Universal Impurity-Induced Bound State in Topological Superfluids

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We predict a universal midgap bound state in topological superfluids, induced by either nonmagnetic or magnetic impurities in the strong scattering limit. This universal state is similar to the lowest-energy Caroli–de Gennes–Martricon bound state in a vortex core, but is bound to localized impurities. We argue that the observation of such a universal bound state can be a clear signature for identifying topological superfluids. We theoretically examine our argument for a spin-orbit coupled ultracold atomic Fermi gas trapped in a two-dimensional harmonic potential by performing extensive self-consistent calculations within the mean-field Bogoliubov–de Gennes theory. A realistic scenario for observing a universal bound state in ultracold ^{40}K atoms is proposed.

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Topological superfluids are of great interest [1]. They are promising candidates that host Majorana fermions [2], which lie at the heart of topological quantum information and computation, due to their exotic non-Abelian exchange statistics [3–5]. To date, there have been a number of proposals for practical realizations of topological superfluids, including $p + ip$ superconductors [6,7], surfaces of three-dimensional topological insulators [8–10] or one-dimensional (1D) spin-orbit coupled nanowires [11,12] in proximity to an s-wave superconductor, and two-dimensional (2D) [13–16] or 1D [17–19] spin-orbit coupled atomic Fermi gases near Feshbach resonances. All these proposals are appealing and are to be examined experimentally. In fact, recent experimental results on the tunneling spectroscopy of semiconductor InSb nanowires in a magnetic field placed in contact with a superconducting electrode [20] may already suggest the existence of topological superfluids and Majorana fermions. However, unambiguous characterizations of the topological properties of the nanowires are still missing.

In this Letter, we propose that a universal midgap bound state, induced by strong nonmagnetic or magnetic impurity scattering, could provide a clear signature for the existence of topological superfluids. In the solid state, impurities are widely known to serve as an important local probe that characterizes the quantum state of hosting systems [21]. Individual impurities have been used to determine the superconducting pairing symmetry of unconventional non-s-wave superconductors [22] and to demonstrate Friedel oscillations on a Be(0001) surface [23]. In strongly correlated many-body systems, they may be employed to pin one of the competing orders [24]. Here, unique to topological superfluids, we predict that a single impurity with a sufficiently strong scattering strength can create a universal midgap state bound to the impurity. It resembles the lowest-energy Caroli–de Gennes–Martricon (CdGM) bound state inside a vortex core [25]. For small order parameters, where the bound state energy E is nearly zero, the wave function of the universal bound state is found to closely follow the symmetry of that of Majorana fermions [16].

In our work, the emergence of a universal impurity-induced bound state is examined theoretically in an interacting spin-orbit coupled ultracold atomic Fermi gas in 2D harmonic traps [16]. We perform numerically extensive self-consistent calculations by using the fully microscopic Bogoliubov–de Gennes (BdG) theory, to explore the details of the universal bound state. This specific choice of topological superfluids is motivated by the recent realization of spin-orbit coupling in atomic Fermi gases of ^{40}K [26] and ^{6}Li atoms [27]. Benefiting from the high controllability in the interaction, geometry, and purity in cold-atom experiments, 2D spin-orbit coupled atomic Fermi gases are arguably the best candidate for observing the predicted universal bound state. Our results, however, should be applicable as well to various topological superfluids that are believed to exist in the solid state. We propose a realistic scenario for creating a universal bound state in ^{40}K atoms and discuss briefly the relevance of our results to other solid state systems.

Mean-field BdG equation.—To start, we consider a trapped 2D atomic Fermi gas with a Rashba-type spin-orbit coupling and a Zeeman field h, which is believed to be a topological superfluid when the Zeeman field exceeds a threshold h_c [16]. The model Hamiltonian of the system is given by $\mathcal{H} = \int d\mathbf{r}[\mathcal{H}_0(\mathbf{r}) + \mathcal{H}_I(\mathbf{r}) + \mathcal{H}_{\rm imp}(\mathbf{r})]$, where

$$\mathcal{H}_0(\mathbf{r}) = \sum_{\sigma=\uparrow,\downarrow} \psi_\sigma^\dagger \mathcal{H}_\sigma^S(\mathbf{r})\psi_\sigma + [\psi_\uparrow^\dagger V_{SO}(\mathbf{r})\psi_\downarrow + \text{H.c.}] \quad (1)$$

