{7/15} (\theta_1 - \theta_2) \cdot \left[ T_{2/5} (\theta_1 - \theta_2) \right]^3 T_{2/15} (\theta_1 - \theta_2) \left[ T_{1/15} (\theta_1 - \theta_2) \right]^2 / \left\{ P_{11/30} (\theta_1 - \theta_2) \right\} \cdot P_{7/15} (\theta_1 - \theta_2) P_{2/15} (\theta_1 - \theta_2) \left[ P_{2/3} (\theta_1 - \theta_2) \right]^2 P_{1/3} (\theta_1 - \theta_2) \cdot \left[ P_{2/5} (\theta_1 - \theta_2) \right]^2 P_{3/5} (\theta_1 - \theta_2) P_{1/15} (\theta_1 - \theta_2) P_{14/15} (\theta_1 - \theta_2) \right\} \] (A.9)

\[ F_{ab}^\sigma (\theta_1, \theta_2) = \left\{ c_{12}^0 + c_{12}^1 \cosh (\theta_1 - \theta_2) + c_{12}^2 \cosh^2 (\theta_1 - \theta_2) \right\} \cdot \left( \frac{T_{4/5} (\theta_1 - \theta_2) T_{3/5} (\theta_1 - \theta_2) T_{7/15} (\theta_1 - \theta_2) T_{4/15} (\theta_1 - \theta_2)}{P_{4/5} (\theta_1 - \theta_2) P_{3/5} (\theta_1 - \theta_2) P_{7/15} (\theta_1 - \theta_2) P_{4/15} (\theta_1 - \theta_2)} \right) \] (A.10)

\[ F_{ac}^\sigma (\theta_1, \theta_2) = \left\{ c_{13}^0 + c_{13}^1 \cosh (\theta_1 - \theta_2) + c_{13}^2 \cosh^2 (\theta_1 - \theta_2) + c_{13}^3 \cosh^3 (\theta_1 - \theta_2) \right\} \cdot \left( \frac{T_{29/30} (\theta_1 - \theta_2) T_{7/10} (\theta_1 - \theta_2) T_{13/30} (\theta_1 - \theta_2)}{P_{29/30} (\theta_1 - \theta_2) P_{7/10} (\theta_1 - \theta_2) P_{23/30} (\theta_1 - \theta_2)} \right) \cdot \left( \frac{T_{1/10} (\theta_1 - \theta_2) T_{11/30} (\theta_1 - \theta_2)}{P_{1/10} (\theta_1 - \theta_2) P_{11/30} (\theta_1 - \theta_2) P_{19/30} (\theta_1 - \theta_2)} \right)^2 \] (A.11)

\[ F_{bc}^\sigma (\theta_1, \theta_2) = \left\{ c_{23}^0 + c_{23}^1 \cosh (\theta_1 - \theta_2) + c_{23}^2 \cosh^2 (\theta_1 - \theta_2) = \right\} \cdot \left( \frac{T_{25/30} (\theta_1 - \theta_2)}{P_{25/30} (\theta_1 - \theta_2) P_{19/30} (\theta_1 - \theta_2)} \right) \cdot \left( \frac{T_{19/30} (\theta_1 - \theta_2) T_{9/30} (\theta_1 - \theta_2) \left[ T_{7/30} (\theta_1 - \theta_2) \right]^2}{P_{9/30} (\theta_1 - \theta_2) P_{7/30} (\theta_1 - \theta_2) P_{23/30} (\theta_1 - \theta_2)} \right) \cdot \left( \frac{T_{13/30} (\theta_1 - \theta_2) T_{15/30} (\theta_1 - \theta_2)}{P_{13/30} (\theta_1 - \theta_2) P_{17/30} (\theta_1 - \theta_2) P_{15/30} (\theta_1 - \theta_2)} \right) \] (A.12)

where

\[ T_\lambda (\theta) = \exp \left\{ 2 \int_0^\infty \frac{dt \cosh [(\lambda - 1/2) t]}{t \cosh (t/2) \sinh t} \sin^2 \left( \frac{i \pi - \theta}{2 \pi} \right) \right\} \] (A.13)
and

\[ P_\lambda(\theta) = \frac{\cos(\lambda \pi) - \cosh \theta}{2 \cos^2(\lambda \pi/2)} \]  (A.14)

and all coefficients \( \{c^k_{ij}\} \) in above expressions can be found in Ref. [57], which explicit values are,

\[ c^0_{11}, c^1_{11} = -10.19307727, -2.09310293. \]
\[ c^0_{22}, c^2_{32}, c^3_{32}, c^5_{22} = -500.2535896, -791.3745549, -338.8125724, -21.48559881. \]
\[ c^0_{33}, c^2_{33}, c^3_{33}, c^5_{33}, c^7_{33} = -87821.70785, -267341.1276, -301093.9432, -150512.4122, -30166.99117, -1197.056497. \]
\[ c^0_{12}, c^1_{12}, c^2_{12} = -70.2921893519, -71.792063506, -7.9790221816. \]
\[ c^0_{13}, c^1_{13}, c^2_{13}, c^3_{13} = -7049.622303, -13406.48877, -6944.416956, -5822.557366. \]
\[ c^0_{23}, c^2_{23}, c^3_{23}, c^5_{23} = -3579.556465, -8436.850081, -6618.297073, -1846.579035, -92.73452314. \]

The relevant three-particle form factor of the \( E_8 \) model is,

\[ F^\sigma_{aaa}(\theta_1, \theta_2, \theta_3) = Q^\sigma_{aaa}(\theta_1, \theta_2, \theta_3) \frac{F^\text{min}_{aa}(\theta_1 - \theta_2)}{(e^{\theta_1} + e^{\theta_2}) D_{aa}(\theta_1 - \theta_2)} \]  (A.15)

\[ \frac{F^\text{min}_{aa}(\theta_1 - \theta_3)}{(e^{\theta_1} + e^{\theta_3}) D_{aa}(\theta_1 - \theta_3)} \frac{F^\text{min}_{aa}(\theta_2 - \theta_3)}{(e^{\theta_2} + e^{\theta_3}) D_{aa}(\theta_2 - \theta_3)} \]  (A.16)

where \([16, 57]\)

\[ \frac{F^\text{min}_{aa}(\theta_1 - \theta_j)}{D_{aa}(\theta_i - \theta_j)} = \left\{ -i \sinh \left( \frac{\theta_i - \theta_j}{2} \right) \right\} \frac{T_{2/3}(\theta_i - \theta_j) T_{2/5}(\theta_i - \theta_j) T_{1/15}(\theta_i - \theta_j)}{P_{2/3}(\theta_i - \theta_j) P_{2/5}(\theta_i - \theta_j) P_{1/15}(\theta_i - \theta_j)} \]  (A.17)
and [89]

\[ Q^\sigma_{aaa} (\theta_1, \theta_2, \theta_3) = 1148.690509 e^{3\theta_1} + 46.76252978 e^{4\theta_1 + \theta_2} + 1148.690509 e^{3\theta_2} + 3703.911733 e^{\theta_1 + 2\theta_2} + 46.76252978 e^{4\theta_1 + 2\theta_2 - 2\theta_3} + 4.354182251 e^{4\theta_1 + \theta_2 - 2\theta_3} + 46.76252978 e^{3\theta_1 + 2\theta_2 - 2\theta_3} + 30.148257928 e^{\theta_1 + 3\theta_2 - \theta_3} + 46.76252978 e^{4\theta_2 - \theta_3} + 1148.690509 e^{2\theta_1 + 2\theta_2 - \theta_3} + 604.2577928 e^{\theta_1 + 3\theta_2 - \theta_3} + 46.76252978 e^{4\theta_2 - \theta_3} + 1148.690509 e^{3\theta_3} + 3703.911733 e^{2\theta_1 + \theta_3} + 4.354182251 e^{4\theta_1 - 2\theta_2 + \theta_3} + 604.2577928 e^{\theta_1 - 2\theta_2 + \theta_3} + 6286.815608 e^{\theta_1 + \theta_2 + \theta_3} + 3703.911733 e^{2\theta_2 + \theta_3} + 4.354182251 e^{-2\theta_1 + 4\theta_2 + \theta_3} + 3703.911733 e^{\theta_1 + 2\theta_3} + 46.76252978 e^{3\theta_1 - 2\theta_2 + 2\theta_3} + 1148.690509 e^{2\theta_1 - \theta_2 + 2\theta_3} + 3703.911733 e^{2\theta_2 + 2\theta_3} + 1148.690509 e^{-\theta_1 + 2\theta_2 + 2\theta_3} + 46.76252978 e^{-2\theta_1 + 3\theta_2 + 2\theta_3} + 46.76252978 e^{2\theta_1 - 2\theta_2 + 3\theta_3} + 604.2577928 e^{\theta_1 - \theta_2 + 3\theta_3} + 604.2577928 e^{-\theta_1 + \theta_2 + 3\theta_3} + 46.76252978 e^{-2\theta_1 + 2\theta_2 + 3\theta_3} + 46.76252978 e^{-\theta_1 + 4\theta_3} + 4.354182251 e^{\theta_1 - 2\theta_2 + 4\theta_3} + 46.76252978 e^{-\theta_2 + 4\theta_3} + 4.354182251 e^{-2\theta_1 + \theta_2 + 4\theta_3} \]

(A.18)

**A.3 Derivation of \( S_{1,1} (\omega, q) \)**

\( S_{1,1} \) is calculated using the finite volume regularization scheme [60,90]. We have

\[ D_{00} = \langle \sigma \rangle_0^2, \quad \text{and} \]

\[ D_{11}(x,t) = \int_{-\infty}^{\infty} \frac{d\theta_1}{2\pi} \int_{-\infty}^{\infty} \frac{d\theta_1'}{2\pi} F_2^\sigma (\theta_1 + i\pi, \theta_1') F_2^\sigma (\theta_1' + i\pi, \theta_1) \cdot \]

\( e^{-\beta \Delta_1 \cosh \theta_1} e^{-i(\Delta_1 \sinh \theta_1 - \Delta_2 \sinh \theta_1')} x \cdot e^{-i(\Delta_2 \cosh \theta_1' - \Delta_1 \cosh \theta_1)} t + \]

\[ + 2 \langle \sigma \rangle_0 F_2^\sigma \int_{-\infty}^{\infty} \frac{d\theta}{2\pi} e^{-\beta \Delta_1 \cosh \theta_1} \]

(A.18)
From now until $D_{22}$, we will focus on the time-dependent parts, i.e., the connected pieces of the correlation functions. The time-independent parts, i.e., the disconnected pieces, will be discussed after the analysis on time-dependent parts of $D_{22}$. Then from $S_{11}$, we have

$$S_{11}(q, \omega) = \int d\theta_1 d\theta_1' F_2^\sigma(\theta_1 + i\pi, \theta_1') F_2^\sigma(\theta_1' + i\pi, \theta_1) e^{-\beta \Delta_1 \cosh \theta_1} \cdot \delta(q + \Delta_1 \sinh \theta_1 - \Delta_2 \sinh \theta_1') \delta(\omega + \Delta_1 \cosh \theta_1 - \Delta_2 \cosh \theta_1')$$

(A.19)

Denote

$$\begin{cases}
    y = \Delta_1 \sinh \theta_1 - \Delta_2 \sinh \theta_1' \\
    z = \Delta_1 \cosh \theta_1 - \Delta_2 \cosh \theta_1'
\end{cases}$$

(A.20)

then

$$d\theta_1 d\theta_1' = \left| \frac{\partial (\theta_1, \theta_1')}{\partial (y, z)} \right| dydz = \frac{dydz}{\Delta_1 \Delta_2 \sqrt{\cosh^2 (\theta_1 - \theta_1') - 1}}$$

(A.21)

Noticing the fact that the integral ranges for new variables $y$ and $z$ run from $-\infty$ to $+\infty$, so the integral in the structure factor can be easily done, which is

$$S_{11}(q, \omega) = \int d\theta_1 d\theta_1' F_2^\sigma(\theta_1 + i\pi, \theta_1') F_2^\sigma(\theta_1' + i\pi, \theta_1) \cdot \delta(q + \Delta_1 \sinh \theta_1 - \Delta_2 \sinh \theta_1') \delta(\omega + \Delta_1 \cosh \theta_1 - \Delta_2 \cosh \theta_1') e^{-\beta \Delta_1 \cosh \theta_1}$$

(A.22)

$$= \left. \frac{F_2^\sigma(\theta_1 + i\pi, \theta_1') F_2^\sigma(\theta_1' + i\pi, \theta_1) e^{-\beta \Delta_2 \cosh \theta_1' e^{\beta \omega}}}{\Delta_1 \Delta_2 \sqrt{\cosh^2 (\theta_1 - \theta_1') - 1}} \right|_{\theta_1 - \theta_1' = \alpha}$$

$$+ \left. \frac{F_2^\sigma(\theta_1 + i\pi, \theta_1') F_2^\sigma(\theta_1' + i\pi, \theta_1) e^{-\beta \Delta_2 \cosh \theta_1' e^{-\beta \omega}}}{\Delta_1 \Delta_2 \sqrt{\cosh^2 (\theta_1 - \theta_1') - 1}} \right|_{\theta_1 - \theta_1' = -\alpha}$$

(A.23)

$$= \left. \frac{|F_2^\sigma(\alpha + i\pi, 0)|^2 e^{-\beta \Delta_1 \cosh \theta_1_+}}{\Delta_1 \Delta_2 \sqrt{\cosh^2 \alpha - 1}} \right. + \left. \frac{|F_2^\sigma(-\alpha + i\pi, 0)|^2 e^{-\beta \Delta_1 \cosh \theta_1_-}}{\Delta_1 \Delta_2 \sqrt{\cosh^2 \alpha - 1}} \right.$$
where

$$\Gamma \equiv \cosh \alpha = \cosh(\theta_1 - \theta'_1) = \frac{\Delta^2_1 + \Delta^2_2 - (\omega^2 - q^2)}{2\Delta_1 \Delta_2}$$  \hfill (A.25)$$

$$\cosh \theta_{1\pm} = \frac{\omega \Delta_1 - \omega \Delta_2 \Gamma \pm q \Delta_2 \sqrt{\Gamma^2 - 1}}{q^2 - \omega^2}$$  \hfill (A.26)$$

In the equal sign of Eq. (A.23) we have used the fact that the form factor is only dependent on the difference between any two rapidities. For numerical calculations, we take advantage of the symmetry properties described in Eq. (A.24).

## A.4 \(S_{1,1}(\omega, q)\) of two same-mass 1-particle state

In Eq. (A.22), the \(q\) integration followed by the \(\theta'_1\) integration gives rise to

$$S_{11}(\omega) = \frac{2}{\Delta_i} \cdot \int d\theta_1 \left\{ \left| F_2^\sigma (\theta_1 - \theta'_1(\theta_1, \omega) + i\pi, 0) \right|^2 e^{-\beta \Delta_i \cosh \theta_1} \right\} \sqrt{\left( \cosh \theta_1 + \frac{\omega}{\Delta_i} \right)^2 - 1}$$  \hfill (A.27)$$

Then we make a further simple variable transform \(\cosh \theta_1 = x - \omega_i\) \((\omega_i = \omega/(2\Delta_i))\), we have

$$S_{1,1}(\omega_i)_{\Delta_1=\Delta_2=\Delta_i} = \frac{2e^{\omega/(2T)}}{\Delta} \int_{1+\omega_i}^{\infty} dx \frac{(F(\omega, q_-(x)) + F(\omega, q_+(x))) \exp \left\{ -\frac{\Delta_i}{T} x \right\}}{\sqrt{(x + 1 + \omega_i)(x + 1 - \omega_i)(x - 1 + \omega_i)(x - 1 - \omega_i)}}$$  \hfill (A.28)$$

where \(\omega_i = \omega/(2\Delta_i)\), and

$$F(\omega_i, q_\pm(x)) = |F_2^\sigma (\arccosh[1 + \lambda(\omega_i, x)] + i\pi, 0)|$$  \hfill (A.30)$$
with

\[ \lambda(\omega_i, x) = \left( -\omega_i^2 + x^2 - 1 \pm \sqrt{(x - 1 - \omega_i)(x - 1 + \omega_i)(x + 1 + \omega_i)(x + 1 - \omega_i)} \right) \]

(A.31)

We can also get Eq. (A.29) by making variable transform \( x = -\omega/(2\Delta_i) + (q/(2\Delta_i)) \cdot \sqrt{(q^2 - \omega^2 + 4\Delta_i^2)/(q^2 - \omega^2)} \) for the \( q \) integration over Eq. (A.24). The exponential-decaying factor in the integrand of Eq. (A.29) indicates that the dominant contribution come from the regime where \( x \) is close to \( 1 + \omega_i \). Since \( \omega_i \) is small, in this regime we can approximate \( F(\omega_i, q\pm(x)) \) as

\[ F(\omega_i, q\pm(x)) \approx |F^\sigma_{2}(i\pi, 0)|_{\Delta_1=\Delta_2=\Delta_i}^2 (i = a, b, c, d, e, f, g, h) \]

(A.32)

Then we have

\[ S_{1,1}(\omega \to 0, \omega/\Delta_i \ll 1)|_{\Delta_1=\Delta_2=\Delta_i} \]

(A.33)

\[ \approx \frac{4e^{\omega/(2T)}}{\Delta_i} \int_{1+\omega_i}^{\infty} dx \frac{|F^\sigma_{2}(i\pi, 0)|^2 \exp \left\{ -\frac{\Delta_i}{T} x \right\}}{\sqrt{(x + 1 + \omega_i)(x + 1 - \omega_i)(x - 1 + \omega_i)(x - 1 - \omega_i)}} \]

(A.34)

\[ \approx \left\{ \begin{array}{ll}
\frac{2|F^\sigma_{2}(i\pi, 0)|^2}{\Delta_i} e^{-\Delta_i/T} \{ -\ln \frac{\omega}{4T} - \gamma_E + \cdots \cdots \} (\omega \ll T \ll \Delta_i) \\
\frac{2e^{-\Delta_i/T}|F^\sigma_{2}(i\pi)|^2}{\Delta_i} \left\{ \sqrt{\frac{\pi T}{2}} - \frac{\sqrt{\pi}}{4} \left( \frac{T}{2} \right)^{3/2} + \cdots \cdots \right\} (T \ll \omega \ll \Delta_i)
\end{array} \right. \]

(A.35)

where \( |F^\sigma_{2}(i\pi, 0)|_{\Delta_1=\Delta_2=\Delta_a}^2 \approx 65. \)
A.5 Derivation of $S_{1,2}(\omega, q)$

We again use the finite volume regularization scheme \[60,90\], and have

\[ D_{12}(x, t) = C_{12} - Z_1 C_{01} \]  
(A.36)

\[ = \frac{1}{2} \int_{C_+} \frac{d\theta_1}{2\pi} \int_{-\infty}^{\infty} \frac{d\theta'_1}{2\pi} \int_{-\infty}^{\infty} \frac{d\theta'_2}{2\pi} F_3^{\sigma}(\theta_1 + i\pi, \theta'_1, \theta'_2) F_3^{\sigma}(\theta_1 + i\pi, \theta'_1, \theta'_2) \]  
(A.37)

\[ e^{-\Delta_a} \cosh \theta_1 e^{-ix\Delta_a}(\sinh \theta_1 - \sinh \theta'_1 - \sinh \theta'_2) e^{-it\Delta_a}(\cosh \theta'_1 + \cosh \theta'_2 - \cosh \theta_1) \]  
(A.38)

\[ = \frac{1}{2} \int_0^{\infty} \frac{d\theta'_1}{2\pi} \int_{-\infty}^{\infty} \frac{d\theta'_2}{2\pi} \]  
(A.39)

\[ \{ e^{-\Delta_a} \cosh \theta'_1 e^{i\Delta_a x} \sinh \theta'_2 e^{-it\Delta_a} \cosh \theta'_2 \} \]  
(A.40)

\[ - (F_1^{\sigma})^2 \int_{-\infty}^{\infty} \frac{d\theta'_1}{2\pi} \int_{-\infty}^{\infty} \frac{d\theta'_2}{2\pi} e^{-\Delta_a} \cosh \theta'_1 e^{i\Delta_a x} \sinh \theta'_2 e^{-it\Delta_a} \cosh \theta'_2 . \]  
(A.41)

\[ (\Delta_a x \cosh \theta'_1 + \Delta_a (i\beta + t) \sinh \theta'_1) [S(\theta'_1 - \theta'_2) - 1] \]  
(A.42)

\[ - (F_1^{\sigma})^2 \int_{-\infty}^{\infty} \frac{d\theta'_1}{2\pi} e^{-\Delta_a} \cosh \theta'_1 e^{i\Delta_a x} \sinh \theta'_2 e^{-it\Delta_a} \cosh \theta'_2 \]  
(A.43)

where $C_+$ is used to denote the integration contour from $-\infty$ to $\infty$ slightly above the real axis on the rapidity complex plane, and \[60,90\]

\[ F_3^{\sigma}(\theta_1 + i\pi, \theta'_1, \theta'_2) = \frac{i \left( 1 - S(\theta'_1 - \theta'_2) \right) F_3^{\sigma}}{\theta_1 - \theta'_1} + \frac{i \left( S(\theta'_1 - \theta'_2) - 1 \right) F_3^{\sigma}}{\theta_1 - \theta'_2} + F_3^{\sigma}(\theta_1 + i\pi|\theta'_1, \theta'_2) \]  
(A.44)

where $S_{aa}$ is the scattering matrix for $a-a$ channel, and $F_3^{\sigma}(\theta_1 + i\pi|\theta'_1, \theta'_2)$ is regular on real axis.