is the single-particle Hamiltonian density in the presence of Rashba spin-orbit coupling $V_{SO}(\mathbf{r}) = -i\lambda(\partial_y + i\partial_x)$, $\mathcal{H}_I(\mathbf{r}) = U_0\psi_\uparrow^\dagger(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r})$ represents the interaction, and $\mathcal{H}_{\text{imp}}(\mathbf{r}) = \sum_{\sigma=\uparrow,\downarrow}\psi_\sigma^\dagger V_{\text{imp}}^\sigma(\mathbf{r})\psi_\sigma$ describes the potential scattering due to the impurity. Here, $\psi_{\uparrow,\downarrow}^\dagger$ are respectively the creation field operators for the spin-up and spin-down atoms and $\mathcal{H}_\sigma^S(\mathbf{r}) \equiv -\hbar^2\nabla^2/(2M) + M\omega^2r^2/2 - \mu - h\sigma_z$ is the single-particle Hamiltonian in a 2D harmonic trapping potential $M\omega^2r^2/2$, in reference to the chemical potential μ. We have used the standard s-wave contact interaction between atoms with opposite spins, whose strength U_0 is to be regularized by the binding energy of the two-body bound state E_a [16,28]. For computational simplicity, we place an impurity at the origin and consider either a deltalike scattering potential, $V_{\text{imp}}^\sigma(\mathbf{r}) = V_{\text{imp}}^\sigma\delta(r)$, or a Gaussian-shape potential with width d, $V_{\text{imp}}^\sigma(\mathbf{r}) = [V_{\text{imp}}^\sigma/(\pi d^2)]\exp[-r^2/d^2]$. In the case of a magnetic impurity, we take the potential strength $V_{\text{imp}}^\uparrow = -V_{\text{imp}}^\downarrow = -V_{\text{imp}}$, while for the nonmagnetic impurity, $V_{\text{imp}}^\uparrow = V_{\text{imp}}^\downarrow = -V_{\text{imp}}$. We have checked both positive and negative values of V_{imp} and have observed very similar results at large $|V_{\text{imp}}|$. Hereafter, we focus on the case with $V_{\text{imp}} > 0$.

We solve the low-energy fermionic quasiparticles of the model Hamiltonian by using the standard mean-field BdG approach, $\mathcal{H}_{\text{BdG}}\Psi_\eta(\mathbf{r}) = E_\eta\Psi_\eta(\mathbf{r})$, where

$$\mathcal{H}_{\text{BdG}} = \begin{bmatrix} \mathcal{H}_\uparrow^S(\mathbf{r}) + V_{\text{imp}}^\uparrow(\mathbf{r}) & V_{SO}(\mathbf{r}) & 0 & -\Delta(\mathbf{r}) \\ V_{SO}^\dagger(\mathbf{r}) & \mathcal{H}_\downarrow^S(\mathbf{r}) + V_{\text{imp}}^\downarrow(\mathbf{r}) & \Delta(\mathbf{r}) & 0 \\ 0 & \Delta^*(\mathbf{r}) & -\mathcal{H}_\uparrow^S(\mathbf{r}) - V_{\text{imp}}^\uparrow(\mathbf{r}) & V_{SO}^\dagger(\mathbf{r}) \\ -\Delta^*(\mathbf{r}) & 0 & V_{SO}(\mathbf{r}) & -\mathcal{H}_\downarrow^S(\mathbf{r}) - V_{\text{imp}}^\downarrow(\mathbf{r}) \end{bmatrix} \quad (2)$$

is the BdG Hamiltonian, $\Psi_\eta(\mathbf{r}) = [u_{\uparrow\eta}, u_{\downarrow\eta}, v_{\uparrow\eta}, v_{\downarrow\eta}]^T$, and E_η are the Nambu spinor wave functions and energies for quasiparticles, respectively. Within the mean field, the order parameter takes the form $\Delta(\mathbf{r}) = -(U_0/2)\sum_\eta[u_{\uparrow\eta}v_{\downarrow\eta}^*f(E_\eta) + u_{\downarrow\eta}v_{\uparrow\eta}^*f(-E_\eta)]$ and, is to be solved self-consistently together with the atomic densities, $n_\sigma(\mathbf{r}) = (1/2)\sum_\eta[|u_{\sigma\eta}|^2f(E_\eta) + |v_{\sigma\eta}|^2f(-E_\eta)]$. Here $f(x) \equiv 1/(e^{x/k_BT} + 1)$ is the Fermi distribution function at temperature T. The chemical potential μ, implicit in $\mathcal{H}_\sigma^S(\mathbf{r})$, can be determined by the total number of atoms N using the number equation $\int d\mathbf{r}[n_\uparrow(\mathbf{r}) + n_\downarrow(\mathbf{r})] = N$. As the impurity is placed at the origin $r = 0$, the BdG Hamiltonian preserves rotational symmetry. Therefore, we take $\Delta(\mathbf{r}) = \Delta(r)$ and decouple the BdG equation into different angular momentum channels indexed by an integer m, with which the quasiparticle wave functions become $[u_{\uparrow\eta}(r), u_{\downarrow\eta}(r)e^{i\varphi}, v_{\uparrow\eta}(r)e^{i\varphi}, v_{\downarrow\eta}(r)]e^{im\varphi}/\sqrt{2\pi}$. By expanding $u_{\sigma\eta}(r)$ and $v_{\sigma\eta}(r)$ in the basis of 2D harmonic oscillators, the solution of the BdG equation converts to a matrix diagonalization problem. Numerically we have to truncate the summation over energy levels η. This is done by introducing a high energy cutoff E_c, above which a local density approximation is used for high-lying wave functions [29]. We have checked that such a hybrid procedure is numerically very efficient.

For the results presented here, we have solved self-consistently the BdG equation for a cloud with $N = 400$ atoms at zero temperature. In 2D harmonic traps, it is convenient to use the Fermi radius $r_F = (4N)^{1/4}\sqrt{\hbar/(M\omega)}$ and Fermi energy $E_F = \hbar^2k_F^2/(2M) = \sqrt{N}\hbar\omega$ as the units for length and energy, respectively. The strength of the impurity scattering potential V_{imp}^σ will be measured in units of $r_F^2E_F$. We have taken an interaction parameter $E_a = 0.2E_F$ and a spin-orbit coupling strength $\lambda k_F/E_F = 1$. With these parameters, the whole Fermi cloud becomes a topological superfluid when the Zeeman field is larger than a threshold $h_c \simeq 0.57E_F$ [16]. Let us first consider the localized impurities with a deltalike scattering potential $V_{\text{imp}}^\sigma\delta(r)$.

Emergence of a universal impurity bound state.—According to Anderson's theorem [30], a conventional s-wave superfluid can barely be affected by nonmagnetic impurities. In contrast, magnetic impurities can break the time-reversal symmetry of the superfluid and act as pair breakers, leading to the appearance of a midgap state—the so-called Yu-Shiba state—which is bound to localized impurities inside the pairing gap [31,32]. The energy of such a midgap bound state is determined by the strength of the impurity scattering potential V_{imp}. As V_{imp} increases, the Yu-Shiba state moves from the upper gap edge to the lower gap edge for the spin-up atoms and moves oppositely for the spin-down atoms. In the presence of Rashba spin-orbit coupling, we have confirmed numerically that the above statements continue to hold, even under a Zeeman field, if the Fermi cloud is not a topological superfluid. For a typical parameter $h = 0.2E_F$, with an increase of the strength of the magnetic impurity, we find that the position of the Yu-Shiba state moves very quickly from one gap edge to the other.

In contrast, once the Zeeman field is beyond the threshold h_c so that the whole Fermi cloud becomes a topological