For $x = 0$, it’s easy to see that the last three terms do not contribute to low-
frequency \((\omega \ll \Delta_a)\) response of local DSF. From the first integration we have

\[
S_{12}(q, \omega) = \frac{1}{2} \int \frac{d\hbar}{2\pi} \int_{-\infty}^{\infty} d\theta_1' \int_{-\infty}^{\infty} d\theta_2' F_3^\sigma (\theta_1 + i\pi + i\varepsilon, \theta_1', \theta_2') \cdot 
\]

\[\cdot F_3^\sigma (\theta_1 + i\pi + i\varepsilon, \theta_1', \theta_2') \delta (q + \Delta_a \sinh \theta_1 - \Delta_a (\sinh \theta_1' + \sinh \theta_2')) \cdot \]

\[\cdot \delta (\omega + \Delta_a \cosh \theta_1 - \Delta_a (\cosh \theta_1' + \cosh \theta_2')) \tag{A.45}\]

The energy-momentum conservation yields

\[
\begin{align*}
0 &= q + \sinh \theta_1 - \sinh \theta_1' - \sinh \theta_2' \\
0 &= \omega + \cosh \theta_1 - \cosh \theta_1' - \cosh \theta_2' 
\end{align*} \tag{A.46}
\]

For \(F_{3rc}^\sigma\) we can integrate out \(\theta_1'\) and \(\theta_2'\), yielding (because the masses of three particles are equal to each other, \(S_{21}(q, \omega) = S_{12}(q, \omega)\))

\[
S_{(12)+(21)}(q, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\theta_1}{\sqrt{(f(\tilde{\omega}, \tilde{q}, \theta_1) - 1)^2 - 1}} F_{3rc}^\sigma (\theta_1 + i\pi | \ln z_+, \ln z_-) F_{3rc}^\sigma (\theta_1 + i\pi | \ln z_-, \ln z_+) e^{-\beta \Delta_a \cosh \theta_1} \tag{A.47}
\]

with

\[
z_\pm = \frac{1}{2} (\tilde{\omega} + \cosh \theta + \tilde{q} + \sinh \theta) \left(1 \pm 2 \sqrt{1 - 2/f(\tilde{\omega}, \tilde{q}, \theta)}\right), \tag{A.48}
\]

and

\[
f(\tilde{\omega}, \tilde{q}, \theta) = \left[ (\tilde{\omega} + \cosh \theta)^2 - (\tilde{q} + \sinh \theta)^2 \right] / 2 \tag{A.49}
\]

where \(\tilde{\omega} = \omega/\Delta_a\) and \(\tilde{q} = q/\Delta_a\). The energy-momentum conservation gives constraint: \(f(\tilde{\omega}, \tilde{q}, \theta) \geq 2\), i.e., \((\tilde{\omega} - \tilde{q})e^{2\theta} + (\tilde{\omega}^2 - \tilde{q}^2 - 3)e^\theta + \tilde{\omega} + \tilde{q} \geq 0\). This constraint allows zero in the denominator of the integrand in Eq. (A.47), which is a branch point. This can be clearly shown after a variable transform \(e^\theta \to x\) and expanding \(x\) around the zeros.
Thus the integration will smooth out the superficial singularity leaving us a regular integration over \( \theta \). Furthermore, if \( \tilde{\omega} > \tilde{q} \geq 0 \), we can get the constraint for rapidity
\[ 0 < 2e^\theta < -\frac{\tilde{\omega}^2-\tilde{q}^2-3}{\tilde{\omega}-\tilde{q}} - \sqrt{\left(\frac{\tilde{\omega}^2-\tilde{q}^2-3}{\tilde{\omega}-\tilde{q}}\right)^2 - 4\frac{\tilde{\omega}+\tilde{q}}{\tilde{\omega}-\tilde{q}}} \text{ or } 2e^\theta > -\frac{\tilde{\omega}^2-\tilde{q}^2-3}{\tilde{\omega}-\tilde{q}} + \sqrt{\left(\frac{\tilde{\omega}^2-\tilde{q}^2-3}{\tilde{\omega}-\tilde{q}}\right)^2 - 4\frac{\tilde{\omega}+\tilde{q}}{\tilde{\omega}-\tilde{q}}}. \]

However, it’s easy to see in these two ranges that, because \( \tilde{\omega} \ll 1 \), we will have \( \cosh \theta \sim 1/\tilde{\omega} \), making it negligible in the zero frequency limit. If \( \tilde{\omega} \leq \tilde{q} \), we get constraint on the rapidity of \( \theta \) as (without loss of generality we choose \( \tilde{\omega} > 0 \)):
\[ 0 < 2e^\theta < \left[(\tilde{\omega}^2-\tilde{q}^2-3) + \sqrt{(\tilde{\omega}^2-\tilde{q}^2-1)(\tilde{\omega}^2-\tilde{q}^2-9)}\right]/(\tilde{q} - \tilde{\omega}) \equiv \mu(\tilde{\omega}, \tilde{q}). \]

We can then determine the maximum of \( \mu(\tilde{\omega}, \tilde{q}) \) to be located at \( \tilde{q}_m = \sqrt{(3 - \tilde{\omega})(1 - \tilde{\omega})} \); again recalling \( \tilde{\omega} \ll 1 \), we have \( \cosh \theta \gtrsim 2 - \tilde{\omega} \). This indicates that a small region of \( \tilde{q} \) exists, in which \( \cosh \theta \) is a little smaller than 2. Therefore, we will include in numerical calculations the channels \( D_{1,2} + D_{2,1} \). For the leftover two parts in Eq. (A.44), we have
\[
\begin{align*}
\frac{i(1 - S(\theta_1' - \theta_2')) F_1^\sigma}{\theta_1 - \theta_1' + i\varepsilon} &= P\frac{i(1 - S(\theta_1' - \theta_2')) F_1^\sigma}{\theta_1 - \theta_1'} - i\pi\delta(\theta_1 - \theta_1'), \quad (A.50) \\
\frac{i(S(\theta_1' - \theta_2') - 1) F_1^\sigma}{\theta_1 - \theta_2' + i\varepsilon} &= P\frac{i(S(\theta_1' - \theta_2') - 1) F_1^\sigma}{\theta_1 - \theta_2'} - i\pi\delta(\theta_1 - \theta_2'). \quad (A.51)
\end{align*}
\]

Here \( P \) denotes principal value integration. The parts of \( F_3^\sigma(\theta_1 + i\pi + i\varepsilon, \theta_1', \theta_1')F_3^\sigma(\theta_1 + i\pi + i\varepsilon, \theta_2', \theta_1') \) have no contributions; after integrating over \( \theta_1' \) or \( \theta_2' \), it only leaves us \( e^{-i\Delta_a \cosh \theta_1} \); since \( \omega \ll \Delta_a \), it vanishes for the local low-frequency dynamics. For the parts of \( F_3^\sigma(\theta_1 + i\pi + i\varepsilon, \theta_1', \theta_2')F_3^\sigma(\theta_1 + i\pi + i\varepsilon, \theta_2', \theta_1') \) containing \( 1/(\theta_1 - \theta_1' + i\varepsilon)^2 \), we can finish an integration by part, leaving us only a simple principal-value integration. We can repeat the discussions for the part having delta function, and show that it does not have any contribution. Consider now all the left over parts in...
Since they are all principal-value-type integration, they do not encounter any singularity. Following the discussion on the integration containing integrand of \( F_{3}^{3}(\theta_1 + i\pi + i\epsilon, \theta_1', \theta_2') \) \( F_{3}^{3}(\theta_1 + i\pi + i\epsilon, \theta_2', \theta_1') \), they will have similar contributions, and thus they will be included in our numerical calculations. The calculations for the other two channels \( aa - b \) and \( aa - c \) are similar.

### A.6 Calculation of \( D_{22} \)

Using the finite volume regularization scheme [60,90], we have

\[
D_{aa,aa} (x, t) = C_{22} - Z_1 C_{11} + (Z_1^2 - Z_2) C_{00} = I_1 + I_2 + I_3 + I_4 + I_5 + I_6 + I_7 + I_8 \quad (A.52)
\]

We analyze the integrals in \( D_{aa,aa} \) one by one. In all following analysis, we focus on the low-frequency regime. (High-frequency regime is relatively straightforward, where the steepest descent method can be applied directly.) The three integrals \( I_1, I_2 \) and \( I_3 \) are time-independent:

\[
I_1 = -2 \int \frac{d\theta_1}{2\pi} F_{2}^{\sigma}(i\pi, 0) \langle \sigma \rangle e^{-2\beta \Delta_a \cosh \theta_1} \quad (A.53)
\]

\[
I_2 = \frac{1}{2} \int \frac{d\theta_1 d\theta_2}{(2\pi)^2} (F_{2}^{\sigma}(i\pi, 0))^2 e^{-\beta \Delta_a (\cosh \theta_1 + \cosh \theta_2)} \quad (A.54)
\]

\[
I_3 = \int \frac{d\theta_1 d\theta_2}{(2\pi)^2} F_{4s}^{\sigma}(\theta_1, \theta_2) \langle \sigma \rangle e^{-\beta \Delta_a (\cosh \theta_1 + \cosh \theta_2)} \quad (A.55)
\]

where

\[
F_{4s}^{\sigma}(\theta_1, \theta_2) = \lim_{\varepsilon \to 0} F_{4}^{\sigma}(\theta_1 + i\pi + \varepsilon, \theta_2 + i\pi + \varepsilon, \theta_2, \theta_1) = 2i F_{2}^{\sigma}(\theta_2 + i\pi, \theta_1) \frac{[S_{aa}(\theta_1 - \theta_2) - S_{aa}(\theta_2 - \theta_1)]}{\theta_1 - \theta_2} + F_{4rc}^{\sigma}(\theta_2 + i\pi, \theta_1 + i\pi | \theta_2, \theta_1) \quad (A.56)
\]
Since \(\lim_{z \to 0} \left[ (S_{aa}(z) - S_{aa}(-z)) / z \right] = 2S'_{aa}(0)\) is finite, and \(F_{4rc}^a\) is a regular function on real axis \([60, 90]\), the whole integrand in \(I_3\) is regular. As we mentioned before we will return to the discussion of these constant parts.

The integral \(I_4\) is

\[
I_4 = -\int \int \frac{d\theta_1 d\theta_1'}{(2\pi)^2} (F_2^a(\theta_1 + i\pi, \theta_1'))^2 \cdot e^{-2\beta \Delta a \cosh \theta_1} \cdot e^{-ix \Delta a (\sinh \theta_1 - \sinh \theta_1')} \cdot e^{-it \Delta a (\cosh \theta_1' - \cosh \theta_1)}
\]

\[\text{(A.57)}\]

\(I_4\) has the same integral structure as seen in the calculation of \(S_{11}\), except for a different thermal weight-factor. So we will have a similar \(\ln(\omega/T)\) divergence in the low-frequency regime as in \(S_{11}\). However, it is associated with a \(e^{-2\Delta a / T}\) factor, and thus negligible compared with \(S_{11}\).

The integral \(I_5\) is

\[
I_5 = -\int \int \frac{d\theta_1 d\theta_2}{(2\pi)^2} (F_2^a(\theta_2 + i\pi, \theta_1))^2 \cdot e^{-\beta \Delta a (\cosh \theta_1 + \cosh \theta_2)} \cdot e^{-ix \Delta a (\sinh \theta_2 - \sinh \theta_1)} \cdot e^{-it \Delta a (\cosh \theta_1 - \cosh \theta_2)}
\]

\[\text{(A.58)}\]

Again we have a similar integrand structure as in \(S_{11}\), and therefore the divergence in the low-frequency regime in \(I_5\) will not be stronger than \(\ln(\omega/T)\); the thermal factor \(e^{-2\Delta a / T}\) again makes it negligible compared with \(S_{11}\).
The integral $I_6$ is $I_6^{(1)} + I_6^{(2)}$, with

$$I_6^{(1)} = \int \int \frac{d\theta_1 d\theta_2}{(2\pi)^2} \int \frac{d\theta'_1}{2\pi} (F_2^\sigma(\theta_1 + i\pi, \theta'_1))^2 \left(1 - S(\theta'_1 - \theta_1)S(\theta_1 - \theta_2)\right)$$

$$(-\Delta ax \cosh \theta_1 + \Delta ax \sinh \theta_1) e^{-\beta \Delta ax (\cosh \theta_1 + \cosh \theta_2)} e^{-ix\Delta ax (\sinh \theta_2 - \sinh \theta'_1)} .$$

$$I_6^{(2)} = -\int \int \frac{d\theta_1 d\theta_2}{(2\pi)^2} \int \frac{d\theta'_1}{2\pi} (F_2^\sigma(\theta_1 + i\pi, \theta'_1))^2 \varphi(\theta'_1 - \theta_1)S(\theta'_1 - \theta_1)S(\theta_1 - \theta_2)$$

$$e^{-\beta \Delta ax (\cosh \theta_1 + \cosh \theta_2)} e^{-ix\Delta ax (\sinh \theta_2 - \sinh \theta'_1)} e^{-it\Delta ax (\cosh \theta'_1 - \cosh \theta_2)}$$

where

$$\varphi(\theta'_1 - \theta_1)S(\theta'_1 - \theta_1)S(\theta_1 - \theta_2)$$

$$= -\frac{i}{S(\theta'_1 - \theta_1)} \frac{dS(\theta'_1 - \theta_1)}{d\theta'_1} S(\theta'_1 - \theta_1)S(\theta_1 - \theta_2)$$

$$= -iS(\theta_1 - \theta_2) \frac{dS(\theta'_1 - \theta_1)}{d\theta'_1}$$

We will see that combining $I_6^{(1)}$ and part of $I_8$ gives zero contribution to the local dynamics. So we consider $I_6^{(2)}$. Since the time-space oscillation factor in $I_6^{(2)}$, $e^{-ix\Delta ax (\sinh \theta_2 - \sinh \theta'_1)} e^{-it\Delta ax (\cosh \theta'_1 - \cosh \theta_2)}$, is independent of rapidity $\theta_1$, and the leftover integrand is regular on the real axis, we can apply the steepest descent method for $\theta_1$ with saddle point at $\theta_1 = 0$,

$$I_6^{(2)} \sim \sqrt{\frac{T}{\Delta ax}} e^{-\Delta ax/T} \int \int \frac{d\theta_1 d\theta'_1}{(2\pi)^2} (F_2^\sigma(i\pi, \theta'_1))^2 S(-\theta_2) \left[ i \frac{dS(\theta'_1)}{d\theta'_1} \right] .$$

$$e^{-\beta \Delta ax \cosh \theta_2} e^{-ix\Delta ax (\sinh \theta_2 - \sinh \theta'_1)} e^{-it\Delta ax (\cosh \theta'_1 - \cosh \theta_2)}$$
The leftover integral has similar structure as in $S_{11}$ and, in low-frequency regime,

$$
\left| I_6^{(2)}(\omega) \right| \sim \sqrt{\frac{T}{\Delta_a}} \frac{e^{-2\Delta_a/T} e^{\omega/2T} |F_2^g(i\pi, 0)|^2}{\Delta_a} S(0) S'(0) \ln \frac{\omega}{4T} \quad (\omega \ll T \ll \Delta_a).
$$

(A.64)

Thus, its contribution to the low-energy local dynamics is negligible compared with $S_{11}$.

The integral $I_7$ is

$$
I_7 = 2 \int \int \frac{d\theta_1 d\theta_2}{(2\pi)^2} P \int \frac{d\theta'_1}{2\pi} F^g_{4\text{ss}}(\theta_1 + i\pi, \theta_2 + i\pi|\theta'_1, \theta_1) F^g_2(\theta_2 + i\pi, \theta'_1)
$$

$$
e^{-\beta\Delta_a(\cosh \theta_1 + \cosh \theta_2)} e^{-ix\Delta_a(\sinh \theta_2 - \sinh \theta'_1)} e^{-it\Delta_a(\cosh \theta'_1 - \cosh \theta_2)}
$$

(A.65)

where

$$
F^g_{4\text{ss}}(\theta_1 + i\pi, \theta_2 + i\pi|\theta'_1, \theta_1) = i \frac{(S_{aa}(\theta_1 - \theta_2) + 1)}{\theta_1 - \theta'_1} F^g_2(\theta_2 + i\pi, \theta'_1) + F^g_{4\text{rc}}(\theta_1 + i\pi, \theta_2 + i\pi|\theta'_1, \theta_1)
$$

(A.66)

Consider the part containing $F^g_{4\text{rc}}(\theta_1 + i\pi, \theta_2 + i\pi|\theta'_1, \theta_1)$. Since $F^g_{4\text{rc}}(\theta_1 + i\pi, \theta_2 + i\pi|\theta'_1, \theta_1)$ is not singular on the real axis, this part of the integration behaves similarly as that in $I_6^{(2)}$, making its contribution negligible in the low-frequency regime. Consider next the part containing $\frac{i(S_{aa}(\theta_1 - \theta_2) + 1)}{\theta_1 - \theta'_1} F^g_2(\theta_2 + i\pi, \theta'_1)$. The integration here is still well defined in the sense of principal-value integration over $\theta'_1$. Recall the definition of principal-value integration:

$$
P \int_L \frac{h(\tau)}{\tau - t} d\tau = \int_L \frac{h(\tau) - h(t)}{\tau - t} d\tau + h(t) \ln \frac{b - t}{t - a}
$$

(A.67)

where $t$ lies on curve $L$ (not at end points). Since $\theta'_1$ integration is on real axis,

$$
P \int_R \frac{h(\theta'_1)}{\theta_1 - \theta'_1} d\theta'_1 = P \int_{-\infty}^{\infty} \frac{h(\theta'_1)}{\theta_1 - \theta'_1} d\theta'_1 = - \int_L \frac{h(\theta'_1) - h(\theta_1)}{\theta'_1 - \theta_1} d\tau
$$

(A.68)
In our case,

\[ h(\theta') = i \left( S_{aa}(\theta_1 - \theta_2) + 1 \right) \left[ F_2^\sigma(\theta_2 + i\pi, \theta_1') \right]^2 e^{i\Delta_a x \sinh \theta'_1} e^{-i\Delta_a \cosh \theta'_1} \]  

The function associated with \( e^{-\beta \Delta_a \cosh \theta_1} \) is not singular on real axis. Thus we can apply steepest decent method for \( \theta_1 \), leaving us \( \theta'_1 \) and \( \theta_2 \) integrations as

\[ I_7 \sim 2 \sqrt{\frac{T}{\Delta_a}} e^{-\beta \Delta_a} \int \frac{d\theta_2 d\theta'_1}{(2\pi)^2} \frac{i [S_{aa}(\theta_2) + 1]}{\theta'_1} \left[ \left( F_2^\sigma(\theta_2 + i\pi, \theta'_1) \right)^2 - \left( F_2^\sigma(\theta_2 + i\pi, 0) \right)^2 \right] e^{-\beta \cosh \theta_2} e^{-i\Delta_a x (\sinh \theta_2 \sinh \theta'_1)} e^{-it\Delta_a \cosh \theta'_1} \]  

(A.70)

For the leftover integration, we encounter a structure similar as in \( S_{11} \). Therefore the part involving principal-value integration gives contribution at the order of

\[ \frac{1}{\Delta_a} \sqrt{\frac{T}{\Delta_a}} e^{-2\Delta_a/T} |F_2^\sigma(i\pi, 0)|^2 \ln \frac{\omega}{4T} \]. Combining with the other part’s contribution we have

\[ I_7(\omega) \sim \frac{1}{\Delta_a} \sqrt{\frac{T}{T}} e^{-2\Delta_a/T} |F_2^\sigma(i\pi, 0)|^2 \ln \frac{\omega}{4T} \quad (\omega \ll T \ll \Delta_a) \]  

(A.71)

We conclude that \( I_7 \)'s contribution to low-energy local dynamics is negligible compared with \( S_{11} \).

The integral \( I_8 \) is

\[ I_8 = \frac{1}{4} \int \int \int \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^4} F_4^\sigma(\theta_2 + i\pi, \theta_1 + i\pi, \theta'_1, \theta'_2) F_4^\sigma(\theta_1 + i\pi, \theta_2 + i\pi, \theta'_2, \theta'_1) e^{-\beta \Delta_a (\cosh \theta_1 + \cosh \theta_2)} e^{-i\Delta_a x (\sinh \theta_1 + \sinh \theta_2 - \sinh \theta'_1 - \sinh \theta'_2)} e^{-it\Delta_a (\cosh \theta'_1 + \cosh \theta'_2 - \cosh \theta_1 - \cosh \theta_2)} \]  

(A.72)
where

\[
\begin{align*}
F_4^\sigma (\theta_2 + i\pi, \theta_1 + i\pi, \theta_1', \theta_2') &\quad F_4^\sigma (\theta_1 + i\pi, \theta_2 + i\pi, \theta_2', \theta_1') \\
&= F_4^\sigma_{4rc} (\theta_2 + i\pi, \theta_1 + i\pi|\theta_1' + i\varepsilon, \theta_2' + i\varepsilon) \cdot \\
&\quad \cdot F_4^\sigma_{4rc} (\theta_1 + i\pi, \theta_2 + i\pi|\theta_2' + i\varepsilon, \theta_1' + i\varepsilon) \\
+ &\quad F_4^\sigma_{4rc} (\theta_2 + i\pi, \theta_1 + i\pi|\theta_1' + i\varepsilon, \theta_2' + i\varepsilon) \cdot \\
&\quad \cdot \left[ \frac{E}{\theta_1 - \theta_2' - i\varepsilon} + \frac{F}{\theta_1 - \theta_1' - i\varepsilon} + \frac{G}{\theta_2 - \theta_2' - i\varepsilon} + \frac{H}{\theta_2 - \theta_1' - i\varepsilon} \right] \\
+ &\quad F_4^\sigma_{4rc} (\theta_1 + i\pi, \theta_2 + i\pi|\theta_1' + i\varepsilon, \theta_2' + i\varepsilon) \cdot \\
&\quad \cdot \left[ \frac{A}{\theta_2 - \theta_1' - i\varepsilon} + \frac{B}{\theta_2 - \theta_2' - i\varepsilon} + \frac{C}{\theta_1 - \theta_1' - i\varepsilon} + \frac{D}{\theta_1 - \theta_2' - i\varepsilon} \right] \\
+ &\quad \frac{AH}{(\theta_2 - \theta_1' - i\varepsilon)^2} + \frac{BG}{(\theta_2 - \theta_2' - i\varepsilon)^2} + \frac{CF}{(\theta_1 - \theta_1' - i\varepsilon)^2} + \frac{DE}{(\theta_1 - \theta_2' - i\varepsilon)^2} \\
+ &\quad \frac{AE + DH}{(\theta_2 - \theta_1' - i\varepsilon)(\theta_1 - \theta_2' - i\varepsilon)} + \frac{AF + CH}{(\theta_2 - \theta_1' - i\varepsilon)(\theta_1 - \theta_1' - i\varepsilon)} \\
+ &\quad \frac{AG + BH}{(\theta_2 - \theta_2' - i\varepsilon)(\theta_1 - \theta_1' - i\varepsilon)} + \frac{BE + DG}{(\theta_2 - \theta_2' - i\varepsilon)(\theta_1 - \theta_1' - i\varepsilon)} \\
+ &\quad \frac{BF + CG}{(\theta_2 - \theta_2' - i\varepsilon)(\theta_1 - \theta_1' - i\varepsilon)} + \frac{CE + DF}{(\theta_1 - \theta_1' - i\varepsilon)(\theta_1 - \theta_2' - i\varepsilon)}
\end{align*}
\]
with

\[ A = i \left[ S (\theta_2 - \theta_1) - S (\theta'_2 - \theta'_1) \right] F^\sigma \left( \theta_1 + i\pi, \theta'_2 \right) ; \]

\[ B = i \left[ S (\theta'_1 - \theta'_2) S (\theta_2 - \theta_1) - 1 \right] F^\sigma \left( \theta_1 + i\pi, \theta'_1 \right) ; \]

\[ C = i \left[ 1 - S (\theta_2 - \theta_1) S (\theta'_1 - \theta'_2) \right] F^\sigma \left( \theta_2 + i\pi, \theta'_2 \right) ; \]

\[ D = i \left[ S (\theta'_1 - \theta'_2) - S (\theta_2 - \theta_1) \right] F^\sigma \left( \theta_2 + i\pi, \theta'_1 \right) ; \]

\[ E = i \left[ S (\theta_1 - \theta_2) - S (\theta'_2 - \theta'_1) \right] F^\sigma \left( \theta_2 + i\pi, \theta'_1 \right) ; \]

\[ F = i \left[ S (\theta'_2 - \theta'_1) S (\theta_1 - \theta_2) - 1 \right] F^\sigma \left( \theta_2 + i\pi, \theta'_2 \right) ; \]

\[ G = i \left[ 1 - S (\theta_1 - \theta_2) S (\theta'_2 - \theta'_1) \right] F^\sigma \left( \theta_1 + i\pi, \theta'_1 \right) ; \]

\[ H = i \left[ S (\theta'_2 - \theta'_1) - S (\theta_1 - \theta_2) \right] F^\sigma \left( \theta_1 + i\pi, \theta'_2 \right) \] (A.82)

From Eq. (A.75) we have \((q \text{ and } \omega \text{ has been rescaled by } \Delta_a)\)

\[ I^{(1)}_8 (\omega, q) = \frac{1}{\Delta^2_a} \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^2} F_{4rc}^\sigma (\theta_2 + i\pi, \theta_1 + i\pi | \theta'_1, \theta'_2) \cdot \]

\[ \cdot F_{4rc}^\sigma (\theta_1 + i\pi, \theta_2 + i\pi, \theta'_1, \theta'_2) \delta (q + \sinh \theta_1 + \sinh \theta_2 - \sinh \theta'_1 - \sinh \theta'_2) \cdot \]

\[ \cdot \delta (\omega + \cosh \theta_1 + \cosh \theta_2 - \cosh \theta'_1 - \cosh \theta'_2) \] (A.83)

\[ = \frac{1}{\Delta^2_a} \int \frac{d\theta_1 d\theta_2}{(2\pi)^2} \cdot \]

\[ F_{4rc}^\sigma (\theta_2 + i\pi, \theta_1 + i\pi | \theta'_1, \theta'_2) F_{4rc}^\sigma (\theta_1 + i\pi, \theta_2 + i\pi, \theta'_1, \theta'_2) e^{-\Delta_a (\cosh \theta_1 + \cosh \theta_2)} \]

\[ \left\{ \left[ \frac{(\omega + \cosh \theta_1 + \cosh \theta_2)^2 - (q + \sinh \theta_1 + \sinh \theta_2)^2}{2} - 1 \right]^2 - 1 \right\}^{1/2} \]

\[ \Rightarrow \]

\[ I^{(1)}_8 (\omega) = \frac{1}{\Delta_a} \int dq \int \frac{d\theta_1 d\theta_2}{(2\pi)^2} \]

\[ F_{4rc}^\sigma (\theta_2 + i\pi, \theta_1 + i\pi | \theta'_1, \theta'_2) F_{4rc}^\sigma (\theta_1 + i\pi, \theta_2 + i\pi, \theta'_1, \theta'_2) e^{-\Delta_a (\cosh \theta_1 + \cosh \theta_2)} \]

\[ \left\{ \left[ \frac{(\omega + \cosh \theta_1 + \cosh \theta_2)^2 - (q + \sinh \theta_1 + \sinh \theta_2)^2}{2} - 1 \right]^2 - 1 \right\}^{1/2} \] (A.84)

where \(\theta'_1\) and \(\theta'_2\) are functions of \(\theta_1\) and \(\theta_2\). Then we can apply steepest descent
method on \( I_8^{(1)}(\omega) \), leading to (unlike \( S_{11} \), here \( \theta_1 \) and \( \theta_2 \) are independent of \( q \) and \( \omega \)),

\[
I_8^{(1)}(\omega) \sim \frac{F_{4rc}(i\pi, i\pi|0,0)^2}{\Delta_a} \frac{T}{\Delta_a} e^{-2\Delta_a/T} \int dq \frac{1}{\sqrt{\left(\frac{(\omega+2)^2-q^2}{2} - 1\right)^2 - 1}} \quad (A.85)
\]

The allowed integral range of \( q \) can be determined by

\[
\left(\frac{(\omega+2)^2-q^2}{2} - 1\right)^2 - 1 \geq 0 \Rightarrow (\omega^2 + 4\omega - q^2) \left[\frac{1}{4} (\omega^2 + 4\omega - q^2) + 1\right] \geq 0 \Rightarrow
\]

\[
(q^2 - \omega^2 - 4\omega) (q^2 - 4\omega - \omega^2 - 4) \geq 0 \Rightarrow q^2 \geq 4 + \omega^2 + 4\omega \quad \text{or} \quad q^2 \leq \omega^2 + 4\omega \quad (A.86)
\]

Using evenness of the integrand as a function of \( q \) (so the integral over \( q \) can be shrunk to \((0, \infty)\)) and making variable transform \( z = \omega^2 + 4\omega - q^2 \), we have

\[
I_8^{(1)}(\omega) \sim \frac{F_{4rc}(i\pi, i\pi|0,0)^2}{\pi \Delta_a} \frac{T}{\Delta_a} e^{-2\Delta_a/T} \left( \int_{4}^{\infty} dz + \int_{-(4\omega + \omega^2)}^{0} \frac{dz}{\sqrt{(z + 4\omega + \omega^2)(z - 4)}} \right) \int dq \frac{1}{\sqrt{(z + 4\omega + \omega^2)(z - 4)}} \frac{z}{\sqrt{a}}
\]

\[
= \frac{F_{4rc}(i\pi, i\pi|0,0)^2}{\pi \Delta_a} \frac{T}{\Delta_a} e^{-2\Delta_a/T} \left[ \frac{2(iK(-4/a) + K(1 + 4/a))}{\sqrt{a}} + K(-a/4) \right] \quad (a \ll 1)
\]

\[
= \frac{F_{4rc}(i\pi, i\pi|0,0)^2}{\pi \Delta_a} \frac{T}{\Delta_a} e^{-2\Delta_a/T} \left\{ \pi - \frac{\pi}{16} a + \frac{9\pi}{1024} a^2 + \ldots \right\} \quad (a \ll 1)
\]

\[
= \frac{F_{4rc}(i\pi, i\pi|0,0)^2}{\pi \Delta_a} \frac{T}{\Delta_a} e^{-2\Delta_a/T} \left\{ 1 - \frac{1}{4} \frac{\omega}{\Delta_a} + \ldots \right\} \quad (A.87)
\]

where \((a = \omega^2 + 4\omega)\). Therefore, \( I_8^{(1)} \) is negligible for the low-energy local dynamics compared with \( S_{11} \).

For Eqs. (A.76,A.77), all terms have a similar structure, so we can just focus on...
one of them.

\[
I_8^{(2)} = \frac{1}{4} \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^4} F^\sigma_{4rc} (\theta_2 + i\pi, \theta_1 + i\pi|\theta'_1 + i\varepsilon + \theta'_2 + i\varepsilon) \frac{E}{\theta_1 - \theta'_2 - i\varepsilon}
\]

\[
e^{-\beta \Delta_n (\cosh \theta_1 + \cosh \theta_2)} e^{-i \Delta_n x (\sinh \theta_1 + \sinh \theta_2 - \sinh \theta'_1 - \sinh \theta'_2)} e^{-i t \Delta_n (\cosh \theta'_1 + \cosh \theta'_2 - \cosh \theta_1 - \cosh \theta_2)}
\]

\[
= I_8^{(2),1} + I_8^{(2),2}
\]  

(A.88)

where

\[
I_8^{(2),1} = \frac{1}{4} P \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^4} F^\sigma_{4rc} (\theta_2 + i\pi, \theta_1 + i\pi|\theta'_1 + i\varepsilon + \theta'_2 + i\varepsilon) \frac{E}{\theta_1 - \theta'_2}
\]

\[
e^{-\beta \Delta_n (\cosh \theta_1 + \cosh \theta_2)} e^{-i \Delta_n x (\sinh \theta_1 + \sinh \theta_2 - \sinh \theta'_1 - \sinh \theta'_2)} e^{-i t \Delta_n (\cosh \theta'_1 + \cosh \theta'_2 - \cosh \theta_1 - \cosh \theta_2)}
\]  

(A.89)

and

\[
I_8^{(2),2} = \frac{1}{4} i \pi \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^4} F^\sigma_{4rc} (\theta_2 + i\pi, \theta_1 + i\pi|\theta'_1 + i\varepsilon + \theta'_2 + i\varepsilon) E\delta(\theta_1 - \theta'_2)
\]

\[
e^{-\beta \Delta_n (\cosh \theta_1 + \cosh \theta_2)} e^{-i \Delta_n x (\sinh \theta_1 + \sinh \theta_2 - \sinh \theta'_1 - \sinh \theta'_2)} e^{-i t \Delta_n (\cosh \theta'_1 + \cosh \theta'_2 - \cosh \theta_1 - \cosh \theta_2)}
\]  

(A.90)

For \(I_8^{(2),1}\), the principal value integral structure will be similar as that appearing in \(I_7\). Similar analysis can be applied to \(I_8^{(2),1}\), leading to a non-singular contribution in the low-frequency regime (it’s a four-fold integration similar to that appearing in \(I_8^{(1)}\)). As for \(I_8^{(2),2}\), it’s easy to get

\[
I_8^{(2),2} = \frac{1}{4} i \pi \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^4} F^\sigma_{4rc} (\theta_2 + i\pi, \theta_1 + i\pi|\theta'_1, \theta'_2) E|_{\theta_1 = \theta'_2}.
\]

\[
e^{-\beta \Delta_n (\cosh \theta_1 + \cosh \theta_2)} e^{-i \Delta_n x (\sinh \theta_2 - \sinh \theta'_2)} e^{-i t \Delta_n (\cosh \theta'_1 - \cosh \theta_2)}
\]  

(A.91)

where \(E|_{\theta_1 = \theta'_2} = i |S(-\theta_2) - S(-\theta'_2)| F^\sigma_{2} (\theta_2 + i\pi, \theta'_2)\). We encounter similar integral structure as shown in \(I_6^{(2)}\). Thus, this part’s contribution will be of the same order as
that appearing in $I^{(2)}_6$. Therefore the contribution from $I^{(2)}_8$ to the low-energy local dynamics is negligible compared with $S_{11}$.

For Eqs. (A.78–A.81), let’s first consider the parts containing terms similar to the following:

$$AE + DH \over (\theta_2 - \theta'_1 - i\varepsilon) (\theta_1 - \theta'_2 - i\varepsilon)$$  \hspace{1cm} (A.92)

Other five similar terms will have contribution at the same order of this one. For this one we have

$$AE + DH \over (\theta_2 - \theta'_1 - i\varepsilon) (\theta_1 - \theta'_2 - i\varepsilon) = P \over \theta_2 - \theta'_1 \over 1 \over \theta_1 - \theta'_2 \over i\pi\delta(\theta_1 - \theta'_2) (AE + DH) + (A.93)$$

$$P \over \theta_1 - \theta'_2 i\pi\delta(\theta_2 - \theta'_1) (AE + DH) - \pi^2\delta(\theta_2 - \theta'_1) \delta(\theta_1 - \theta'_2) (AE + DH) (A.94)$$

For the first term we will encounter similar structure as $I^{(1)}_8$, and for the second and third terms we will encounter similar structure as $I^{(2)}_8$. It is also easy to calculate

$$\pi^2\delta(\theta_2 - \theta'_1) \delta(\theta_1 - \theta'_2) (AE + DH) = 0.$$ Thus, the total contribution from the term containing $AE + DH \over (\theta_2 - \theta'_1 - i\varepsilon)(\theta_1 - \theta'_2 - i\varepsilon)$ is negligible. This applies to other similar terms, in which there can exist non-vanishing terms of two multiples of delta functions. The terms having this kind of structure will have similar integral structure as $S_{11}$, after integrating over the two delta functions. But the thermal factor $e^{-2\Delta_a/T}$ makes this negligible.

We next discuss last terms which have a similar structure as

$$AH \over (\theta_2 - \theta'_1 - i\varepsilon)^2$$  \hspace{1cm} (A.95)
Such terms can formerly be handled as follows,

\[
\frac{AH}{(\theta_2 - \theta'_1 - i\varepsilon)^2} \rightarrow \text{Integration by part} \rightarrow \int \frac{1}{\theta'_1 - \theta_2 + i\varepsilon} \partial\theta'_1 (AH \cdots) \quad (A.96)
\]

Combining the contributions from four such terms with that appearing in \( I^{(1)}_6 \) will yield zero contribution to the low-energy local dynamics. Explicitly we have

\[
AH = - [S(\theta_2 - \theta_1) - S(\theta'_1 - \theta'_2)] F_2^\sigma (\theta_1 + i\pi, \theta'_2) \cdot \\
\cdot [S(\theta'_2 - \theta'_1) - S(\theta_1 - \theta_2)] F_2^\sigma (\theta_1 + i\pi, \theta'_1) \\
= [2 - S(\theta_2 - \theta_1)S(\theta'_2 - \theta'_1) - S(\theta_1 - \theta_2)S(\theta'_1 - \theta'_2)] (F_2^\sigma (\theta_1 + i\pi, \theta'_2))^2
\]

\[
\Rightarrow \frac{1}{4} \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^4} \frac{AH}{(\theta_2 - \theta'_1 - i\varepsilon)^2} K_{tx}^{(\beta)} (\theta_1, \theta_2) (\theta'_1, \theta'_2) \\
= \frac{1}{4} \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^4} \frac{AH K_{tx}^{(\beta)} (\theta_1, \theta_2) (\theta'_1, \theta'_2)}{\theta_2 - \theta'_1 - i\varepsilon} \bigg|_{\theta'_1 = \infty} + \\
\frac{1}{4} \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^4} \frac{1}{\theta'_1 - \theta_2 + i\varepsilon} \left[ K_{tx}^{(\beta)} \partial\theta'_1 (AH) + AH \left( \partial\theta'_1 K_{tx}^{(\beta)} \right) \right] \\
= \frac{1}{4} \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^4} \left[ P \frac{1}{\theta'_1 - \theta_2} - i\pi \delta (\theta'_1 - \theta_2) \right] \left[ K_{tx}^{(\beta)} \partial\theta'_1 (AH) + AH \left( \partial\theta'_1 K_{tx}^{(\beta)} \right) \right] \\
(A.98)
\]

where

\[
K_{tx}^{(\beta)} (\theta_1, \theta_2, \theta'_1, \theta'_2) = \\
e^{-\beta \Delta_a (\cosh \theta_1 + \cosh \theta_2)} e^{-i\Delta_a x (\sinh \theta_1 + \sinh \theta_2 - \sinh \theta'_1 - \sinh \theta'_2)} e^{-it\Delta_a (\cosh \theta'_1 + \cosh \theta'_2 - \cosh \theta_1 - \cosh \theta_2)}
(A.99)
\]

Let’s focus on the following integral (all other integrals will have similar features as before),

\[
\frac{1}{4} \int \frac{d\theta_1 d\theta_2 d\theta'_1 d\theta'_2}{(2\pi)^4} \left[ -i\pi \delta (\theta'_1 - \theta_2) \right] \left[ K_{tx}^{(\beta)} \partial\theta'_1 (AH) \right] \\
(A.100)
\]
where

\[[-i\pi \delta (\theta_1' - \theta_2)] \left[ AH \left( \partial_{\theta_1'} K_{tx}^{(b)} \right) \right] \]

\[= \pi \delta (\theta_1' - \theta_2) \left[ 2 - S(\theta_2 - \theta_1)S(\theta_2' - \theta_2) - S(\theta_1 - \theta_2)S(\theta_2 - \theta_2') \right] \]

(A.101)

\[
(F_2^\sigma (\theta_1 + i\pi, \theta_2'))^2 \left( x \Delta_a \cosh \theta_2 - t \Delta_a \sinh \theta_2 \right) K_{tx}^{(b)} (\theta_1 \theta_2 | \theta_1 \theta_1')
\]

Substituting the above results back into the integral, and after finishing the integration over the delta function we can re-label the integral variables as follows

\[\theta_1 \leftrightarrow \theta_2 \text{ and } \theta_1' \rightarrow \theta_1'\] (A.102)

we get

\[
\frac{1}{4} \int \frac{d\theta_1 d\theta_2 d\theta_1' d\theta_2'}{(2\pi)^4} \left[ [-i\pi \delta (\theta_1' - \theta_2)] \left[ AH \left( \partial_{\theta_1'} K_{tx}^{(b)} \right) \right] \right] =
\]

\[
\frac{1}{8} \int \frac{d\theta_1 d\theta_2 d\theta_1'}{(2\pi)^3} \left[ 2 - S(\theta_1 - \theta_2)S(\theta_1' - \theta_1) - S(\theta_2 - \theta_1)S(\theta_1 - \theta_1') \right] \]

\[
(F_2^\sigma (\theta_1 + i\pi, \theta_2'))^2 \left( x \Delta_a \cosh \theta_2 - t \Delta_a \sinh \theta_2 \right) K_{tx}^{(b)} (\theta_1 \theta_2 | \theta_1 \theta_1')
\]

(A.103)

For the other three similar terms, one can get a similar integral as above for the part we are interested in. These parts can be combined with that appearing in \(I_6^{(1)}\) and yield

\[
I_c(x, t) \equiv I_{8\text{part}}^{(1)} + I_6^{(1)} = \frac{1}{2} \int \frac{d\theta_1 d\theta_2 d\theta_1'}{(2\pi)^3} \left[ S(\theta_1 - \theta_2)S(\theta_1' - \theta_1) - S(\theta_2 - \theta_1)S(\theta_1 - \theta_1') \right] \]

\[
(F_2^\sigma (\theta_1 + i\pi, \theta_2'))^2 \left( x \Delta_a \cosh \theta_2 - t \Delta_a \sinh \theta_2 \right) K_{tx}^{(b)} (\theta_1 \theta_2 | \theta_1 \theta_1')
\]

(A.104)

\[
\Rightarrow \quad I_c(\omega) = \frac{1}{2} \int \frac{d\theta_1 d\theta_2 d\theta_1'}{(2\pi)^3} u(\theta_1, \theta_2, \theta_1', \omega)
\]

(A.105)
with
\[ u(\theta_1, \theta_2, \theta'_1, \omega) = (F_2^\theta (\theta_1 + i\pi, \theta'_2))^2 e^{-\beta \Delta_a (\cosh \theta_1 + \cosh \theta_2)} e^{-i \Delta_a (\cosh \theta'_1 - \cosh \theta_2)}. \]

\[ \cdot [S(\theta_1 - \theta_2)S(\theta'_1 - \theta_1) - S(\theta_2 - \theta_1)S(\theta_1 - \theta'_1)] \frac{2\pi \delta [\omega - \Delta_a (\cosh \theta'_1 - \cosh \theta_2)]}{\omega - \Delta_a (\cosh \theta'_1 - \cosh \theta_2)} \]

(A.106)

Because
\[ u(-\theta_1, -\theta_2, -\theta'_1, \omega) = -u(\theta_1, \theta_2, \theta'_1, \omega), \]
we have \( I_c(\omega) = 0 \).

Combining all of the above, we conclude that (except for the time-independent parts in \( I_8 \), see below) there are no singularities in the frequency dependence that are stronger than that of \( S_{11} \), and the thermal factor \( e^{-2\Delta_a/T} \) makes \( S_{22} \) to be negligible compared to \( S_{11} \).

### A.7 Contributions of disconnected parts up to \( D_{22} \)

At \( x \to \infty \) we expect following cluster properties,
\[ \langle \sigma(x,t)\sigma(0,0) \rangle_T \sim \langle \sigma(0,0) \rangle_T^2 \] (A.108)

Applying the Leclair-Mussardo formula [91] for the single-point function \( \langle \sigma(0,0) \rangle_T \) in Eq. (A.108), we can get the part which contributes time-independent pieces in the two-point correlation function \( \langle \sigma(x,t)\sigma(0,0) \rangle_T \). Indeed in the \( E_8 \) model, up to \( e^{-3\Delta_i/T} \) (\( i = a, b, c \)), the time independent parts up to \( D_{22} \) can be summed over to
\langle \sigma \rangle_{2}^{T,i} + O(e^{-3\Delta_i/T}) \text{ with}

\langle \sigma \rangle_{T,i} = \langle \sigma \rangle_0 + \int \frac{d\theta_1}{2\pi} F_{2}^{\sigma}(i\pi, 0)e^{-\beta \Delta_i \cosh \theta_1} - \int \frac{d\theta_1}{2\pi} F_{2}^{\sigma}(i\pi, 0)e^{-2\beta \Delta_i \cosh \theta_1}

+ \frac{1}{2} \int \int \frac{d\theta_1 d\theta_2}{(2\pi)^2} F_{4s}^{\sigma}(\theta_1, \theta_2)e^{-\beta \Delta_i (\cosh \theta_1 + \cosh \theta_2)} + O(e^{-3\Delta_i/T}) \ (i = a, b, c)

(A.109)

It’s easy to see that \langle \sigma \rangle_{T,i} above is term-by-term corresponding to Leclair-Mussardo formula [91]. We thus expect that, when summing over to infinite terms of the expansion series, the contribution from all of these space-time independent terms will sum over to \langle \sigma(0, 0) \rangle_{T}^{2}. In other words, none of the time-independent terms in the two-point correlation function will appear in the two-point connected correlation function.
Appendix B

Appendix for thermodynamics near quantum critical point in itinerant magnetic systems

B.1 Some formulas

Logarithm gamma function and digamma function can be expressed as [92],

\[
\ln \Gamma(z) = (z - 1/2) \ln z + (\ln 2\pi)/2 + 2 \int_0^\infty \frac{\arctan(t/z) dt}{e^{2\pi t} - 1} \quad (B.1)
\]
\[
\psi(z) = \frac{d\ln \Gamma(z)}{dz} = -\frac{1}{2z^2} + \ln z - \int_0^\infty \frac{2t dt}{(t^2 + z^2)(e^{2\pi t} - 1)} \quad (B.2)
\]

and generalized Riemann zeta function is [92],

\[
\zeta(s, z) = \frac{z^{-s}}{2} + \frac{z^{1-s}}{s-1} + 2 \int_0^\infty \frac{(z^2 + y^2)^{-s/2} \sin(s\theta)}{e^{2\pi y} - 1} dy \quad \text{where } \theta = \arctan(y/z) \Rightarrow
\]
\[
\zeta(2, z) = \frac{1}{2z^2} + \frac{1}{z} + \int_0^\infty \frac{2\sin 2\theta}{z^2 + y^2} \frac{dy}{e^{2\pi y} - 1} \quad (B.3)
\]
\[
= \frac{1}{2z^2} + \frac{1}{z} + \int_0^\infty \frac{4zy}{(z^2 + y^2)^2} \frac{dy}{e^{2\pi y} - 1} \quad (B.4)
\]

When \(|z|\) is large (\(|z| \to \infty\)),

\[
\ln \Gamma(z) \sim (z - 1/2) \ln z + (\ln 2\pi)/2 + \sum_{r=1}^n \frac{(-1)^{r-1} B_r}{2r(2r-1)} z^{-2r+1} + O(z^{-2n-1}) (B.5)
\]
\[
\psi(z) \sim -\frac{1}{2z} + \ln z - \sum_{r=1}^n \frac{(-1)^{r-1} B_r}{2r} z^{-2r} + O(z^{-2n-2}) \quad (B.6)
\]
\[
\zeta(2, z) = \frac{d\psi(z)}{dz} \sim \frac{1}{2z^2} + \frac{1}{z} + \sum_{r=1}^n (-1)^{r-1} B_r z^{-2r-1} + O(z^{-2n-3}) \quad (B.7)
\]
Figure B.1: Feynman diagrams for the free energy of the QLGT to the quadratic order in $u$ in bare loop-perturbative expansion. The cross symbol is used to denote the bare coupling $u$. $F_G$ here is bare Gaussian free energy, the two loop diagram represents bare two-loop contribution $F_u$, and the two three-loop diagrams contribute to $F_{u^2}$.