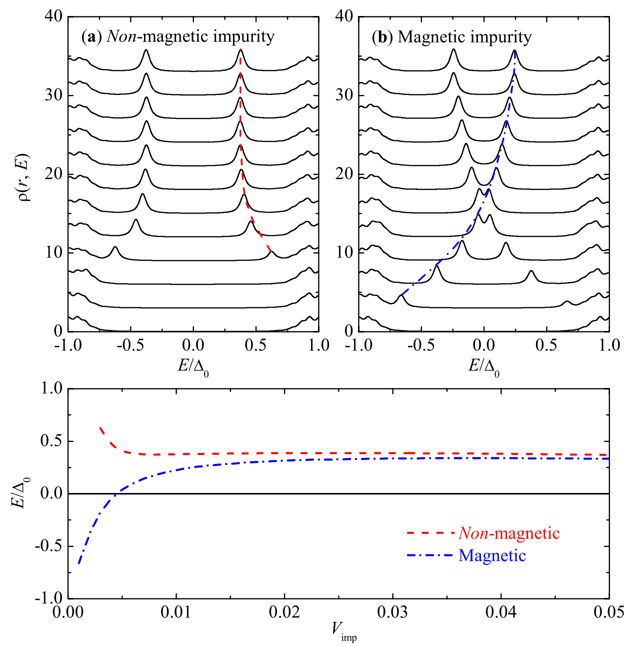

FIG. 1 (color online). Bound states induced by a nonmagnetic deltalike impurity (a) and by a magnetic deltalike impurity (b), $V^{\sigma}_{\rm imp}(\mathbf{r}) = V^{\sigma}_{\rm imp}\delta(r)$, in a topological superfluid at $h = 0.7E_F$, as shown by the peaks in the total local density of states (LDOS) $\rho(r, E)$ at $k_F r = 2$. Here, $\rho(r, E) = \sum_\sigma \rho_\sigma(\mathbf{r}, E)$ and $\rho_\sigma(\mathbf{r}, E) = (1/2)\sum_\eta[|u_{\sigma\eta}|^2\delta(E - E_\eta) + |v_{\sigma\eta}|^2\delta(E + E_\eta)]$. The dashed and dash-dotted lines highlight the resonance peak position or the energy of bound states. From bottom to top, the impurity strength increases from $V_{\rm imp} = 0$ to $0.011r_F^2E_F$, in steps of $0.001r_F^2E_F$. The curves are offset for clarity, except for the lowest curve at $V_{\rm imp} = 0$. (c) The energy of bound states as a function of the impurity strength, in units of the gap parameter at the trap center in the absence of impurity, $\Delta_0 \simeq 0.307E_F$.

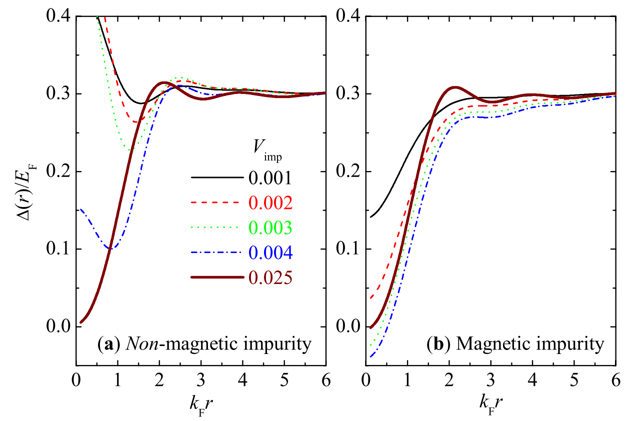

FIG. 2 (color online). Gap parameter as a function of impurity strength $V_{\rm imp}$ (in units of $r_F^2E_F$), for a nonmagnetic impurity (a) and for a magnetic impurity (b). In the limit of strong impurity scattering, the gap parameter has the same spatial distribution, whether the impurity is nonmagnetic or magnetic.

superfluid, we observe an entirely different behavior, as revealed in Fig. 1. For nonmagnetic impurities, an unexpected bound state appears from one gap edge as the impurity strength is larger than a critical strength $V_{\rm imp} \gtrsim 0.004r_F^2E_F$. As $V_{\rm imp}$ increases, the bound state moves towards, but never reaches, zero energy. In fact, its energy saturates quickly to $E \simeq 0.11E_F \simeq \Delta_0^2/E_F$, where $\Delta_0 \simeq 0.307E_F$ is the gap parameter at the trap center in the absence of an impurity. For magnetic impurities, the dependence of the position of the Yu-Shiba state on the impurity strength is also strongly modified: at large impurity scattering, the Yu-Shiba state now moves to $E \simeq \Delta_0^2/E_F$, nearly at the same energy as the new bound state induced by strong nonmagnetic impurities. This coincidence in the energy of bound states clearly indicates that in topological superfluids a universal bound state emerges in the limit of strong impurity scattering.

Origin of the universal state.—The appearance of bound states implies that the gap parameter would be strongly depleted close to the impurity. In Fig. 2, we examine the spatial profile of the order parameter near the impurity. For a weak nonmagnetic impurity, as shown in Fig. 2(a), the gap parameter is already strongly modified at $V_{\rm imp} \gtrsim 0.004r_F^2E_F$. Seen as a scattering potential for Bogoliubov quasiparticles [25], the gap parameter hence starts to accommodate a bound state. For a weak magnetic impurity [Fig. 2(b)], the pair-breaking effect is always significant enough to induce a Yu-Shiba bound state, as anticipated. In the strong scattering limit, it is remarkable that the gap parameter acquires a universal spatial profile, despite the type and strength of the impurities. It is fully depleted at the impurity site and has a very similar distribution as the gap parameter inside a vortex core. Therefore, we anticipate that the observed universal bound state would resemble the well-known CdGM vortex-core bound states [25]. Indeed, the energy of the universal impurity state, $E \simeq \Delta_0^2/E_F$, is of the same order as that of the CdGM bound states.