As a result, we have following useful asymptotic formulas,

\[ 2 \int_0^\infty \frac{\arctan \left( \frac{t}{z} \right) dt}{e^{2\pi t} - 1} \sim \sum_{r=1}^n \frac{(-1)^{r-1}B_r}{2r(2r-1)} z^{-2r+1} + O(z^{-2n-1}) \quad (|z| \to \infty) \quad (B.8) \]

\[ \int_0^\infty \frac{2tdt}{(t^2 + z^2)(e^{2\pi t} - 1)} \sim \sum_{r=1}^n \frac{(-1)^{r-1}B_r}{2r} z^{-2r} + O(z^{-2n-2}) \quad (|z| \to \infty) \quad (B.9) \]

\[ \int_0^\infty \frac{4zy}{(z^2 + y^2)^2 e^{2\pi y} - 1} dy \sim \sum_{r=1}^n (-1)^{r-1}B_r z^{-2r-1} + O(z^{-2n-3}) \quad (|z| \to \infty) \quad (B.10) \]

where $B_r (r = 1, 2, 3, \cdots)$ are Bernoulli coefficients. Eq. (B.8,B.9,B.10) will be used in following sections.

B.2 Perturbation calculation for the bare free energy density

We will perform bare free energy density calculation for $d3z2$ systems in this section.

B.2.1 Bare perturbation series for free energy density

For our purpose we expand the bare free energy density to $u^2$ as it is shown in Fig.(B.1),

\[ F \sim F_G + \frac{u}{\pi} + \frac{u^2}{2} + \frac{u^2}{\pi} + O(u^3) \]
\[ F = F_G + F_u + F_{u^2} + \cdots \]  

where \( F_G \) and \( F_u \) are the same as Eq. (3.8) and Eq. (3.9), and

\[
F_{u^2} = -u^2 \left[ 4n^2(n+8)I^2J + 4n(n+2) \int_0^{\beta} d\tau \int d^d x \langle \phi(\tau,x)\phi(0,0) \rangle \right]^4
\]  

(B.12)

with

\[
J = 2 \int_0^{\Lambda} \frac{d^dq}{(2\pi)^d} \int_0^{\Gamma_q} d\varepsilon \frac{d\varepsilon}{\pi} \coth \left( \frac{\varepsilon}{2T} \right) \left( \frac{\varepsilon}{\Gamma_q} \right) \left( r_0 + (q\xi_0)^2 \right) \left( \frac{r_0 + (q\xi_0)^2}{(\varepsilon/\Gamma_q)^2 + (r_0 + (q\xi_0)^2)^2} \right)^2
\]  

(B.13)

In the following we will specifically calculate critical behavior of bare free energy for \( d3z2 \) systems. First let’s give an estimation for the second term in the bracket of Eq. (B.12). After some calculations we get its leading behaviors in QC (Eq. (B.47)) are \( T^{7/2} \) at infrared limit, and \( T^5 \) at ultraviolet limit. And furthermore in FL (Eq. (B.59)) its leading behaviors are \( \delta^{7/2} \) at both infrared and ultraviolet limits. Since the integrand in Eq. (B.24) is not singular in the intermediate regime, which indicates the contribution from intermediate regime is finite and a crossover between infrared and ultraviolet limits. As a result, the contribution from the second term in the bracket of Eq. (B.12) is subleading in QC and FL. For avoiding unnecessary complication we will not consider this term in following discussions. In the detailed discussions of critical behavior of \( d3z2 \) in QCR and FLR in following two subsections, we will only focus on scalar case, i.e., \( n = 1 \).
Figure B.2: Sunflower Feynman diagram for the most singular one at the order of $u^N$ in bare perturbative loop expansion, where each small ring is corresponding to self-connection of two legs in each four-leg vertex, and the big ring is corresponding to the connections of all left over two legs of all $N$ four-leg vertexes.

B.2.2 Sunflower diagrams in bare loop perturbative series

At the order of $u^N$ in bare perturbative loop expansion, there are $N$ four-leg vertexes connecting with each other forming into a large number of connected Feynman diagrams. One important connected diagram among them is sunflower diagram shown in Fig. (B.2), where each small ring is corresponding to self-connection of two legs in each four-leg vertex, i.e., $I$, and the big ring is corresponding to the connections of all left over two legs of all $N$ four-leg vertexes. We denote the big ring in this sunflower diagram as $J_N$, which is proportional to $T \sum_{\omega_l} \int \frac{d^d q}{(2\pi)^d} (r_0 + (q\xi_0)^2 + |\omega_l|/\Gamma_\omega)^N$. The explicit formula for sunflower diagram at the order of $u^N$ is

$$-\frac{T}{2} \frac{1}{N!} I^N \frac{d^N}{dr_0^N} \sum_{\omega_l} \int \frac{d^d q}{(2\pi)^d} \ln \left( r_0 + (q\xi_0)^2 + |\omega_l|/\Gamma_\omega \right) = \frac{1}{N!} I^N \frac{d^N}{dr_0^N} F_G$$  (B.14)
Then we can do re-summation over all of this kind of diagrams of free energy as follows [93,94],

$$\sum_{N=0}^{\infty} \left( \frac{1}{N!} I^N \frac{d^N}{dr_0^N} F_G \right) = F_G(r_0 + I) \quad (B.15)$$

which indicates we can formally get a closed form after re-summation of sunflower diagrams. We shall see sunflower diagrams are singular diagrams in each order of $u$. Furthermore for systems above upper critical dimension the re-summation of sunflower diagrams can remove superficial singularities at each order of $u$, giving us a renormalized free energy in the form of Eq. (B.15).

### B.2.3 Critical behavior of bare free energy in the quantum critical regime

$$F_{d3z2}^{QC} = F_G^{QC} + F_u^{QC} + F_{u^2}^{QC} + \cdots \quad (B.16)$$

where

$$F_G^{QC} \sim n \left( \frac{\sigma}{4\pi} \Lambda_0 - \frac{\sigma}{\pi} \Lambda_0 r_0^{5/2} + \frac{\sigma}{\sqrt{2}} r_0^{3/2} - \frac{\pi\sigma}{6} r_0^{3/2} t + \frac{\sigma}{4\sqrt{2}} r_0^{1/2} t^2 + \cdots \right) \quad (B.17)$$

$$F_u^{QC} \sim un(n+2) \left( \frac{\sigma^2}{18} + \frac{2\sigma^2}{3} t^{3/2} - \frac{\pi\sigma^2}{3\sqrt{2}} r_0^{1/2} t + \cdots \right) \quad (B.18)$$

$$F_{u^2}^{QC} \sim -4u^2 n(n+8) \left( \frac{\sigma^3}{72\sqrt{2}} + \frac{\sigma^3}{18\sqrt{2}} t^{1/2} + \frac{\pi\sigma^3}{72} r_0^{-1/2} t + \cdots \right) + \cdots \quad (B.19)$$

with $\sigma = NK_3\Gamma_0$.

By observing Eq (B.19), we can see, starting from $u^2$, it exists infrared divergence in QCR when bare parameter $r_0$ is zero. This infrared divergence comes from Matsubara zero-modes contribution. And actually all linear in temperature terms in this bare
series are from Matsubara zero-mode contribution. And these singular terms are from sunflower diagrams contributions. So now we can apply the re-summation formula Eq. (B.15), where the big circle now is corresponding to $J_N(\omega_l = 0)$ proportional to $T \int d^4q/(r_0 + (q\xi_0)^2)^N$. After finishing the summation, the infrared divergence finally disappears, giving us Matsubara zero-modes of free energy proportional to $F(\omega_l = 0) \sim T(r_0 + I(T, r_0, u))^{3/2} = T(r_0 + u\sigma/\sqrt{2} + u\sqrt{2}\sigma t^{3/2})^{3/2}$, where we find the bare mass is renormalized by $u\sigma/\sqrt{2}$, and gets a thermal part $u\sqrt{2}\sigma t^{3/2})^{3/2}$.

After setting the renormalized mass (non-thermal part) at quantum critical point, then we get a $u^{3/2}t^{13/4}$ sub-leading correction to total free energy.

From Eq. (B.18) we find at linear order in $u$ the free energy has singular $t^{3/2}$ mass-independent term, which gives singular contribution to specific heat coefficient when temperature is taken zero-temperature limit. And this singular behavior will become more and more serious when we calculate higher-order loop-perturbative terms. Similar trick for removing infrared divergence can be used to remove these singular behaviors by summing sunflower diagrams shown in Fig.(B.2). But this time each big ring is associated with the bare-mass-independent temperature-dependent terms in bare perturbation series, in this way, we can get a re-summation proportional to $(I + t)^{5/2} \sim (u\sigma/\sqrt{2} + u\sqrt{2}\sigma t^{3/2} + t)^{5/2}$, which finally formally removes those singular terms appearing in the bare-loop-perturbative expansion series.
B.2.4 Critical behavior of bare free energy in the Fermi liquid regime

\[ F_{d_{3z2}}^{FL} = F_{G}^{FL} + F_{u}^{FL} + F_{u^2}^{FL} + \ldots \]  \hspace{1cm} (B.20)

where

\[ F_{G}^{FL} \sim n \left( \frac{\sigma}{4\pi} \Lambda \xi_0 - \frac{\sigma \pi}{6} \Lambda \xi_0 t^2 + \frac{\pi^2 \sigma}{12} r_0^{1/2} t^2 + \ldots \right) \]  \hspace{1cm} (B.21)

\[ F_{u}^{FL} \sim un(n + 2) \left( \frac{\sigma^2}{18} + \frac{\sqrt{2} \pi^2 \sigma^2}{36} r_0^{3/2} (t/r_0)^2 + \ldots \right) \]  \hspace{1cm} (B.22)

\[ F_{u^2}^{FL} \sim -4u^2 n(n + 8) \left( \frac{\sigma^3}{72\sqrt{2}} + \left( \frac{\pi^2 \sigma^3}{864} r_0^{1/2} + \frac{\pi^2 \sigma^3}{144} r_0^{3/2} \right) (t/r_0)^2 + \ldots \right) \]  \hspace{1cm} (B.23)

Because in $FL \delta \gg t$, as a result, there is no infrared divergence from Matsubara zero modes. Nevertheless, from second term of Eq. (B.22) we find specific heat coefficient is divergent when we take bare-zero-mass limit. And this kind of divergences become more and more serious when we follow sunflower diagrams order by order. Again after applying re-summation formula Eq. (B.15), we remove the singularities, getting this part of diagrams proportional to $(r_0 + l)^{1/2} t^2 = (r_0 + u \sigma/(3\sqrt{2}) + \pi^2 \sigma r_0^{3/2} (t/r_0)^2/12)^{1/2} t^2$.

B.2.5 Remarks on re-summation of bare perturbation series vs. renormalization group calculation

A direct implication of above discussions in FLR and QCR is that the divergences appearing in each order of bare loop expansion is superficial, which can be removed by a re-summation of a special series of Feynman diagrams, and finally giving us
Figure B.3: Two other singular diagrams at the order of $u^N$ in bare perturbative loop expansion.

real perturbation series in $u$. However we only showed the removal of superficial singularities in sunflower-diagram series. It’s easy to see there exit lots of other types of superficial singularities in bare-loop-expansion series. Fig. (B.3) shows two other types of singular diagrams at the order of $u^N$ in bare perturbative loop expansion. And these other types of singular diagrams require cleverer re-summations of special groups of Feynman diagrams, which indicates the inconvenience of bare perturbative calculation. In principle once re-summations can run through all Feynman diagrams we will get complete physical information of the system. However, the above re-summation technique is more dependent on special choice of re-summing Feynman diagrams, which in general is not systematically. This difficulty can be conquered by RG calculation as we shall see. Although it’s still an open problem on re-summation of what kinds of Feynman diagrams in RG calculation, essentially RG calculation is also a kind of "re-summation" of Feynman diagrams, and furthermore this "re-summation" is systematically controllable. In following appendixes we will see the
RG calculation can systematically give us perturbation series in $u$, where the singular term appearing in previous order of renormalized loop expansion will be canceled in following order of renormalized loop expansion, which will be specifically demonstrated to the first-order-in-$u$ RG calculation. And at the first time we give out correct formula for renormalized free energy to linear order in $u$.

B.2.6 Calculation of an order-$u^2$ loop diagram

In this section we give detailed calculation on the other loop diagram besides sunflower diagram at $u^2$ order of bare loop expansion for $d3\xi2$ systems. For calculating that diagram let’s first calculate $\langle \phi(\tau, x)\phi(0, 0) \rangle$.

$$
\langle \phi(\tau, x)\phi(0, 0) \rangle = \frac{1}{\beta V} \sum_{\omega_1, q} e^{i \hat{q} \cdot \hat{x}} e^{-i \omega \tau} \frac{\delta + q^2 + |\omega|}{\Gamma_0}.
$$

$$
= \int_{0}^{\Lambda} \frac{d^3 q}{(2\pi)^3} e^{i \hat{q} \cdot \hat{x}} \frac{1}{\beta} \sum_{\omega_1} \frac{e^{-i \omega \tau}}{\delta + q^2 + |\omega|} \frac{\varepsilon}{\Gamma_0}
$$

$$
= \frac{1}{2\pi^2 x} \int_{0}^{\Lambda} q \sin(qx) dq \int_{0}^{\tau_0} \frac{d\varepsilon}{\pi} \frac{\varepsilon}{(\varepsilon/\Gamma_0)^2 + (\delta + q^2)^2} \frac{\cosh \left[ (\beta/2 - \tau)\varepsilon \right]}{\sinh \left[ \beta \varepsilon/2 \right]} \tag{B.24}
$$

But

$$
\int_{0}^{\tau_0} \frac{d\varepsilon}{\pi} \frac{\varepsilon}{(\varepsilon/\Gamma_0)^2 + (\delta + q^2)^2} \frac{\cosh \left[ (\beta/2 - \tau)\varepsilon \right]}{\sinh \left[ \beta \varepsilon/2 \right]} \tag{B.25}
$$

$$
\int_{0}^{T} \frac{d\varepsilon}{\pi} \frac{\varepsilon}{(\varepsilon/\Gamma_0)^2 + (\delta + q^2)^2} \frac{\cosh \left[ (\beta/2 - \tau)\varepsilon \right]}{\sinh \left[ \beta \varepsilon/2 \right]} \tag{B.26}
$$

$$
= \int_{A_1}^{\tau_0} \frac{d\varepsilon}{\pi} \frac{\varepsilon}{(\varepsilon/\Gamma_0)^2 + (\delta + q^2)^2} \frac{\cosh \left[ (\beta/2 - \tau)\varepsilon \right]}{\sinh \left[ \beta \varepsilon/2 \right]} \tag{B.27}
$$
where

$$A_1 \approx \int_0^T \frac{d\varepsilon}{\pi} \frac{\varepsilon/\Gamma_0}{(\varepsilon/\Gamma_0)^2 + (\delta + q^2)^2} \frac{1}{\beta\varepsilon/2} = \frac{2T}{\pi} \tan^{-1} \left( \frac{t}{\delta + q^2} \right)$$  \hspace{1cm} (B.28)$$

with \( t = T/\Gamma_0 \). And

$$B_1 \approx \int_T^{\Gamma_0} \frac{d\varepsilon}{\pi} \frac{\varepsilon/\Gamma_0}{(\varepsilon/\Gamma_0)^2 + (\delta + q^2)^2} \left( e^{-\tau \varepsilon} + e^{-(\beta - \tau)\varepsilon} \right)$$  \hspace{1cm} (B.29)$$

In Eq. (B.29), if \( \tau \) is closer to zero than \( \beta \), then \( e^{-\tau \varepsilon} \) is leading term; if \( \tau \) is close to \( \beta \), then \( e^{-(\beta - \tau)\varepsilon} \) is leading term. Since these two situations are symmetry in estimation of Eq. (B.29), we will choose the first situation for following calculation. The first situation indicates \( \tau < 1/(2T) \), for convenience, let’s re-define \( \tau \) as \( \tau = \alpha \beta = \alpha/T \) with \( \alpha < 1/2 \), thus

$$B_1 \approx \int_T^{\Gamma_0} \frac{d\varepsilon}{\pi} \frac{\varepsilon/\Gamma_0}{(\varepsilon/\Gamma_0)^2 + (\delta + q^2)^2} \left( e^{-\tau \varepsilon} \right)$$

$$\approx \int_T^{T/\alpha} \frac{d\varepsilon}{\pi} \frac{\varepsilon/\Gamma_0}{(\varepsilon/\Gamma_0)^2 + (\delta + q^2)^2} \left( 1 - \alpha\varepsilon/T \right)$$  \hspace{1cm} (B.30)$$

As a result,

$$\frac{1}{2\pi^2x} \int_0^\Lambda dq \sin(qx)B_1$$

$$\approx \frac{1}{2\pi^2x} \int_0^\Lambda dq \sin(qx) \int_t^{t/\alpha} \frac{d\varepsilon}{\pi} \frac{\varepsilon}{\varepsilon^2 + (\delta + q^2)^2}$$

$$= \frac{\Gamma_0}{4\pi^3x} \int_0^\Lambda q \sin(qx) \ln \left[ 1 + \frac{(1/\alpha)^2 - 1}{1 + (\delta/t + q^2/t)^2} \right] dq$$  \hspace{1cm} (B.31)$$

$$\approx 2\Gamma_0 \ln \left[ 1/\alpha \right] - \sqrt{\delta x} \cos(\sqrt{\delta x}) + \sin(\sqrt{\delta x})$$

$$+ \frac{T}{4\pi^3x} \int_0^{\Lambda/\sqrt{t}} q \sin(q\sqrt{t}x) \ln \left[ 1 + \frac{(1/\alpha)^2}{1 + q^2} \right] dq$$  \hspace{1cm} (B.32)$$

Eq. (B.28), Eq. (B.32) and Eq. (B.33) will be used in following discussion in QC and FL.
Asymptotic behavior of $\langle \phi(\tau, x)\phi(0, 0) \rangle$ in QC

In QC we have $t \gg \delta$, then from Eq. (B.28),

$$\frac{1}{2\pi^2 x} \int_0^\Lambda dq \sin(qx) A_1 \approx \frac{T}{\pi^3 x} \int_0^\Lambda q \sin(qx) \frac{\tan^{-1}(1/(\delta/t + q^2/t))}{\delta + q^2} dq \quad (B.34)$$

$$\approx \frac{T}{4\pi x} e^{-\sqrt{\delta x}} + \frac{2\Gamma_0^{1/2} T^{1/2} \cos(\sqrt{t}x)}{\pi^3 x^2} + O(x^3) \quad (\delta \ll T, \ x \gtrsim 1/\sqrt{t}) \quad (B.35)$$

From integration in Eq. (B.33), since in QC, $\sqrt{\delta/t} \ll 1 < 1/\alpha$, thus at low-T limit, we have

$$\frac{T}{4\pi^3 x} \int_{\sqrt{\delta/t}}^{\Lambda/\sqrt{t}} q \sin(q\sqrt{tx}) \ln \left[ 1 + \frac{(1/\alpha)^2}{1 + q^2} \right] dq \quad (B.36)$$

$$\approx \frac{T}{4\pi^3 x} \int_0^{\infty} q \sin(q\sqrt{tx}) \ln \left[ 1 + \frac{1/\alpha^2}{1 + q^2} \right] dq \quad (B.37)$$

$$\approx T^{1/2} \frac{\Gamma_0^{1/2} e^{-\sqrt{t}x}}{4\pi^2 x^2} \quad (x \gtrsim 1/\sqrt{t}, \ \tau < \beta/2) \quad (B.38)$$
On the other hand at short distance limit \( x \sim 1/\Lambda \), we have (setting \( \delta = 0 \))

\[
\langle \phi(\tau, x)\phi(0, 0) \rangle \approx \int_0^\Lambda \frac{d^3q}{(2\pi)^3} \int_0^{T_0} \frac{d\epsilon}{\pi} \frac{\epsilon/\Gamma_0}{(\epsilon/\Gamma_0)^2 + (\delta + q^2)^2} \frac{\cosh[(\beta/2 - \tau)\epsilon]}{\sinh[\beta\epsilon/2]} \tag{B.39}
\]

\[
= \frac{1}{2\pi^3} \int_0^1 d\epsilon \frac{\cosh[(1/(2t) - \tau\Gamma_0)\epsilon]}{\sinh[\epsilon/(2t)]} \int_0^\Lambda q^2 \frac{d^3q}{\epsilon^2 + q^4} \tag{B.40}
\]

\[
\approx \frac{1}{2\pi^3} \int_0^1 d\epsilon \frac{\cosh[(1/(2t) - \tau\Gamma_0)\epsilon]}{\sinh[\epsilon/(2t)]} \int_0^\infty q^2 \frac{d^3q}{\epsilon^2 + q^4} \tag{B.41}
\]

\[
= \frac{\Gamma_0}{4\sqrt{2\pi^2}} t^{3/2} \int_0^{1/t} d\epsilon \sqrt{\epsilon} \frac{e^{-(\tau/\beta)\epsilon} + e^{-(1-\tau/\beta)\epsilon}}{1 - e^{-\epsilon}} \tag{B.42}
\]

\[
\approx \frac{\Gamma_0}{4\sqrt{2\pi^2}} t^{3/2} \int_0^\infty d\epsilon \sqrt{\epsilon} \frac{e^{-(\tau/\beta)\epsilon} + e^{-(1-\tau/\beta)\epsilon}}{1 - e^{-\epsilon}} e^{-\epsilon} \tag{B.43}
\]

\[
= \frac{\Gamma_0}{2\sqrt{2\pi^5/2}} t^{3/2} \left\{ \zeta(3/2, \tau/\beta + 1/2(\beta\Gamma_0)) + \zeta(3/2, 1 - \tau/\beta + 1/2(\beta\Gamma_0)) \right\} \tag{B.44}
\]

\[
\approx \frac{\Gamma_0}{2\sqrt{2\pi^5/2}} t^{3/2} \left\{ \zeta(3/2, \tau/\beta) + \zeta(3/2, 1 - \tau/\beta) \right\} \tag{B.45}
\]

\[
\approx \frac{\Gamma_0}{2\sqrt{2\pi^5/2}} t^{3/2} + \zeta(3/2) \frac{\Gamma_0 t^{3/2}}{\sqrt{2\pi^5/2}} + O \left( (\tau/\beta)^2 \right) \tag{B.46}
\]

From Eq. (B.33), Eq. (B.35), Eq. (B.38), and Eq. (B.46), we get leading asymptotic behavior for the other loop diagram at the order of \( u^2 \) as follows,

\[
\int_0^\beta d\tau \int d^4x \langle \phi(\tau, x)\phi(0, 0) \rangle^4 \sim \left\{ \int_\tau d\tau \int_{x \gtrsim \sqrt{\Gamma_0}} d^4x \left( \frac{\Gamma_1^{1/2} T^{1/2} \cos(\sqrt{\tau}x)}{\pi^{3/2}} \right)^4 \right\} \tag{B.47}
\]

**Asymptotic behavior of \( \langle \phi(\tau, x)\phi(0, 0) \rangle \) in FL**

In FL, we have \( \delta \gg t \), then from Eq. (B.28)

\[
\frac{T}{\pi^3} \int_0^\Lambda q \sin(qx) A_1 dq \approx \left\{ \begin{array}{ll}
\frac{T^2}{4\pi^2 T_0} e^{-\sqrt{x}/x} \left( x \gtrsim 1/\sqrt{\delta} \gg 1/\Lambda \right) \\
\frac{T^2}{2\pi^2 T_0} \left( \frac{\pi/2 \sqrt{x}}{\sqrt{x} - \frac{2}{\Lambda} + \frac{\delta}{\Lambda^2} + \cdots} \right) \left( 1/\Lambda \lesssim x \lesssim 1/\sqrt{\delta} \right)
\end{array} \right. \tag{B.48}
\]
Furthermore, since $t/\delta \ll 1$ (temperature can be chosen as zero in $FL$), so it’s natural to choose $t/\delta < \alpha$, then from Eq. (B.32) we have

$$\Gamma_0 \approx \frac{\Gamma_0}{4\pi^3 x} \int_0^\Lambda q \sin(qx) \ln \left[ 1 + \frac{(1/\alpha)^2 - 1}{1 + (\delta/t + q^2/t)^2} \right] dq \quad (B.49)$$

$$\approx \frac{\Gamma_0}{4\pi^3 x} \int_0^\Lambda q \sin(qx) \ln \left[ 1 + \frac{1/\alpha^2}{(\delta/t)^2 (1 + q^2/\delta)^2} \right] dq \quad (B.50)$$

$$= \frac{1}{4\pi^3 x \delta^2 \Gamma_0 \tau^2} \int_0^\Lambda \frac{q \sin(qx)}{(1 + q^2/\delta)^2} dq \quad (B.51)$$

but

$$\int_0^\Lambda \frac{q \sin(qx)}{(1 + q^2/\delta)^2} dq \approx \int_0^{\sqrt{\delta/2}} q \sin(qx) dq + \int_0^{\sqrt{\delta/2}} \frac{dqq \sin qx}{2q^2/\delta + (q^2/\delta)^2} \quad (B.52)$$

$$\approx \int_0^{\sqrt{\delta/2}} q \sin(qx) dq + \delta^2 \int_0^{\sqrt{\delta/2}} \frac{\sin qx}{q^3} dq + \delta \int_0^{\Lambda} \frac{\sin qx}{q} dq \quad (B.53)$$

$$= -\frac{\sqrt{\delta/2}}{x} \cos \left( \sqrt{\delta/2} x \right) + \frac{\sin \left( \sqrt{\delta/2} x \right)}{x^2} + \delta^2 \int_0^{\sqrt{\delta/2}} \frac{\sin qx}{q^3} dq + \frac{\delta}{2} \int_0^{\Lambda} \frac{\sin qx}{q} dq \quad (B.54)$$

Since we are discussing critical behavior, so $\delta$ is also small, then the later two integration is at the order of $\delta$, which is sub-leading compared with the front two terms. As a result,
\[
\frac{\Gamma_0}{4\pi^3x} \int_0^\Lambda dq \sin(qx)(B_1)
\approx \frac{1}{4\pi^3x\delta^2\Gamma_0\tau^2} \left( \frac{\sin\left(\sqrt{\frac{\delta}{2}}x\right)}{x^2} - \sqrt{\frac{\delta}{2}}\cos\left(\sqrt{\frac{\delta}{2}}x\right) \right)
\approx \begin{cases} 
\frac{\sqrt{2}\cos\left(\frac{\sqrt{\delta}}{2}x\right)}{8\pi^3x^2\delta^{3/2}\Gamma_0\tau^2} & (x \gtrsim \sqrt{2/\delta}, t/\delta < \tau/\beta) \\
\frac{1}{48\sqrt{2}\pi^3\delta^{3/2}\Gamma_0\tau^2} & (x \lesssim \sqrt{2/\delta}, t/\delta < \tau/\beta)
\end{cases}
\]

Collecting above results, we get leading asymptotic behaviors for the other three-loop diagram $FL$ (using Eq. (B.58)),

\[
\int_0^\beta d\tau \int d^d x \langle \phi(\tau, x)\phi(0, 0) \rangle^4 \sim \begin{cases} 
\int_\tau d\tau \int_{x \gtrsim \sqrt{2/\delta}} d^d x \left( \frac{\sqrt{2}\cos\left(\frac{\sqrt{\delta}}{2}x\right)}{8\pi^3x^2\delta^{3/2}\Gamma_0\tau^2} \right)^4 & (t < \beta/2, t/\delta < \tau/\beta) \\
\int_\tau d\tau \int_{1/\Lambda}^{1/\Lambda} d^d x \left( \frac{1}{48\sqrt{2}\pi^3\delta^{3/2}\Gamma_0\tau^2} \right)^4 & (t < \beta/2, t/\delta < \tau/\beta)
\end{cases}
\]

### B.3 RG equation for the free energy to the linear order in the quartic coupling parameter

In this Appendix, we show the details of the perturbative RG approach to the quantum Landau-Ginzburg model. We show the RG equations for different parameters. In particular, we extend the RG calculation on the free energy beyond the Gaussian level, which is able to take account of all contributions to the free energy in the linear order of the quartic coupling parameter $u$.

We introduce a sliding parameter $b > 1$ in scale transformation, which separates the degrees of freedom into the high-energy/short-wavelength part $k = (\Lambda/b, \Lambda)$, $\epsilon =$
After integrating out the high-energy part, we can obtain the effective action for the low-energy degrees of freedom at the new length scale $b/\Lambda$. This provides a systematic method to capture the low-energy/long-wavelength physics associated with the critical point. The dependence of different physical parameters on the scale transformation is described by a set of RG equations. We first consider free energy at the one loop level corresponding to the single circle in Fig. (3.2). To the linear order in coupling $u$, they are found to be \[18, 19, 95\]

\[
\frac{dt(b)}{d\ln b} = zt(b) \tag{B.60}
\]

\[
\frac{d\delta(b)}{d\ln b} = \frac{1}{\nu} \delta(b) + 4u(b)(n + 2)f^{(2)}(t(b), \delta(b)) \tag{B.61}
\]

\[
\frac{du(b)}{d\ln b} = [4 - (d + z)] u(b) \]

\[
-4u^2(b)(n + 8)f^{(4)}(t(b), \delta(b)) \tag{B.62}
\]

\[
\frac{dF(b)}{d\ln b} = (d + z)F(b) - \frac{1}{2} nNT^* f^{(0)}(t(b), \delta(b)) \tag{B.63}
\]
where $\nu = 1/2$, $N = 1/\xi_0^d$, $t = T/T^*$, $\delta(b = 1) = r_0$ and $T^* = \Gamma_0$ in this model and,

$$f^{(0)}(t, \delta) = K_d(\Lambda\xi_0)^{d+z-2} \int_0^1 \frac{d\tilde{\xi}}{2t} \coth \left( \frac{\Lambda\xi_0}{2t} \right) \tan^{-1} \frac{\tilde{\xi}}{\delta + (\Lambda\xi_0)^2}$$

$$+ \frac{2}{\pi} \int_0^{\Lambda\xi_0} \frac{d^d\tilde{q}}{(2\pi)^d} \frac{q^{z-2}}{2t} \coth \left( \frac{q^{z-2}}{2t} \right) \tan^{-1} \frac{1}{\delta + q^2} \tag{B.64}$$

$$f^{(2)}(t, \delta) = K_d(\Lambda\xi_0)^{d+z-2} \int_0^1 \frac{d\tilde{\xi}}{2t} \coth \left( \frac{\Lambda\xi_0}{2t} \right) \tan^{-1} \frac{\tilde{\xi}}{\delta + (\Lambda\xi_0)^2 + \tilde{\xi}^2}$$

$$+ \frac{2}{\pi} \int_0^{\Lambda\xi_0} \frac{d^d\tilde{q}}{(2\pi)^d} \frac{q^{z-2}}{2t} \coth \left( \frac{q^{z-2}}{2t} \right) \tan^{-1} \frac{1}{(\delta + q^2)^2 + 1} \tag{B.65}$$

$$f^{(4)}(t, \delta) = -\frac{\partial f^{(2)}(t, \delta)}{\partial \delta} \tag{B.66}$$

where $\tilde{\xi} = \xi/T^* = \xi/\Gamma_0$, $\tilde{q} = q\xi_0$ and $K_d = \int \delta(q - 1)d^dq/(2\pi)^d$.

The free energy in this order can be calculated by integrating Eq. (B.63), which is

$$F_{RG} = -nNT^* \int_0^\infty dx e^{-(d+z)x} f^{(0)}[te^{x}, re^{x/\nu}] \tag{B.67}$$

where $\delta(b) = r(b)b^{1/\nu} = r(e^x)e^{x/\nu}$, and $\delta(b)|_{b=1} = r_0 = \delta$.

We show in the following that this is equivalent to the free energy of a renormalized Gaussian model, i.e., with the bare parameter $r$ replaced by renormalized mass term $r(T)$.

Without the loss of generality, we set $\Lambda\xi_0 = 1$ and rewrite Eq. (B.67) as

$$F_{RG} = -CK_d \int_0^\infty e^{-(d+z)x} dx \int_0^1 \frac{d\xi}{\pi} \coth \left( \frac{\xi}{2te^{x}} \right) \tan^{-1} \frac{\xi}{re^{x/\nu} + 1}$$

$$- F_0 \frac{2}{\pi} \int_0^\infty e^{-(d+z)x} dx \int_0^1 \frac{d^d\tilde{q}}{(2\pi)^d} \frac{q^{z-2}}{2te^{x}} \coth \left( \frac{q^{z-2}}{2te^{x}} \right) \tan^{-1} \frac{1}{re^{x/\nu} + q^2} \tag{B.68}$$

where $C = nNT^*$. For part $A$, we take a variable transformation $e^{-zx} \rightarrow x$ and
get

\[ A = -\frac{CK_d}{z\pi} \int_0^1 x^{d/z} dx \int_0^1 dy \coth \frac{xy}{2t} \tan^{-1} \frac{yx^{1/\nu}}{r + x^{1/\nu}}, \quad (B.69) \]

while for part \(B\), we take the variable transformation

\[
\begin{align*}
q & \rightarrow \frac{q}{x} \\
e^{xz/q^2} & \rightarrow x
\end{align*}
\]

and obtain

\[ B = -\frac{2CK_d}{z\pi} \int_0^1 dq q^{-3} \int_{1/q^2}^{\infty} \frac{dx}{x} \frac{dx}{x^{d/z} \coth \frac{1}{2t} \tan^{-1} \frac{1}{r + x^{1/\nu}} + 1} \quad (B.71) \]

During the above derivation we have used the fact in Gaussian universality \(\nu = 1/2\).

Make further variable transformation \(x \rightarrow 1/x\) and \(1/q^2 \rightarrow y\) then,

\[
B = -\frac{CK_d}{z\pi} \int_0^1 dx \int_1^{1/y^{z/2}} dy \int_0^{1/x^{d/z}} \frac{dy}{x^{d/z}} \coth \frac{xy}{2t} \tan^{-1} \frac{yx^{1/\nu} y}{r + x^{1/\nu}} \quad (B.72)
\]

\[
= -\frac{CK_d}{z\pi} \int_0^1 dx \int_1^{1/x^{2/z}} dy \int_0^{1/x^{d/z}} \frac{dy}{x^{d/z}} \coth \frac{xy}{2t} \tan^{-1} \frac{yx^{1/\nu} y}{r + x^{1/\nu}} \quad (B.73)
\]

From Eq.(B.72) to Eq.(B.73) we keep integral area invariant, and the boundary is \(xy^{z/2} = 1 \Leftrightarrow x^{2/z} y = 1\). Combine Eq.(B.69) and Eq.(B.72), we have

\[
F_{RG}^G = -\frac{CK_d}{z\pi} \int_0^1 x^{d/z} dx \int_0^{1/x^{d/z}} dy \coth \frac{xy}{2t} \tan^{-1} \frac{yx^{1/\nu} y}{r + x^{1/\nu}} \quad (B.74)
\]

The do variable transformation \(q = x^{1/z}\) and \(\varepsilon = \Gamma_q q^2 y\), we finally have (using \(\Lambda \xi_0 = 1\))

\[
F_G^{RG} = -n \int_0^\Lambda \frac{d^d q}{(2\pi)^d} \int_0^{\Gamma_q} \frac{d\varepsilon}{2\pi} \coth \frac{\varepsilon}{2t} \tan^{-1} \frac{\varepsilon/\Gamma_q}{r(t) + (q\xi_0)^2} \quad (B.75)
\]
which is Gaussian form of free energy in Eq. (3.8) with bare parameter \( r_0 \) replaced by renormalized parameter \( r(t) \).

We now turn to the analysis of two-loop contribution to the free energy corresponding to the second diagram in Fig (3.2). Let’s start from bare free energy to linear order in \( u \)

\[
F = F_G + un(n + 2)I^2 \equiv F_G + F_u
\]  

(B.76)

where

\[
I = \frac{2}{n} \frac{\partial F_G}{\partial \delta} = -2 \int_0^\Lambda \frac{d^dq}{(2\pi)^d} \int_0^{\Gamma_q} \frac{d\varepsilon}{2\pi} \coth \frac{\varepsilon}{2T} \frac{\varepsilon}{\Gamma_q} \frac{\varepsilon/\Gamma_q}{(\varepsilon/\Gamma_q)^2 + (\delta + (q\xi_0)^2)^2}
\]

(B.77)

Now let’s perform RG calculation on

\[
H \equiv - \int_0^\Lambda \frac{d^dq}{(2\pi)^d} \int_0^{\Gamma_q} \frac{d\varepsilon}{2\pi} \coth \frac{\varepsilon}{2T} \frac{\varepsilon}{\Gamma_q} \frac{\varepsilon/\Gamma_q}{(\varepsilon/\Gamma_q)^2 + (\delta + (q\xi_0)^2)^2}
\]  

(B.78)

We have

\[
H \equiv H' - H_\Lambda \ln b
\]

(B.79)

where

\[
H_\Lambda = \Lambda^d K_d \int_0^{\Gamma_\Lambda} \frac{d\varepsilon}{2\pi} \coth \frac{\varepsilon}{2T} \frac{\varepsilon}{\Gamma_\Lambda} \frac{\varepsilon/\Gamma_\Lambda}{(\varepsilon/\Gamma_\Lambda)^2 + (\delta + (\Lambda\xi_0)^2)^2}
\]

(B.80)

and

\[
H' = - \int_0^{\Lambda'/b} \frac{d^dq}{(2\pi)^d} \int_0^{\Gamma_q} \frac{d\varepsilon}{2\pi} \coth \frac{\varepsilon}{2T} \frac{\varepsilon}{\Gamma_q} \frac{\varepsilon/\Gamma_q}{(\varepsilon/\Gamma_q)^2 + (\delta + (q\xi_0)^2)^2}
\]

(B.81)
Using rescaling

\[ \varepsilon' = b^z \varepsilon, \quad T = Tb^z, \quad \delta' = b^2 \delta \quad \text{and} \quad q' = bq \]  

(B.82)

Then we have

\[ H' \equiv b^{2-(d+z)}H'' - \left( b^{2-(d+z)} \ln b \right) H_\Gamma \]  

(B.83)

where

\[ H_\Gamma = \frac{1}{\pi} \int_0^\Lambda \frac{d^dq}{(2\pi)^d} \cosh \frac{\Gamma q}{2T} \frac{\Gamma q}{\Gamma + (\delta + (q\xi_0)^2)^2} \]  

(B.84)

So after RG, we get

\[ H = b^{2-(d+z)}H'' - \ln b \left( H_A + H_\Gamma b^{2-(d+z)} \right) \]  

(B.85)

Then

\[ F_u = 4un(n+2) \left\{ b^{2-(d+z)}H'' - \ln b \left( H_A + H_\Gamma b^{2-(d+z)} \right) \right\}^2 \]  

(B.86)

After combining with RG results at single loop level Eq. (B.63), we get RG equation for free energy to the two-loop approximation,

\[ \frac{dF(b)}{d\ln b} = (d+z)F(b) - \left( \frac{1}{2} nNT^* f^{(0)} - 4un(n+2)2H \left( H_A + H_\Gamma \right) \right) \]  

(B.87)

Let’s do some further simplification on the terms of \( H, H_A, \) and \( H_\Gamma \) by applying \( \tilde{\varepsilon} = \varepsilon/\Gamma_A \) and \( \tilde{q} = q'\xi_0 \),

\[ H_A = \frac{1}{\xi_0^d} K_d \Gamma_0 (\Lambda\xi_0)^{d+z-2} \cdot \int_0^1 \frac{d\tilde{\varepsilon}}{2\pi} \coth \frac{\tilde{\varepsilon}(\Lambda\xi_0)^{z-2}}{2T} \frac{\tilde{\varepsilon}}{\tilde{\varepsilon}^2 + (\delta + (\Lambda\xi_0)^2)^2} \]  

(B.88)
\[
H_\Gamma = \frac{1}{\xi_0^d} \Gamma_0 \int_0^{\Lambda \xi_0} d^d \hat{q} \int_0^{d\hat{q}} \hat{q}^{-2} \coth \left( \frac{\hat{q}^{-2}}{2t} \right) \frac{1}{1 + (\delta' + \hat{q}^2)^2} \quad (B.89)
\]

\[
\Rightarrow \quad 2 (H_\Lambda + H_\Gamma) \equiv NT^* f^{(2)}(t, \delta) \quad (B.90)
\]

where \( f^{(2)}(t, \delta) \) is just Eq. (B.65). And

\[
2H = NT^* \int_0^{\Lambda \xi_0} d^d \hat{q} \int_0^{d\hat{q}} \hat{q}^{-2} \int_0^1 \frac{d\hat{\xi}}{\pi} \coth \left( \frac{\hat{q}^{-2}}{2t} \right) \frac{\hat{\xi}^{2-2}}{\hat{\xi}^2 + (\delta + \hat{q}^2)^2} \equiv NT^* h(t, \delta) \quad (B.91)
\]

\[
\Rightarrow \quad 4un(n + 2)2H'' (H_\Lambda + H_\Gamma) = 2n(n + 2)(NT^*)^2 uh(t, \delta) f^{(2)}(t, \delta) \quad (B.92)
\]

\[
\Rightarrow \quad \frac{dF(b)}{d\ln b} = (d + z) F(b) - \left( \frac{1}{2} n NT^* f^{(0)}(b) - 2n(n + 2)(NT^*)^2 u(b) h(b) f^{(2)}(b) \right) \quad (B.93)
\]
B.4 Asymptotic behaviors for running parameter $r(b)$

From Eq. (B.61), Eq. (B.65), and notifying $\delta(b) = b^{1/\nu} r(b)$, then for leading contribution we have

$$ r(b) = r_0 + 4(n+2)uK_d \int_0^{\ln b} dx e^{(4-(d+z)-1/\nu)x} , $$

$$ \cdot \int_0^1 d\varepsilon \coth \frac{\varepsilon}{2te^{2x}} \ln (1 + \frac{1}{(r(t)e^{2x} + 1)^2}) $$

$$ \approx r_0 + 4(n+2)uK_d \int_0^\infty dx e^{(2-(d+z))x} \frac{1}{2} \ln \left( 1 + \frac{1}{(r(t)e^{2x} + 1)^2} \right) $$

$$ + 4(n+2)uK_d \int_0^{\ln b} dx e^{(4-(d+z)-1/\nu)x} , $$

$$ \cdot \int_0^1 d\varepsilon \left( \coth \frac{\varepsilon}{2te^{2x}} - 1 \right) \frac{\varepsilon}{\varepsilon^2 + (r(t)e^{2x} + 1)^2} $$

Taking cutoff at $t(b) = b^{2}t = 1$, then it’s easy to get running parameter in Fermi liquid region and quantum critical region respectively as follows

$$ r(b) \sim \begin{cases} 
  d2z2, & r_0 + (n+2) \ln 2 \frac{K_2}{\pi} u + 2(n+2) \frac{K_2}{\pi} ur_0 \ln r_0 + (n+2) \frac{2\pi K_2}{3} \frac{1}{r} ut^2 \\
  d3z2, & r_0 + \frac{2}{3}(n+2) \ln 2 \frac{K_3}{\pi} u - \frac{2(n+2)K_3}{\pi} ur_0 + (n+2) \frac{2\pi K_3}{3} \frac{1}{r} ut^2 \\
  d2z3, & r_0 + \frac{2}{3}(n+2) \ln 2 \frac{K_2}{\pi} u - \frac{2(n+2)K_2}{\pi} ur_0 + (n+2) \frac{2\pi K_2}{3} \frac{1}{r} ut^2 \\
  d3z3, & r_0 + \frac{n+2}{2} \ln 2 \frac{K_3}{\pi} u - \frac{5(n+2)K_3}{8\pi} ur_0 + \frac{2(n+2)\pi K_3}{3} \frac{1}{r} ut^2 
\end{cases} $$

(B.96)

and in quantum critical region we have

$$ r(b) \sim \begin{cases} 
  d2z2, & r_0 + (n+2) \ln 2 \frac{K_2}{\pi} u + 2(n+2) \frac{K_2}{\pi} ur_0 \ln r_0 + \frac{(n+2)K_2}{3} ut \\
  d3z2, & r_0 + \frac{2}{3}(n+2) \ln 2 \frac{K_3}{\pi} u - \frac{2(n+2)K_3}{\pi} ur_0 + \frac{2\sqrt{2\pi}(n+2)K_3}{3} ut^{3/2} \\
  d2z3, & r_0 + \frac{2}{3}(n+2) \ln 2 \frac{K_2}{\pi} u - \frac{2(n+2)K_2}{\pi} ur_0 + \frac{2(n+2)K_2}{9} ut \\
  d3z3, & r_0 + \frac{n+2}{2} \ln 2 \frac{K_3}{\pi} u - \frac{5(n+2)K_3}{8\pi} ur_0 + \frac{(2n)^{1/3}(n+2)\pi K_3}{4} ut^{4/3} 
\end{cases} $$

(B.97)

In Eqs. (B.96, B.97), the $r_0$ is bare tuning parameter, the control parameter will be $r_0$ adding with the constant part which is linear order in $u$. 
B.5 The singular contribution in the free energy of the renormalized Gaussian model

Push system closing to QCP, then $b = e^x$ goes to infinity, then we have renormalized free energy to linear order in $u$,

$$F(t, r) = \frac{1}{2} n N T^* \int_0^{\ln b} e^{-(d+z)x} f^{(0)}(te^{zx}, r(e^x)e^{x/\nu}) dx$$

$$-2n(n + 2)(NT^*)^2 u \int_0^{\ln b} e^{4 - 2(d+z)x} h(te^{zx}, r(e^x)e^{x/\nu}) f^{(2)}(te^{zx}, r(e^x)e^{x/\nu}) dx$$ (B.98)

Denote the Gaussian part and quartic correction part as

$$F_G^{RG}(t, r(t)) \equiv \frac{1}{2} n N T^* \int_0^{\ln b} e^{-(d+z)x} f^{(0)}(te^{zx}, r(e^x)e^{x/\nu}) dx$$ (B.99)

$$F_u^{RG}(t, r(t)) \equiv -2n(n + 2)(NT^*)^2 u \int_0^{\ln b} e^{4 - 2(d+z)x} h(te^{zx}, r(e^x)e^{x/\nu}) f^{(2)}(te^{zx}, r(e^x)e^{x/\nu}) dx$$ (B.100)

For Gaussian part after subtracting the contribution of zero-point fluctuations we have

$$F_G^{RG}(t, r(t)) - F_G^{RG}(0, r(0))$$

$$= F_G^{RG}(t, r(t)) - F_G^{RG}(0, r(t)) + F_G^{RG}(0, r(t)) - F_G^{RG}(0, r(0))$$

$$\equiv F_{regular}^{G, RG} + F_{singular}^{G, RG}$$ (B.101)

In Appendix B.6 we show clearly $F_{regular}^{G, RG} \equiv F_G^{RG}(t, r(t)) - F_G^{RG}(0, r(0))$ gives similar scaling behaviors as it’s discussed in Ref [4, 18, 19] so now let’s focus on $F_{singular}^{G, RG} \equiv F_G^{RG}(0, r(t)) - F_G^{RG}(0, r(0))$ in Gaussian part. When temperature is low, this term
can be rewritten as

\[
F_{\text{singular}}^{G, RG} = F_{G}^{RG}(0, r(t)) - F_{G}^{RG}(0, r(0)) \\
\approx \frac{1}{2} n NT^* \int_{0}^{\ln b} e^{-(d+z)x} e^{2x} \frac{\partial f(0)(0, r(r^x)e^{x/y})}{\partial r} \bigg|_{r(t)=r(0)} dx(r(t) - r(0))(B.102)
\]

From the integral structure of \(f^{(2)}\) in Eq. (B.65), it’s easy to find the first integral is the leading term. And for convenience we denote \(2n(n + 2)(NT^*)^2 uf^{(2)}(0, r(0)) \frac{Kd}{\pi} = A\). We stop scales at \(t(b) = b^2 t = 1\), and then apply variable transformation \(x' = e^{-zx}\), then we have (only calculate leading term in \(f^{(2)}\))

\[
F_{\text{singular}}^{G, RG} = \frac{A}{d + z - 2} \left\{ 1 - l^{(d+z-2)/z} \right\} \frac{1}{z} (2t)^{(d+z-2)/z} \int_{1/2}^{1/(2t)} y^{(d-2)/z} \left( \ln \alpha - \frac{1}{2\alpha} - \psi(\alpha) \right) dy (B.104)
\]

where \(\alpha = y/\pi + (r(t)/(2t)^{2/z})(y^{1-2/z}/\pi)\). Since all of our calculation is based on 1st order in \(u\), so we need to find out which part of quartic term may give out such term. Since \(h(0, r)\) does not give out the term we need, so a natural choice is to finish the integration when the the integration over \(h\) is chosen as \(h(t, r) - h(0, r)\), when temperature is low enough, again we may choose \(f^{(2)}\) in quartic part as \(f^{(2)}(0, r(0))\), at this situation we have (same variable transformation will be applied as we did in
Gaussian singular part)
\[
F_{u}^{RG} \sim -A \cdot \nabla \int_0^{\ln b} e^{(4-2(d+z))x} dx \int_0^1 q^{d+z-3} dq \int_0^1 d\varepsilon \frac{2\varepsilon}{(e^{\varepsilon q^2/(t)} - 1)(\varepsilon^2 + (r(t)e^{\varepsilon q^2} + q^2)^2)}
\]
\[
= -\frac{A}{z} \int_t^1 x^{(2d+z-4)/z} dx \int_0^1 q^{d+z-3} dq \int_0^1 d\varepsilon \frac{2\varepsilon}{(e^{\varepsilon q^2/(t)} - 1)(\varepsilon^2 + (r(t)/x^{2/z} + q^2)^2)}
\]
\[
\sim -A \frac{(2t)^{2d+2z-4}}{z} \cdot \nabla \int_1^{1/(z-2)} q^{d+z-3} x^{2(2d+2z-4)} dq \int_1^{q^{2/(2t)}} y^{2d-4/2} + 1 dy \left( \ln \beta - \frac{1}{2\beta} - \psi(\beta) \right)
\]
(B.105)

where \( \beta = yq^2/\pi + r(yq^2)^{1-2/2} / (\pi(2t)^{2/2}) \).

Then in quantum critical region, we have
\[
F_{s}^{G.RG} \sim \begin{cases} \frac{A}{d+z-2} \left\{ 1 - t^{(d+z-2)/z} \right\} , & d = 3, z = 2, \\ \frac{A\pi^2}{18} \sqrt{\frac{2}{\pi}} t^{3/2} (QCR) & d = 3, z = 3, \\ \frac{A\pi^2}{24} (2\pi)^{-2/3} t^{4/3} (QCR) & \\ \end{cases}
\]
(B.106)

\[
F_{u}^{RG} \sim -A \frac{(2t)^{2d+2z-4}}{z} \cdot \nabla \int_1^{1/(z-2)} q^{d+z-3} x^{2(2d+2z-4)} dq \int_1^{q^{2/(2t)}} y^{2d-4/2} + 1 dy \left( \ln \beta - \frac{1}{2\beta} - \psi(\beta) \right)
\]
\[
\sim \begin{cases} \frac{A}{d+z-2} \left\{ 1 - t^{(d+z-2)/z} \right\} , & d = 3, z = 2, \\ \frac{A\pi^2}{18} \sqrt{\frac{2}{\pi}} t^{3/2} (QCR) & d = 3, z = 3, \\ \frac{A\pi^2}{24} (2\pi)^{-2/3} t^{4/3} (QCR) & \\ \end{cases}
\]
(B.107)
In Fermi liquid region, we have

$$F^{G,\text{RG}}_{\text{singular}} \sim \frac{A}{d + z - 2} \left\{ 1 - t^{(d+z-2)/z} \right\} \frac{1}{z} \left( 2t \right)^{(d+z-2)/z} \int_{\pi}^{1/(2t)} y^{(d-2)/z} \frac{1}{12\alpha^2} dy \tag{B.108}$$

$$\sim \begin{cases} 
  d = 3, z = 2, & A \frac{\pi^3}{36} t^2 r^{-1/2} (FLR) \\
  d = 2, z = 2, & A \frac{\pi^2}{12} t^2 r^{-1} (FLR) \\
  d = 3, z = 3, & A \frac{\pi^3}{24} t^2 r^{-1} (FLR) \\
  d = 2, z = 3, & A \frac{\pi^3}{36} t^2 r^{-3/2} (FLR) 
\end{cases} \tag{B.109}$$

$$F^{\text{RG}}_u \sim \frac{A (2t)^{2d+2z-4}}{z} . \int_{\frac{1}{z^2}}^{1} q^{d+z-3d-z-2(2d+2z-4)} dq \int_{\frac{1}{2}}^{q^{z-2/(2t)}} y^{2d-4+1} dy \left( \ln \beta - \frac{1}{2\beta} - \psi(\beta) \right) \tag{B.110}$$

$$\sim \begin{cases} 
  z = 2 & \frac{A (2t)^d}{2} \int_{\frac{1}{z^2}}^{1} q^{d-1} dq \int_{\frac{1}{2}}^{q^{z-2/(2t)}} y^{d-1} \frac{1}{12\beta^2} dy \\
  d = 3, z = 2, & -A \frac{\pi^3}{36} t^2 r^{-1/2} (FLR) \\
  d = 2, z = 2, & -A \frac{\pi^2}{12} t^2 r^{-1} (FLR) 
\end{cases} \tag{B.111}$$
and

$$F^{uR}_{\text{G}} \sim -A \frac{(2t)^{2d+2z-4}}{z^2} \int_{1/2}^{1} q^{d+z-3} \frac{q^{-2}}{z} d\xi \int_{1/2}^{q^{-2}/(2t)} y \frac{2d-4}{3} + 1 \frac{1}{12\beta^2} dy$$

(B.114)

$$z=3 \sim -A \frac{(2t)^{2d+2}}{3} \int_{(2\pi)^{1/2}}^{1} q^{d-\frac{1}{3}(2d+2)} d\xi \int_{\pi/q^2}^{q^{-2}/(2t)} y \frac{2d-4}{3} + 1 \frac{1}{12\beta^2} dy$$

(B.115)

$$\begin{align*}
\approx \begin{cases} 
\delta = 3, z = 3, & -\frac{4\xi^2}{24} t^2 r^{-1} (FLR) \\
\delta = 2, z = 3, & -\frac{4\pi^3}{36} t^2 r^{-3/2} (FLR)
\end{cases}
\end{align*}$$

(B.116)

We can see singular contributions from Eqs. (B.106, B.107, B.110, B.113, B.116) can cancel out each other in each respective region! So far we show the singular term appearing in Gaussian part can be canceled out by quartic part, so the simple trick of replacing $\coth$ by $\coth - 1$ in Gaussian part will work. From bare perturbation approach the Gaussian term can be evaluated the same as we’ve done. It is not singular, and has different behaviors in $\delta \gg t$ and $\delta \ll t$ limits. Let’s examine the bare singular part, which actually is just the zero point fluctuations at this situation, and take $d3z2$ systems as examples,

$$F_{G0} = -n \int_{0}^{A} \frac{d^d q}{(2\pi)^d} \int_{0}^{\Gamma_0} \frac{d\varepsilon}{2\pi} \tan^{-1} \frac{\varepsilon}{\Gamma_0} \frac{\varepsilon}{\delta + (q\xi_0)^2}$$

(B.117)

It’s a function of $\delta$ and an upper cutoff. It is similar to phonons where it’s a function of Debye frequency. $\delta$ plays the role as a cutoff as well. Now let’s examine the quartic term $\sim uI^2$. Instead of a direct calculation, we can use $\partial F_{G}/\partial \delta$. Apparently, in either limit, this doesn’t produce more singular terms. For $\partial F_{G0}/\partial \delta$, this simply contributes
the zero-point fluctuations as corrections to $\delta$. Therefore in bare perturbative point of view, the zero-point fluctuations are simply zero-point fluctuations with corrections on the cutoff. Though it aries, this has nothing to do with finite-$T$ thermodynamics. We also can see that there is no singular terms in the perturbative approach (The high orders have singularities for $\int d^3q/(\delta + q^2)^n$ when $\delta = 0$ and $n \geq 2$, which is similar to classical Gaussian model). This is consistent with our RG perturbation calculation where the illusive singular term at RG Gaussian level finally is canceled out by subleading RG terms. This is also natural. It’s not hard to check the origin of singular term of renormalized Gaussian free energy just comes from the ultraviolet limit. We take systems in quantum critical region as examples to show this (calculation in Fermi liquid region is similar). For simplification let’s suppose control parameter $r = 0$, then From Eq.(B.74), we have

$$F_{G, \text{leading}}^{\text{RG}} \sim \int_0^1 \frac{x^{d/z}}{d} dx \int_0^1 dy \coth \frac{yx}{2t} \tan^{-1} \frac{yx^{1/\nu z}}{cut(d+z-2)/z + x^{1/\nu z}} \quad \text{(B.118)}$$

Then the singular part comes from

$$F_{G, \text{singular}}^{\text{RG}} = \int_0^1 \frac{x^{d/z}}{d} dx \int_0^1 \frac{1}{2t} dy \coth \frac{yx}{2t} \tan^{-1} \frac{yx^{1/\nu z}}{cut(d+z-2)/z + x^{1/\nu z}} \quad \text{(B.119)}$$

$$\approx \int_0^1 \frac{x^{d/z}}{d} dx \int_0^1 dy (1 + 2e^{-yx/t}) \tan^{-1} \frac{yx^{1/\nu z}}{cut(d+z-2)/z + x^{1/\nu z}} \quad \text{(B.120)}$$

$$\approx \int_0^1 \frac{x^{d/z}}{d} dx \int_0^1 dy \tan^{-1} \frac{yx^{2/z}}{cut(d+z-2)/z + x^{2/z}} \quad \text{(B.121)}$$

$$\approx \int_0^1 \frac{x^{d/z}}{d} dx \int_0^1 dy \frac{yx^{2/z}}{cut(d+z-2)/z + x^{2/z}} \quad \text{(B.122)}$$

$$= \frac{1}{2} \int_0^1 \frac{x^{(d+2)/z}}{cut(d+z-2)/z + x^{2/z}} dx - 2t^2 \int_0^1 dx \frac{x^{(d+2)/z-2}}{cut(d+z-2)/z + x^{2/z}} \quad \text{(B.123)}$$

We can see the unphysical singularity comes from the first integration of Eq.(B.123)
We can see the singular term \(-z\text{cut}^{(d+z-2)/z}/(2(d+z-2))\) actually comes from the upper limit of \(x\) integration, and this upper limit actually from the beginning of RG flow, which means that this unphysical singularity comes from ultraviolet limit, which is similar as those unphysical ultraviolet divergences in the bare expansion series in Eq. (B.20) and Eq. (B.16). But there are some differences. The bare free energy at Gaussian level actually is regular after subtracting zero-point fluctuations, while the unphysical ultraviolet singularity only happens in higher-order (in \(u\)) contributions.

However, because the renormalized Gaussian picks up contributions from higher-order contributions of bare free energy, so it can be expected that those unphysical ultraviolet singularity will be present even at renormalized Gaussian level. But the essential spirit of this RG procedure is trying to get a low-energy effective theory after integrating out high-energy/momentum contributions, so it should be expected that those unphysical ultraviolet divergences should disappear finally after order by order (in \(u\)) calculations, which is confirmed by the above complete the-first-order in
### B.6 Scaling behaviors of the Free Energy

#### B.6.1 Fermi Liquid Regime

In Fermi liquid region, with our recipe Eq. (3.20)

\[
F(t, r) = -\frac{F_0}{z} \int_{b-z}^{1} dx \frac{d^z}{dz} \int_{0}^{1} d\varepsilon \frac{2}{e^{\varepsilon/t} - 1} \tan^{-1} \frac{\varepsilon}{r(t)/x^{1/z} + 1},
\]

where \( F_0 = nNT^*K_d/\pi \), and transformation of \( e^{-zx} \rightarrow x \) has been applied. In Fermi liquid regime we need only to stop scales at \( t(b) = tb^z = 1 \), then we have

\[
F(t, r) = -\frac{F_0}{z} \int_{t}^{1} dx \frac{d^z}{dz} \int_{0}^{1} d\varepsilon \frac{2}{e^{\varepsilon/t} - 1} \tan^{-1} \frac{\varepsilon}{r(t)/x^{1/z} + 1}
\]

After variable transformation \( x/2t = y \), then \( \varepsilon y = \pi z \) we have [92]

\[
F(t, r) = -\frac{\pi F_0}{z} (2t)^{1+d/z} \int_{1/2}^{1/2t} y^{d/z-1} dy \int_{0}^{1} d\varepsilon \frac{2}{e^{2\pi z} - 1} \tan^{-1} \frac{\pi z}{y(r(t)/(2ty)^{1/z} + 1)}
\]

\[
\approx -\frac{\pi F_0}{z} (2t)^{1+d/z} \int_{1/2}^{1/2t} y^{d/z-1} dy \int_{0}^{\infty} d\varepsilon \frac{2}{e^{2\pi z} - 1} \tan^{-1} \frac{\pi z}{y(r(t)/(2ty)^{1/z} + 1)}
\]

\[
= -\frac{\pi F_0}{z} (2t)^{1+d/z} \int_{1/2}^{1/2t} y^{d/z-1} dy \{\ln(\alpha) + \alpha - (\alpha - 1/2) \ln(\alpha) - \ln(2\pi)/2\}
\]  

where \( \alpha = y(r(t)/(2ty)^{1/z} + 1)/\pi \). In Fermi liquid region \( r/t^{1/z} \gg 1 \), furthermore because \( \nu z \gtrsim 1 \) as a result \( y/y^{1/z} = y^{1-1/z} \gtrsim 1 \) thus \( \alpha = y(r(t)/(2ty)^{1/z} + 1)/\pi \gg \)
1, so to the leading order of the above integration we have

\[
F(t, r) \sim -\frac{\pi F_0}{z} (2t)^{1+d/z} \left( \int_{1/2}^{1/2t} y^{d/z-1} dy \frac{1}{12} \left( \frac{y}{(2y)^{1/z}(2y)^{1/
u z}} + 1 \right) \right)^{-1}
\]

\[
\sim \begin{cases} 
  d = 2, z = 3 : & -\frac{\pi^3}{6} F_0 t^2 / \sqrt{r} + \frac{\pi^2}{3} F_0 t^2 \\
  d = 3, z = 3 : & -\frac{\pi^2}{6} F_0 t^2 \ln(1 + 1/r)
\end{cases} \tag{B.132}
\]

Thus we may immediately get leading critical behavior of entropy in FLR for \(d2z3\) and \(d3z3\) systems as follows

\[
d = 2, z = 3 : S = \frac{\pi^3 F_0 t}{2} r^{-1/2} + O(r) \tag{B.133}
\]

\[
d = 3, z = 3 : S = \frac{\pi^2 F_0 t}{3} \ln(1 + 1/r) \tag{B.134}
\]

\[
= \frac{\pi^2 F_0 t}{3} \ln(1/r) + O(r) \tag{B.135}
\]

From Eq.(B.134,B.135) we see for \(d3z3\) systems the traditional theoretical results \([18, 19]\) (which is only correct when \(r\) is very close to quantum critical point) need to be corrected when \(r\) is large. And actually from our numerical data, we can see \(t \ln(1 + 1/r)\) is the correct scaling behavior for \(d3z3\) systems. And furthermore for both \(d2z3\) and \(d3z3\) systems the second term is negligible because the system stays in Fermi liquid region (in FLR \(r = r + Aur^{(d+z-4)\nu + 1}(t^{1/
u z}/r_c)^2\) and \(t^{1/
u z}/r \ll 1\)).

### B.6.2 Quantum Critical Regime

It’s a little more complicated in quantum critical regime than it in Fermi liquid region, however basic procedure is the same as above. What’s different here is now at first we need to scale temperature to high-T region, which means we will stop RG flow until
$\delta(b) = 1$. Let’s firstly deal with the region where $t(b) \leq 1$. The difficulty here is that we can not always guarantee $\alpha = y \left( r(t)/(2ty)^{1/\nu} + 1 \right)/\pi > 1$ in quantum critical region. We need to divide the integral of $y$ into two regions of $(1/2, \pi)$ and $(\pi, 1/(2t))$, then for the later integral region following similar procedure from Eq.(B.132) we have

$$F_I(t, r) \sim -\frac{\pi F_0}{z} (2t)^{1+d/z} \int_\pi^{1/2t} y^{d/z-1} dy \left\{ \frac{y \left( r(t) \left( 1 \right)/(2y)^{1/\nu} + 1 \right)}{\pi} \right\}^{-1}$$

$$= \begin{cases} 
  d = 2, z = 3 : & -\frac{\pi^2 F_0}{3} t^2 \tan^{-1}(1/\sqrt{r(t)/r(t)}) \\
  + \frac{\pi^2 F_0}{3(2\pi)^{2/3}} t^{5/3} \sqrt{(2\pi t)^{2/3}/r(t)} \tan^{-1}(\sqrt{(2\pi t)^{2/3}/r(t)}) \\
  d = 3, z = 3 : & -\frac{\pi^2 F_0}{6} t^2 \ln \left( 1 + 1/r(t) \right) + \frac{\pi^2 F_0}{6} t^2 \ln \left( 1 + (2\pi t)^{2/3}/r(t) \right) 
\end{cases} \quad (B.136)$$

Then we may get entropy corresponding to $F_I$ as follows

$$d = 2, z = 3 :$$

$$S_I = \frac{\pi^2 F_0}{3} \left( \frac{5}{3(2\pi)^{1/3}} t^{2/3} - 2t \left( 1 - \frac{r}{3} + \frac{Bu}{2\pi} \right) - \frac{r}{6\pi} + But^2 + O(t^2) \right)$$

at $QCP$ $\equiv \frac{\pi^2 F_0}{3} \left( \frac{5}{3(2\pi)^{1/3}} t^{2/3} - 2t \left( 1 + \frac{Bu}{2\pi} \right) + But^2 + O(t^2) \right) \quad (B.137)$

$$d = 3, z = 3 :$$

$$S_I = \frac{\pi^2 F_0}{6} \left( \frac{4}{3} t \ln(1/t) + (2r - 2/3 - 3 \ln(2\pi) - \frac{4}{3(2\pi)^{2/3}} t^{2/3} \right)$$

$$- \frac{8But^{5/3}}{3(2\pi)^{2/3}} + \frac{10But^{7/3}}{3} + O(t^{7/3})$$

at $QCP$ $\equiv \frac{\pi^2 F_0}{6} \left( \frac{4}{3} t \ln(1/t) - (2/3 + 3 \ln(2\pi))t - \frac{8But^{5/3}}{3(2\pi)^{2/3}} + \frac{10But^{7/3}}{3} + O(t^{7/3}) \right) \quad (B.138)$

For $d2z3$ systems since we consider the system in QCR so $r$ is small which means the arctan function approaches to a constant so for $d2z3$ it contains a $t^2$ correction. For $d3z3$ systems because in general we have $2\pi t \ll 1$ (in QCR $r(t) = r + But^{(d+z-4)/z+1}/\nu z$...
and $t^{1/vz}/r_c \gg 1$), so the dominant term will be the first term when temperature is low! We need to finish the integral in the other region of $(1/2, \pi)$ where we need to use a different strategy shown as follows

$$F_{II}(t, r(t)) = -\frac{F_0}{z} (2t)^{1+d/z}$$

$$\int_{1/2}^{\pi} y^{d/z} dy \int_0^1 d\varepsilon \frac{2}{e^{2\varepsilon y} - 1} \tan^{-1} \frac{\varepsilon}{r(t)/(2ty)^{1/z\nu} + 1}$$

$$\approx -\frac{2F_0}{z} (2t)^{1+d/z} \int_{1/2}^{\pi} y^{d/z} dy \int_0^1 d\varepsilon \frac{\varepsilon}{e^{2\varepsilon y} - 1}$$

$$= -\frac{4F_0}{z} t^{1+d/z} \int_1^{2\pi} y^{d/z-1} dy \int_0^y d\varepsilon \frac{\varepsilon}{e^\varepsilon - 1}$$  \hspace{1cm} (B.139)

Following the approximated sign we already used the constraint condition in quantum critical regime and only took the leading order term of $\arctan$. Since $0 \leq \varepsilon \leq y \leq 2\pi$ so we have Bernoulli expansion $\varepsilon/(e^\varepsilon - 1) = \sum_{n=0}^{\infty} \varphi_n \varepsilon^n/n!$ with $\varphi_n$ as Bernoulli coefficients. Then we have

$$F_{II}(t, r) \sim \begin{cases} 
    d = 2, z = 3 : -4c_2/3 F_0 t^{5/3}/3 \\
    d = 3, z = 3 : -4c_1 F_0 t^2/3 
\end{cases}$$  \hspace{1cm} (B.140)

thus leading terms for entropy in this region are

$$S_{II} \sim \begin{cases} 
    d = 2, z = 3 : 20c_2/3 F_0 t^{2/3}/9 \\
    d = 3, z = 3 : 8c_1 F_0 t^{3/3}/3 
\end{cases}$$  \hspace{1cm} (B.141)

where

$$c_d = (2\pi)^{d/z} \sum_{n=0}^{\infty} \frac{\varphi_n ((2\pi)^n+1 - (2\pi)^{-d/z})}{(n+1)!(n+1+d/z)}$$  \hspace{1cm} (B.142)

From Eq.(B.140) the $r-$ and $u-$ independent $t^2$ background term also shows in $d3z3$ systems in QCR. The story does not end here, we need to further stop scale at $\delta(b) = 1$
to reach high-T regime (this does not affect leading behavior in Fermi liquid regime).

For simplicity we will focus on systems with \( d + z > 4 \). At \( t(b_0) = 1 \) i.e. \( b_0 = 1/t^{1/z} \), we have

\[
\delta(b_0) = t^{-1/\nu z} \left( r + 4(n + 2)uBt^{(d+z+1/\nu-4)/z} \right) \tag{B.143}
\]

Continuing the scaling \( t(b) \gg 1 \). We will use \( v(b) \equiv t(b)u(b) \) as scaling parameter. In this region, \( f^2(t) \approx Ct \) and \( f^4(t) \approx Dt \). The RG equations are now given as

\[
\frac{d\delta(b)}{d\ln b} = \frac{1}{\nu} \delta(b) + 4(n + 2)Cv(b) \tag{B.144}
\]

\[
\frac{dv(b)}{d\ln b} = (4 - d)v(b) - 4(n + 8)Dv^2(b)(n + 2) \tag{B.145}
\]

For \( d < 4 \), we can always drop the \( v^2 \) term. Integrating from \( \ln b_0, \ln b \), we have

\[
v(b) = \bar{v}(b/b_0)^{4-d}
\]

with \( \bar{v} = u(b_0)t(b_0) = ut^{(d+z-4)/z} \) for \( d + z > 4 \). Then it follows

\[
\frac{d\delta(b)}{d\ln b} = \frac{1}{\nu} \delta(b) + 4(n + 2)C\bar{v} \left( \frac{b}{b_0} \right)^{4-d} \tag{B.146}
\]

From Eq. (B.146) we may determine stop scaling \( b_* \) for which \( \delta(b_*) = 1 \) as follows:

\[
\frac{b_*}{b_0} \sim \begin{cases} 
  d = 2, z = 3 : t^{-1/3}/u \\
  d = 3, z = 3 : t^{1/3} \left( r + 4(n + 2)uBt^{4/3} \right)^{-1/2}
\end{cases} \tag{B.147}
\]

then

\[
b_*^{z} = \begin{cases} 
  d = 2, z = 3 : u^2t^2 \\
  d = 3, z = 3 : t \left( uBt^{2/3} + r/t^{2/3} \right)^{3/2}
\end{cases} \tag{B.148}
\]
As a result for $d2z3$ systems,

$$F_{III} = -\frac{\pi F_0}{3} (2t)^{5/3} \int_{u^{1/2}}^{1/2} \int_{0}^{1/2} \frac{y^{2/3} dy}{e^{2xy} - 1} \tan^{-1} \frac{\varepsilon}{r(t)/(2ty)^{2/3} + 1}$$

$$\approx -\frac{\pi F_0}{3} (2t)^{5/3} \int_{u^{1/2}}^{1/2} \frac{y^{-1/3}}{r(t)/(2ty)^{2/3} + 1} dy$$

$$\approx -\pi F_0 t^{5/3} \tag{B.149}$$

then

$$S_{III} \sim \frac{5F_0}{3} t^{2/3} \ (d2z3) \tag{B.150}$$

Similarly we can get scaling results for $d3z3$ systems in the region between $(\ln b_*, \ln b_0)$. For simplicity let’s just focus on quantum critical point i.e. $r = 0$ (general discussion is straightforward).

$$F_{III} = -\frac{\pi F_0}{3} (2t)^{2} \int_{(uB)^{3/2}t/2}^{1/2} y dy$$

$$\int_{0}^{1} \frac{d\varepsilon}{e^{2xy} - 1} \tan^{-1} \frac{\varepsilon}{r(t)/(2ty)^{2/3} + 1} \tag{B.151}$$

$$\approx -\frac{\pi F_0}{3} (2t)^{2} \int_{(uB)^{3/2}t/2}^{1/2} \frac{1}{r(t)/(2ty)^{2/3} + 1} dy \tag{B.152}$$

$$\approx -\frac{2\pi F_0}{3} t^{2} \tag{B.153}$$

then

$$S_{III} \sim \frac{4\pi F_0}{3} t \ (d3z3) \tag{B.154}$$

Collect all results in these three integral regions from Eqs.(B.137,B.138,B.141) and Eqs. (B.150,B.155), one may find out the leading scaling behaviors for entropy with corrections, and these analytical results are consistent with numerical results in main context.
Appendix C

Appendix for quantum phase transitions in iso-electronically tuned iron pnictides

C.1 Effective free energy at the large N limit

The corresponding minimum action to incorporate the Ising coupling can be written as \[33,39\]

\[
S = S_2 + S_4
\]

(C.1)

where

\[
S_2 = \sum_{\vec{q}, \omega_l} \left\{ \chi^{-1}_{0, \vec{q}, \omega_l} \left( |\vec{m}_A, \vec{q}, \omega_l|^2 + |\vec{m}_B, -\vec{q}, \omega_l|^2 \right) + 2v \left( q_x^2 - q_y^2 \right) \vec{m}_A, \vec{q}, \omega_l \cdot \vec{m}_B, -\vec{q}, -\omega_l \right\}
\]

(C.2)

\[
S_4 = \int_0^\beta d\tau \int d^2\vec{r} \left\{ u_1 \left[ \left( \vec{m}_A \right)^2 + \left( \vec{m}_B \right)^2 \right] + u_2 \vec{m}_A \vec{m}_B - u_I \left( \vec{m}_A \cdot \vec{m}_B \right)^2 \right\}
\]

(C.3)

where \(\vec{m}_{A/B}(\vec{r}, \tau)\) are \(O(N)\) vector fields of the sublattices of \(A\) and \(B\), and \(\chi^{-1}_{0, \vec{q}, \omega_l} = r + \omega_l^2 + c q^2 + \gamma |\omega_l|\) with \(r = r_0 + wA_Q\). In addition \(u_I \sim J_1^2/J_2^2\) [48]. The anisotropic term in the quadratic action \(S_2\) is invariant under lattice rotation. This becomes clear when we rotate the lattice \(\pi/2\) about a site on sublattice \(A\), which gives \((x, y) \rightarrow (y, -x)\) (or \((q_x, q_y) \rightarrow (q_y, q_{-x})\)), and \(\vec{m}_B \rightarrow -\vec{m}_B\), therefore the anisotropic term has the same symmetry as the lattice when the system is in disorder phase.
The quartic fluctuations can be decoupled as follows (the interaction coefficients of $u_1, u_2, u_I$ have been re-scaled as $u_1/N, u_2/N, u_I/N$) [96],

$$e^{(u_1/N)\int dx \left( \tilde{m}_A \tilde{m}_B \right)^2} = L_1 \int D\Delta_I e^{\int dx \left( -\frac{\Delta_I^2}{u_I} - 2\Delta_I \tilde{m}_A \tilde{m}_B \right)}$$  \hspace{1cm} (C.4)

and

$$e^{-r \sum_{\tilde{q}, \omega_l} \left( \left( \tilde{m}_A, \tilde{q}, \omega_l \right)^2 + \left( \tilde{m}_B, \tilde{q}, \omega_l \right)^2 \right) - \int dx \left\{ (u_1/N) \left( \tilde{m}_A^2 + \tilde{m}_B^2 \right) + (u_2/N) \tilde{m}_A^2 \tilde{m}_B^2 \right\}}$$  \hspace{1cm} (C.5)

$$= L_2 \int D\lambda_A D\lambda_B e^{-i\lambda_A \tilde{m}_A^2 - i\lambda_B \tilde{m}_B^2}$$

with the normalized factors

$$L_1 = \prod_x \sqrt{\frac{u_I/N}{\pi}}, \quad L_2 = \prod_x \sqrt{\frac{(4u_1^2 - u_2^2)/N^2}{4\pi^2}}$$ \hspace{1cm} (C.6)

where $x = (\tau, \vec{r})$ with $\int dx \equiv \int_0^\beta d\tau \int d^2\vec{r}$. Eq. (C.5), for the case with positive quartic couplings, corresponds to the standard Hubbard-Stratonovich transformation. By contrast, Eq. (C.4) describes the case of a negative quartic coupling and a regularization is needed in general [96]. The LHS of Eq. (C.4) is going to diverge after functional integrations over the fields $\tilde{m}_A$ and $\tilde{m}_B$, which indicates that the functional integrals over the fields $\tilde{m}_A$ and $\tilde{m}_B$ can not exchange with the functional integral over the field $\Delta_I$ in the RHS of Eq. (C.4). However, since in our case $u_1$ is larger than $u_I$, when we combine the functional integrals over the LHS’s of Eqs. (C.4,C.5), the total partition function is regular. (Another way of seeing this is that, the solutions to the saddle-point equations are bounded.) As a result, when we deal with the decoupling
over the quartic terms simultaneously, the functional integrals over the fields $\hat{m}_A$ and $\hat{m}_B$ can exchange with those over the conjugate fields of $\Delta_I$, $\lambda_A$ and $\lambda_B$. Hence, after decoupling the quartic terms we can first integrate over the fluctuations in the fields $\hat{m}_A$ and $\hat{m}_B$, leading to the standard procedure of a large-$N$ approach.

To the leading order in $1/N$, we only keep the zeroth mode ($\omega = 0, k = 0$) of order parameters $i\lambda_{A/B}$ and $\Delta_I$. We then integrate over the $N - 1$-component fluctuation fields $\vec{\pi}_{A/B}$ in $\hat{m}_{A/B} = \left(\sqrt{N}\sigma_{A/B}, \vec{\pi}_{A/B}\right)$, leaving us with an effective action as a function of order parameters $\lambda_{A/B}, \sigma_{A/B}$ and $\Delta_I$. Because the sublattices $A$ and $B$ are symmetric, we have $i\lambda_A = \langle m_A^2 \rangle = i\lambda_B = \langle m_B^2 \rangle = m^2$, and $\sigma_A = \pm \sigma_B = \sigma$. Thus to the order of $O(1/N)$ we get the effective free energy as,

$$f = \frac{\Delta_I^2}{u_I} - \frac{(m^2 - r)^2}{2u_1 + u_2} + (m^2 \pm \Delta_I)^2 + g(m^2, \Delta_I)$$  \hspace{1cm} (C.7)

with

$$g(m^2, \Delta_I) = \frac{1}{2} \frac{1}{\beta V} \sum_{\vec{q}, \omega_l} \ln \left[ \left( D^{-1}_{0, \vec{q}, \omega_l} + m^2 \right)^2 - \left( v \left( q_x^2 - q_y^2 \right) + \Delta_I \right)^2 \right]$$  \hspace{1cm} (C.8)

where $D^{-1}_{0, \vec{q}, \omega_l} = \chi^{-1}_{0, \vec{q}, \omega_l} - r$, and we take $+$ when $\sigma_A = \sigma_B = \sigma$, and $-$ when $\sigma_A = -\sigma_B = \sigma$ in the expression of $(m^2 \pm \Delta_I)^2$.

**C.2 Saddle point equations and some general conclusions to the order of O(1/N)**

From Eq. (C.7) we have variational equations w.r.t $\sigma$, $m^2$ and $\Delta_I$,

$$\frac{\partial f}{\partial \sigma} = \frac{\partial f}{\partial \Delta_I} = \frac{\partial f}{\partial m^2} = 0$$  \hspace{1cm} (C.9)
After some manipulations we have (for convenience here we choose the branch of
\( \sigma_A = \sigma_B = \sigma \))

\[(m^2 + \Delta_I) \sigma = 0 \quad \text{(C.10)}\]

\[
\frac{\Delta_I}{u_I} = \frac{m^2 - r}{2u_1 + u_2} - 2\sigma^2 - \frac{1}{2\beta V} \sum_{\vec{q}, i, \omega_l} D^{-1}_{0, \vec{q}, i, \omega_l} + v \left( \frac{1}{q_x^2 - q_y^2} + m^2 + \Delta_I \right) \quad \text{(C.11)}
\]

\[
\frac{\Delta_I}{u_I} = -\frac{m^2 - r}{2u_1 + u_2} + \frac{1}{2\beta V} \sum_{\vec{q}, i, \omega_l} D^{-1}_{0, \vec{q}, i, \omega_l} - v \left( \frac{1}{q_x^2 - q_y^2} + m^2 - \Delta_I \right) \quad \text{(C.12)}
\]

Eqs. (C.11, C.12) imply that in the branch of \( \sigma_A = \sigma_B = \sigma, \Delta_I \leq 0 \). When \( \Delta_I = 0 \), without using Eq. (C.10), after summing over Eq. (C.11) and Eq. (C.12) we immediately have \( \sigma = 0 \), which means the vanishing of \( \Delta_I \) can not happen before vanishing of \( \sigma \).

On the other hand when \( \sigma = 0 \), Eq. (C.11) and Eq. (C.12) merge to one equation, after doing analytic continuation, then setting \( T = 0 \), this combined equation becomes,

\[
\frac{2\Delta_I}{u_I} = \left( \frac{1}{2\pi} \right)^3 \int_{-\Lambda_f}^{\Lambda_f} d^2q \int_0^\infty d\omega \left[ \frac{\gamma \omega}{(\omega^2 - c_1^2)^2 + \gamma^2 \omega^2} - \frac{\gamma \omega}{(\omega^2 - c_0^2)^2 + \gamma^2 \omega^2} \right] \quad \text{(C.13)}
\]

where \( \Lambda_f \) is the Fermi wave vector, and

\[
c_0^2 = (c + v) q_x^2 + (c - v) q_y^2 + m^2 + \Delta_I \quad \text{(C.14)}
\]

\[
c_1^2 = (c - v) q_x^2 + (c + v) q_y^2 + m^2 - \Delta_I \quad \text{(C.15)}
\]

The integration on the right hand side (RHS) of Eq. (C.13) can be done, and the
Eq. (C.13) becomes (see the next section for the detailed calculations)

$$\frac{2\Delta_I}{u_I} = \frac{1}{16\pi^2\sqrt{c^2 - v^2}} \left\{ \gamma \ln \frac{m^2 - \Delta_I}{m^2 + \Delta_I} + i \sqrt{4(m^2 + \Delta_I) - \gamma^2} \ln \frac{\gamma - i \sqrt{4(m^2 + \Delta_I) - \gamma^2}}{\gamma + i \sqrt{4(m^2 + \Delta_I) - \gamma^2}} \right\} + i \sqrt{4(m^2 - \Delta_I) - \gamma^2} \ln \frac{\gamma - i \sqrt{4(m^2 - \Delta_I) - \gamma^2}}{\gamma + i \sqrt{4(m^2 - \Delta_I) - \gamma^2}}$$

(C.16)

Then we can see $\Delta_I = 0$ will be a natural solution for the above equation. If Eq. (C.16) has the other solution $\Delta_I < 0$, then near the transition point we can easily verify breakdown of Eq. (C.16) at the limit of $m^2/\gamma^2 \ll 1$ and $\Delta_I/\gamma^2 \ll 1$, where LHS of Eq. (C.16) is negative while RHS of Eq. (C.16) is positive. And in opposite limit $\gamma^2 \ll m^2$ and $\gamma^2 \ll |\Delta_I|$, Eq. (C.16) has a non-zero solution $m^2 = f(\Delta_I, \gamma)$, however, one can easily verify that at the limits of $\gamma/m^2, \gamma/|\Delta_I| \to 0$, when we substitute the solution back to the free energy, the free energy will be unbounded from below, which means the other solution is un-physical. As a result, there does not exist non-zero solution of Eq. (C.16) in these two limits. Based on these two asymptotic results, we expect that, at zero temperature and to the order $O(1/N)$, vanishing of the magnetic order implies that the Ising order vanishes too. This conclusion is also numerically confirmed.
C.3 Calculation of summations in Eq. (C.11,C.12)

For the summations in Eqs. (C.11,C.12), we have

\[
\frac{1}{2\beta V} \sum_{\vec{q},\omega_{\lambda t}} \frac{1}{D_{\vec{q}}^{-1} + v \left( q_x^2 - q_y^2 \right) + m^2 + \Delta I} = \frac{1}{(2\pi)^3} \int_{-\Lambda_f}^{\Lambda_f} d^2 q \int_0^{\Gamma_0} d\omega \coth \frac{\omega}{2T} \left( \frac{\gamma \omega}{(\omega^2 - c_0^2)^2 + \gamma^2 \omega^2} \right)
\]

(C.17)

\[
\frac{1}{2\beta V} \sum_{\vec{q},\omega_{\lambda t}} \frac{1}{D_{\vec{q}}^{-1} + v \left( q_x^2 - q_y^2 \right) + m^2 - \Delta I} = \frac{1}{(2\pi)^3} \int_{-\Lambda_f}^{\Lambda_f} d^2 q \int_0^{\Gamma_0} d\omega \coth \frac{\omega}{2T} \left( \frac{\gamma \omega}{(\omega^2 - c_0^2)^2 + \gamma^2 \omega^2} \right)
\]

(C.18)

At \( T = 0K \), from Eq. (C.17) we have

\[
\frac{1}{(2\pi)^3} \int_{-\Lambda_f}^{\Lambda_f} d^2 q \int_0^{\Gamma_0} d\omega \coth \frac{\omega}{2T} \left( \frac{\gamma \omega}{(\omega^2 - c_0^2)^2 + \gamma^2 \omega^2} \right) \bigg|_{T=0}
\]

\[
\approx \frac{1}{(2\pi)^3} \int_{-\Lambda_f}^{\Lambda_f} d^2 q \int_0^{\Gamma_0} d\omega \coth \frac{\gamma \omega}{\omega^2 - c_0^2 + \gamma^2 \omega^2}
\]

\[
\approx \frac{1}{(2\pi)^3} \int_{-\Lambda_f}^{\Lambda_f} d^2 q \int_0^{\infty} d\omega \coth \frac{\gamma \omega}{\omega^2 - c_0^2 + \gamma^2 \omega^2}
\]

\[
\approx \frac{1}{(2\pi)^3} \int_{-\Lambda_f}^{\Lambda_f} d^2 q \frac{i}{\sqrt{4c_0^2 - \gamma^2}} \ln \frac{\gamma - i\sqrt{4c_0^2 - \gamma^2}}{\gamma + i\sqrt{4c_0^2 - \gamma^2}}
\]

\[
\approx \frac{\gamma \ln \frac{4(m^2 + \Delta I)}{4c_0^2 + \gamma^2} + i2\sqrt{c_0} \ln \frac{\gamma - i2\sqrt{c_0}}{\gamma + i2\sqrt{c_0}} - i4(m^2 + \Delta I) - \gamma^2 \ln \frac{\gamma - i4(m^2 + \Delta I) - \gamma^2}{\gamma + i4(m^2 + \Delta I) - \gamma^2}}{16\pi^2 \sqrt{c^2 - v^2}}
\]

\[
= G_1
\]

(C.19)

where in the last approximation we have used the approximated condition \( \sqrt{c - v\Lambda_f} \gg \sqrt{c}\Lambda_c \), where the anisotropy is not extremely strong and \( \Lambda_c \) is the low-energy cut-off wave vector for spin excitations. This approximated condition will also be applied for all following calculation. Similarly the integration in Eq. (C.18) can be calculated as
follows,
\[
\frac{1}{(2\pi)^3} \int_{-\Lambda f}^{\Lambda f} d^2q \int_0^{\Gamma_0} d\omega \coth \frac{\omega}{2T} \left( \frac{\gamma\omega}{(\omega^2 - c_1^2)^2 + \gamma^2\omega^2} \right) = \frac{1}{(2\pi)^3} \int_{-\Lambda f}^{\Lambda f} d^2q \int_0^{\Gamma_0} d\omega \frac{\gamma\omega}{(\omega^2 - c_1^2)^2 + \gamma^2\omega^2}
\]
\[
\approx \frac{1}{(2\pi)^3} \int_{-\Lambda f}^{\Lambda f} d^2q \int_0^{\infty} d\omega \frac{i}{\sqrt{4c_1^2 - \gamma^2}} \ln \frac{\gamma - i\sqrt{4c_1^2 - \gamma^2}}{\gamma + i\sqrt{4c_1^2 - \gamma^2}}
\]
\[
\gamma \ln \frac{4(m^2 - \Delta_I)}{4\Lambda_c^2 + \gamma^2} + i2\sqrt{c\Lambda_c} \ln \frac{\gamma - i\sqrt{4m^2 - \Delta_I}}{\gamma + i\sqrt{4m^2 - \Delta_I}} - i\sqrt{4(m^2 - \Delta_I)} - \gamma^2 \ln \frac{\gamma - i\sqrt{4(m^2 - \Delta_I) - \gamma^2}}{\gamma + i\sqrt{4(m^2 - \Delta_I) - \gamma^2}}
\]
\[
\approx \frac{G_2}{16\pi^2\sqrt{c^2 - \nu^2}}
\]
\[
= G_2
\]
\[
(C.20)
\]

Using Eqs. (C.19, C.20), after some integrals, we can get an analytical expression for the free energy as a function of \( \Delta_I, m^2, \sigma \). The central task here is to get a close form of Eq. (C.8). We can tackle the summation as follows,
\[
\frac{\partial g}{\partial \Delta_I} = G_1 - G_2 \equiv g'_\Delta_I; \quad \frac{\partial g}{\partial m^2} = G_1 + G_2 \equiv g''_{m^2}
\]
\[
(C.21)
\]

Then we have
\[
g(\Delta_I, m^2) = \int_0^{\Delta_I} g'_\Delta_I (x, m^2) dx + \int_0^{m^2} g''_{m^2} (0, y) dy
\]
\[
(C.22)
\]

After finish integrations in the above equation, we can get a close form of \( g(\Delta_I, m^2) \). Substituting the close form back into Eq. (C.7), we recover the full free energy expression Eq. (4.7) in Ch. 4.2.
Figure C.1: (a) Illustration of Eq. (4.13); (b) The counterpart for the generic case of $a_{d3z} < 0$ in 3D, illustrating Eq. (C.50), with $\eta = |\delta|/8$.

### C.4 Saddle point equations in the ordered Regime

From Eqs. (C.10,C.11,C.12,C.19,C.20), we can arrive at the following forms of the saddle-point equations in the ordered regime,

\[
- \left( \frac{1}{u_I} - \frac{1}{2u_1 + u_2} \right) |\Delta_I| = \frac{r(w)}{2u_1 + u_2} + \frac{1}{16\pi^2 \sqrt{c^2 - v^2}} \left\{ \gamma \ln \frac{8 |\Delta_I|}{4c\Lambda_c^2 + \gamma^2} + 4\sqrt{\gamma} \Lambda_c \tan^{-1} \left( \frac{2\sqrt{\gamma} \Lambda_c}{\gamma} \right) \right. \\
+ \left. \sqrt{\gamma^2 - 8 |\Delta_I|} \ln \frac{\gamma + \sqrt{\gamma^2 - 8 |\Delta_I|}}{\gamma - \sqrt{\gamma^2 - 8 |\Delta_I|}} \right\} \tag{C.23}
\]

and

\[
2\sigma^2 = \frac{-2 |\Delta_I|}{u_I} + \frac{1}{16\pi^2 \sqrt{c^2 - v^2}} \left\{ \gamma \ln \frac{2 |\Delta_I|}{\gamma^2} + \sqrt{\gamma^2 - 8 |\Delta_I|} \ln \frac{\gamma + \sqrt{\gamma^2 - 8 |\Delta_I|}}{\gamma - \sqrt{\gamma^2 - 8 |\Delta_I|}} \right\} \tag{C.24}
\]
C.5 Nature of the magnetic and Ising transitions at zero temperature

We consider here the concurrent magnetic and Ising transitions at \( T = 0 \). The RG arguments we outlined in the main text suggest that there will be a jump to the order parameters across the transitions, but the jump will be smaller as the damping parameter \( \gamma \) increases. To see how damping affects the transition, we consider the parameter regime where analytical insights can be gained in our large-\( N \) approach. When \( \gamma \) is sufficiently large so that \( x, y \ll 1 \) (definitions of \( x, y \) are given in the main text), it follows from the closed form of free energy [Eq.(7) in the main text] that

\[
\frac{f}{c^{1/2} \Lambda^3_\delta} = -a_0 \left( \frac{r(w)}{c \Lambda^3_\delta} \right)^2 + \frac{\Gamma^3 a_c}{2\pi^2} \mu(w) m_0^2 + 2\Gamma^2 \left( m_0^2 - |\delta_0| \right) \sigma_0^2 + \cdots \tag{C.25}
\]

where in “\( \cdots \)” we temporarily neglect terms at the order of \( O[|\delta_0|^2 \ln |\delta_0|] \) and \( O[m_0^4 \ln m_0^2] \), which will be resumed for getting Eq. (4.13). And \( m_0^2 = m^2/\gamma^2 = (x+y)/2 \), \( \delta_0 = \Delta_I/\gamma^2 = (x-y)/2 \), \( \sigma_0^2 = \sigma^2/ (e^{-1/2} \Lambda_e) \). In addition \( a_c \) and \( a_0, a, \mu(w), \Gamma \) are respectively defined in Eq.(6) and Eq.(14) in the main text. The \( a_c \) here is related to the ellipticity \( \epsilon \) by \( a_c = (\epsilon + 1/\epsilon)/2 \geq 1 \); therefore, a larger \( a_c \) means a stronger anisotropy for the system. From Eq. (C.25), we can observe that if \( r(w) \) is a large positive number, the minimum of the free energy only occurs at \( \sigma_0 = 0 \) and \( m_0 = 0 \), then \( \Delta_I = 0 \), corresponding to the disorder phase of the system as it should be. Eq. (C.25) shows that when the system is deep inside the order phase with \( r_0 < 0 \) and \( |r_0| \gg 1 \), there is no minimum at the origin since \( \mu(w) < 0 \). This implies that when we increase \( r \)
from a large negative value (deep inside the order phase) to certain critical point a phase transition must happen. And this can be made more clear when the system stays in the ordered regime \((\sigma \neq 0)\), where in the limit of \(\eta \equiv |\delta_0| \ll 1\), to the order of \((|\Delta_I|/\gamma^2)^2\), we get Eq. (4.13) in the main text, from which we can see that \(a < 0\) generally holds, which means the maximum of \(A(\eta)\) will be \(\mu_0 = e^{a-1}\) at \(\eta_0 = e^{a-1}\).

The evolution of the equation is illustrated in Fig. C.1(a). When the system is in the ordered regime, i.e., \(r(w)\) is a large negative number, then \(\mu < 0\) and there is a unique global minimum (we focus on the positive branch of Ising order parameter). When \(r(w)\) increases (via increasing \(w\)) to the point that \(\mu = 0\), there is a maximum emerging at the origin while the Ising order shrinks to \(\eta_1 = e^a\). After this, when \(r(w)\) is further increased, the maximum emerges at the origin moves away from the origin with a cusp-type local minimum generated at the origin which can not be covered by Eqs. (C.12,4.13), meanwhile the Ising order shrinks further. And when \(r(w)\) is further increased until \(\mu = \mu_0\), the local maximum and local minimum merge as an inflection point, and the free energy as a function of Ising order will only have a global cusp-type minimum at the origin. Therefore a first order transition happens when \(e^{a-1} < \eta < e^a\) while tuning \(w\) to \(w_c\) such that \(0 < \mu(w_c) < \mu_0\). From Eq. (4.14) we can see larger \(\Gamma\) leads to more negative \(a\), since the transition happens in the regime of \(e^{a-1} < \eta < e^a\), as a result, the first order transition would be exponentially suppressed when \(\Gamma\) becomes larger, implying the transition would become essentially second order when damping becomes strong, which is consistent with RG predictions.
Figure C.2: The evolution of Ising order (a) and antiferromagnetic order (b) as a function of the control parameter $r(w)$ at an extremely strong anisotropy $a_c = 20$ (corresponding ellipticity $\epsilon \approx 0.025$). The jump of the order parameters becomes larger compared with the case of a moderately strong anisotropy $a_c = 2$ (corresponding ellipticity $\epsilon \approx 0.27$) shown in Fig. 2 of the main text.

C.6 The effect of extreme anisotropy

When the anisotropy becomes extremely large, the system effectively becomes 1D, and the effective dimensionality $d + z$ becomes 3; the quartic coupling $-u_I$ will become relevant (as opposed to being marginal) w.r.t. the underlying O(3) QCP, and we expect a stronger degree of first-orderness. Indeed, as shown in Fig. C.2 for an extreme value of anisotropy $a_c = 20$ (corresponding to an extreme ellipticity of $\epsilon = 0.025$), the magnetic order parameter jump becomes sizable.

C.7 The case of three spatial dimensions

In this case, we still have the same saddle-point equation Eq. (C.12), but now we take $q^2 = q_x^2 + q_y^2 + q_z^2$ in $\chi^{-1}_{0, q, \omega_I} = r + \omega_I^2 + cq^2 + \gamma |\omega_I|$. Then at zero temperature the summation in Eq. (C.12) can be calculated as follows (using Eq. (C.18) and working
in the regime of $\Delta_I = -m^2 < 0$).

\[
\frac{1}{2\beta V} \sum_{\tilde{q}, \tilde{w}} D^{-1}_{0, \tilde{q}, \tilde{w}} + v \left(q_x^2 - q_y^2\right) + m^2 - \Delta_I
\]

(C.26)

\[
= \frac{1}{(2\pi)^4} \int_{-\Lambda_f}^{\Lambda_f} d^3q \int_0^{\Gamma_0} d\omega \frac{\gamma \omega}{(\omega^2 - c_T^2) + \gamma^2 \omega^2}
\]

(C.27)

\[
\approx \frac{1}{8\pi^3} \frac{\gamma^2}{c^{1/2} \sqrt{c^2 - v^2}} \int_0^{\Lambda_2^2} dx \frac{i \sqrt{x}}{\sqrt{4x + 4 (m^2 - \Delta_I) - \gamma^2}} \cdot \ln \frac{\gamma - i \sqrt{4x + 4 (m^2 - \Delta_I) - \gamma^2}}{\gamma + i \sqrt{4x + 4 (m^2 - \Delta_I) - \gamma^2}}
\]

(C.28)

\[
= \frac{1}{64\pi^3} \frac{\gamma^2}{c^{1/2} \sqrt{c^2 - v^2}} \int_0^{\Lambda_2} dz \frac{i \sqrt{z}}{\sqrt{z - (1 + \delta)}} \ln \frac{1 - i \sqrt{z - (1 + \delta)}}{1 + i \sqrt{z - (1 + |\delta|)}}
\]

(C.29)

\[
= \frac{1}{64\pi^3} \frac{\gamma^2}{c^{1/2} \sqrt{c^2 - v^2}} \left\{ 2i \int_0^{\Lambda_2} dx \frac{\sqrt{x^2 + 1 - |\delta|} \ln \frac{1 - ix}{1 + ix}}{\sqrt{\delta - 1}} + 2i \int_0^{\Lambda_2} dx \frac{\sqrt{x^2 + 1 - |\delta|} \ln \frac{1 - ix}{1 + ix}}{\sqrt{\delta - 1}} \right\}
\]

(C.30)

where $\Lambda_2 = 4cA^2/\gamma^2 = 4/\Gamma^2$, $\delta = 8\Delta_I/\gamma^2$. Now let’s deal with the two integrals one by one.

\[
I = 2 \int_0^{(1 - |\delta|)^{1/2}} dx \sqrt{1 - |\delta| - x^2} \ln \frac{1 + x}{1 - x}
\]

(C.31)

\[
= 2 (1 - |\delta|)^{1/2} \sum_{n=0}^{\infty} \frac{(-1)^n}{(1 - |\delta|)^n} \left( \begin{array}{c} 1/2 \\ n \end{array} \right) \int_0^{(1 - |\delta|)^{1/2}} dx x^{2n} \ln \frac{1 + x}{1 - x}
\]

(C.32)
\[
\begin{align*}
&= 2 (1 - |\delta|)^{1/2} \sum_{n=0}^{\infty} \frac{(-1)^n}{(1 - |\delta|)^n} \binom{1/2}{n} \cdot \left[ \frac{(1 - |\delta|)^{n+1/2}}{2n + 1} \ln \frac{1 + (1 - |\delta|)^{1/2}}{1 - (1 - |\delta|)^{1/2}} - \int_0^{(1-|\delta|)^{1/2}} \frac{dx x^{2n+1}}{2n + 1} \right] \\
&= 2 \frac{\pi}{4} (1 - |\delta|) \ln \frac{1 + (1 - |\delta|)^{1/2}}{1 - (1 - |\delta|)^{1/2}} + 2 (1 - |\delta|)^{1/2} \cdot \sum_{n=0}^{\infty} \frac{(-1)^n}{(1 - |\delta|)^n} \binom{1/2}{n} \left[ - \int_0^{(1-|\delta|)^{1/2}} \frac{dx x^{2n+1}}{2n + 1} \right] \\
&= 2 \frac{\pi}{4} (1 - |\delta|) \ln \frac{1 + (1 - |\delta|)^{1/2}}{1 - (1 - |\delta|)^{1/2}} + 2 \left[ (1 - |\delta|)^{1/2} + \sqrt{|\delta| - 1} \sinh^{-1} \left( \frac{x}{\sqrt{|\delta| - 1}} \right) \right] \int_0^{(1-|\delta|)^{1/2}} \frac{dx}{1 + x^2} \\
&= 2 \frac{\pi}{4} (1 - |\delta|) \ln \frac{1 + (1 - |\delta|)^{1/2}}{1 - (1 - |\delta|)^{1/2}} + 2 \left[ (1 - |\delta|)^{1/2} + \sqrt{|\delta| - 1} \sinh^{-1} \left( \frac{x}{\sqrt{|\delta| - 1}} \right) \right] \\
&\text{where } \binom{n}{m} \equiv \frac{\Gamma(n+1)}{\Gamma(m+1)\Gamma(n-m+1)} \text{ is the binomial coefficient. But}
\end{align*}
\]
\[ I = -2 \frac{\pi}{4} (1 - |\delta|) \ln \frac{1 + (1 - |\delta|)^{1/2}}{1 - (1 - |\delta|)^{1/2}} + 2 (1 - |\delta|)^{1/2} \frac{i}{4} (1 - |\delta|)^{1/2} \]
\[ \left\{ \pi^2 - 4 \cosh^{-1} \sqrt{|\delta|} \ln \left( -i \left( 1 - \sqrt{|\delta|} \right) / \sqrt{1 - |\delta|} \right) + 4 \text{Li}_2 \left( -i (1 - |\delta|)^{1/2} - \sqrt{|\delta|} \right) - 4 \text{Li}_2 \left( i (1 - |\delta|)^{1/2} + \sqrt{|\delta|} \right) \right\} \] (C.40)

where \( \text{Li}_n(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^n} \) is the polylogarithm function. Substituting Eq. (C.40) back into Eq. (C.37), we have

\[ I = 2 \left\{ -1 + 2 \alpha_0 - 2 \alpha_0 |\delta| + \frac{\pi}{3} |\delta|^{3/2} - \frac{1}{4} |\delta|^2 + O \left( |\delta|^{5/2} \right) \right\} \] (C.41)

Note Eq. (C.40) is an exact result for the integral \( I \) in Eq. (C.30). For simplicity here we only consider the analytic limit at \(|\delta| = 8 |\Delta_t| / \gamma^2 \ll 1\). Within this limit we can get an expansion series of Eq. (C.41) in the order of \(|\delta|\),

\[ I = 2 \left\{ -1 + 2 \alpha_0 - 2 \alpha_0 |\delta| + \frac{\pi}{3} |\delta|^{3/2} - \frac{1}{4} |\delta|^2 + O \left( |\delta|^{5/2} \right) \right\} \] (C.42)

where \( \alpha_0 \approx 0.91596 \) is the Catalan number.

Now let’s calculate the integral \( II \) in Eq. (C.30), which is straightforward in the limit of \(|\delta| = 8 |\Delta_t| / \gamma^2 \ll 1\).

\[ II = 2i \int_{0}^{\sqrt{\lambda}} dx \sqrt{x^2 + 1 - |\delta|} \ln \frac{1 - i x}{1 + i x} \]
\[ = 4 \int_{0}^{\sqrt{\lambda}} dx \sqrt{x^2 + 1} \tan^{-1} x - 2 |\delta| \int_{0}^{\sqrt{\lambda}} dx \frac{\tan^{-1} x}{\sqrt{1 + x^2}} + O \left( |\delta|^2 \right) \] (C.43)
but

\[ 4 \int_{0}^{\sqrt{\Lambda_\gamma}} dx \sqrt{x^2 + 1 \tan^{-1} x} = \pi \Lambda_\gamma - 4 \sqrt{\Lambda_\gamma} + \frac{\pi}{2} \ln \Lambda_\gamma + \frac{\pi}{2} (1 + 2 \ln 2) + 2 - 4\alpha_0 + O \left( \frac{1}{\sqrt{\Lambda_\gamma}} \right) \quad (C.44) \]

and

\[ \int_{0}^{\sqrt{\Lambda_\gamma}} dx \frac{\tan^{-1} x}{\sqrt{x^2 + 1}} = \frac{\pi}{2} \ln 2 - 2\alpha_0 + \frac{\pi}{4} \ln \Lambda_\gamma + O \left( \frac{1}{\sqrt{\Lambda_\gamma}} \right) \quad (C.45) \]

Substituting the results of Eqs. (C.44,C.45) into Eq. (C.43), we have

\[
II = \pi \Lambda_\gamma - 4 \sqrt{\Lambda_\gamma} + \frac{\pi}{2} \ln \Lambda_\gamma + \frac{\pi}{2} (1 + 2 \ln 2) + 2 - 4\alpha_0 \\
- 2 |\delta| \left( \frac{\pi}{2} \ln 2 - 2\alpha_0 + \frac{\pi}{4} \ln \Lambda_\gamma \right) + O \left( \frac{1}{\sqrt{\Lambda_\gamma}} \right) + O(|\delta|^2) \quad (C.46)
\]

Combing the results in Eqs. (C.42,C.46), we finally have

\[
I + II = \pi \Lambda_\gamma - 4 \sqrt{\Lambda_\gamma} + \frac{\pi}{2} \ln \Lambda_\gamma + \frac{\pi}{2} (1 + 2 \ln 2) - \left( \pi \ln 2 + \frac{\pi}{2} \ln \Lambda_\gamma \right) |\delta| \\
+ \frac{\pi}{3} |\delta|^{3/2} + O \left( \frac{1}{\sqrt{\Lambda_\gamma}} \right) + O(|\delta|^2) \quad (C.47)
\]

Substituting Eq. (C.47) into Eq. (C.12), we have

\[
\frac{\alpha_c \Delta_I}{u_I \gamma^2} = \frac{\alpha_c \Delta_I}{(2u_1 + u_2) \gamma^2} + \kappa_0 - \kappa_1 |\delta| + \frac{\pi}{3} |\delta|^{3/2} + O(\delta^2) \quad (C.48)
\]

with \( \alpha_c = 64\pi^3 c^{1/2} \sqrt{c^2 - v^2} \), and

\[
\kappa_0(w) = \frac{\alpha_c r(w)}{(2u_1 + u_2) \gamma^2} + \pi \Lambda_\gamma - 4 \sqrt{\Lambda_\gamma} + \frac{\pi}{2} \ln \Lambda_\gamma + \frac{\pi}{2} (1 + 2 \ln 2) \quad (C.49)
\]

\[
\kappa_1 = \pi \ln 2 + \frac{\pi}{2} \ln \Lambda_\gamma = \pi \ln 2 + \frac{\pi}{2} \ln \frac{4}{1^2}.
\]
Then we have

\[ B(|\delta|) \equiv a_{d_3z^2} |\delta| - \frac{2\pi}{3} |\delta|^{3/2} = \kappa_0(w) \]  

(C.50)

with

\[ a_{d_3z^2} = -\frac{\alpha_c}{4} \left( \frac{1}{u_I} - \frac{1}{2u_1 + u_2} \right) + 2\kappa_1 = -\frac{16\pi^3}{a_e} \left( \frac{c_3^{3/2}}{u_I} - \frac{c_3^{3/2}}{2u_1 + u_2} \right) + 2\kappa_1 \]  

(C.51)

From Eq. (C.50) we can see that the sign of \( a_{d_3z^2} \) will determine the order(s) of the phase transition. If \( a_{d_3z^2} < 0 \), there is no first order transition since Eq. (C.50) always has only one solution; the Ising order parameter will continuously go to zero as we increase the controlled parameter \( w \) in \( \kappa_0(w) \). Fig. C.1(b) illustrates the process for the phase transitions at \( a_{d_3z^2} < 0 \).

If \( a_{d_3z^2} > 0 \), a first order transition can happen, since two solutions of Eq. (C.50) emerge when \( \kappa_0(w) > 0 \). From the LHS of Eq. (C.50), we can determine that \( a_{d_3z^2} > 0 \) can happen either at \( v \approx c \) (i.e., extreme anisotropy) or at extremely small damping rate. In the former case the system is effectively reduced back to the 3D problem, where we roughly recover the 2D results. For the latter case, it is equivalent to changing the effective dimension \( d + z = d + 2 \) to \( d + 1 \). Therefore in both of these two extreme situations, the effective dimension of the system becomes 4; the Ising coupling \( -u_I \) is again marginal, and a first-order transition is to be expected from RG-based considerations. For the problem we are considering, neither case applies.

For the summation in Eq. (C.11), a similar calculation can be carried out. One can easily find that it is \( \delta \)-independent, which is just equal to the \( \delta \)-independent part of the summation in Eq. (C.12). Therefore after summing Eq. (C.11) and Eq. (C.12)
Figure C.3: Evolution of (a) the Ising order parameter and (b) the magnetic order parameter vs. the control parameter at a relatively strong anisotropy, for the 3D case.

Figure C.4: Evolution of (a) the Ising order parameter and (b) the magnetic order parameter vs. the control parameter at an extremely strong anisotropy, and with strong interactions, also in the 3D case.

we will get,

\[
\frac{2\Delta I}{u_I} = -2\sigma^2 + \frac{\gamma^2}{\alpha_c} \left( -\kappa_1 |\delta| + \frac{\pi}{3} |\delta|^{3/2} + O \left( \frac{1}{\sqrt{\Lambda_\gamma}} \right) + O \left( |\delta|^2 \right) \right) \quad (C.52)
\]
i.e.,

\[
\sigma_0 = \frac{\Gamma}{8\pi} \sqrt{\frac{1}{\alpha_c}} \sqrt{\frac{16\pi^3 c^{3/2}}{u_I}} \left( \frac{1}{2} - \kappa_1 \right) |\delta| + \frac{\pi}{6} |\delta|^{3/2} \quad (C.53)
\]

with dimensionless magnetization \(\sigma_0 = c^{1/4} \sigma / \Lambda_c\). From Eq. (C.53) we can see that
when $\delta$ continues goes to zero, magnetization will also continuously go to zero, indicating a second-order magnetic phase transition, and the concurrence of Ising and magnetic phase transitions. From Eqs. (C.50,C.53), we can get Ising order and magnetic order vs. the control parameter $r(w)$ in d3z2 systems in the limit of $|\delta| = 8|\Delta_I|/\gamma^2 \ll 1$, as shown in Figs. (C.3,C.4), where the Ising order $\Delta_I$ and magnetic order $\sigma$ have been respectively re-scaled into dimensionless quantities via $\Delta_I \to \Delta_I/(c\Lambda_c^2)$ and $\sigma \to c^{1/4}\sigma/\Lambda_c = \sigma_0$ (for convenience we also introduce a group of dimensionless parameters $a_{d3z2}^{I} = c^{3/2}/u_I, a_{d3z2}^{\Delta} = c^{3/2}/(2u_1 + u_2), a_c = c/\sqrt{c^2 - v^2}, \Gamma = \gamma/(c^{1/2}\Lambda_c)$).

At moderate strong anisotropy $a_c = 2$ i.e., $\epsilon \approx 0.27$ (Fig. C.3), it shows continuous quantum phase transitions and concurrence of the Ising and magnetic orders when increasing $w$. As in the 2D case we also study the effect of strong anisotropy at $a_c = 20$ i.e., $\epsilon \approx 0.025$ (Fig. C.4), where the continuous phase transitions persist, and the two transitions are concurrent. This is consistent with the RG considerations: given that the effective dimensionality in this case is $d + z = 5$, the quartic coupling $-u_I$ becomes irrelevant w.r.t. to the underlying O(3) transition and will therefore not destabilize the continuous nature of the transition.
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