Now, the formation of the universal bound state can be easily understood from its analogy with the CdGM vortex-core state. As the gap parameter is fully suppressed at the impurity site, we have a local point defect (i.e., vacuum) that is topologically trivial. Due to the topological nature of the Fermi cloud away from the impurity, there would be an interface between the nontopological and topological components, which can host a gapless Majorana edge state [33]. The observed universal impurity state is precisely such a Majorana edge mode. However, its energy is not exactly zero due to the finite confinement of the system [34]. As derived analytically by Stone and Roy [35] (see also Ref. [34]), the dispersion relation of edge states in topological superfluids with a confinement length ξ is given by $E(m) = -(m + 1/2)\Delta_0/(k_F\xi)$. By assuming a characteristic length $\xi \sim \hbar v_F/\Delta_0$ for the gap parameter distribution [25], where v_F is the Fermi velocity, we estimate that $E \sim \Delta_0^2/E_F$, in good agreement with the observed energy of the universal bound state.

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Note added.—After completing this work, we became aware of a related nonself-consistent T-matrix calculation in 1D topological superconductors, which predicted a bound state induced by nonmagnetic impurities [41].

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[1] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).
[2] E. Majorana, Nuovo Cimento **14**, 171 (1937).
[3] A. Kitaev, Ann. Phys. (Amsterdam) **321**, 2 (2006).
[4] C. Nayak, S. Simon, A. Stern, M. Freedman, and S. D. Sarma, Rev. Mod. Phys. **80**, 1083 (2008).
[5] F. Wilczek, Nat. Phys. **5**, 614 (2009).
[6] N. Read and D. Green, Phys. Rev. B **61**, 10 267 (2000).
[7] T. Mizushima, M. Ichioka, and K. Machida, Phys. Rev. Lett. **101**, 150409 (2008).
[8] L. Fu and C. L. Kane, Phys. Rev. Lett. **100**, 096407 (2008).
[9] J. D. Sau, R. M. Lutchyn, S. Tewari, and S. D. Sarma, Phys. Rev. Lett. **104**, 040502 (2010).
[10] J. Alicea, Phys. Rev. B **81**, 125318 (2010).
[11] R. M. Lutchyn, J. D. Sau, and S. D. Sarma, Phys. Rev. Lett. **105**, 077001 (2010).
[12] Y. Oreg, G. Refael, and F. von Oppen, Phys. Rev. Lett. **105**, 177002 (2010).
[13] C. Zhang, S. Tewari, R. M. Lutchyn, and S. D. Sarma, Phys. Rev. Lett. **101**, 160401 (2008).
[14] M. Sato, Y. Takahashi, and S. Fujimoto, Phys. Rev. Lett. **103**, 020401 (2009).
[15] S.-L. Zhu, L. B. Shao, Z. D. Wang, and L. M. Duan, Phys. Rev. Lett. **106**, 100404 (2011).
[16] X.-J. Liu, L. Jiang, H. Pu, and H. Hu, Phys. Rev. A **85**, 021603(R) (2012).
[17] L. Jiang, T. Kitagawa, J. Alicea, A. R. Akhmerov, D. Pekker, G. Refael, J. I. Cirac, E. Demler, M. D. Lukin, and P. Zoller, Phys. Rev. Lett. **106**, 220402 (2011).
[18] X.-J. Liu and H. Hu, Phys. Rev. A **85**, 033622 (2012).
[19] R. Wei and E. J. Mueller, Phys. Rev. A **86**, 063604 (2012).
[20] V. Mourik, K. Zuo, S. M. Frolov, S. R. Plissard, E. P. A. M. Bakkers, and L. P. Kouwenhoen, Science **336**, 1003 (2012); L. P. Rokhinson, X. Liu, and J. K. Furdyna, Nat. Phys. **8**, 795 (2012).
[21] A. V. Balatsky, I. Vekhter, and J.-X. Zhu, Rev. Mod. Phys. **78**, 373 (2006).
[22] E. W. Hudson, K. M. Lang, V. Madhavan, S. H. Pan, H. Eisaki, S. Uchida, and J. C. Davis, Nature (London) **411**, 920 (2001).
[23] P. T. Sprunger, L. Petersen, E. W. Plummer, E. Lægsgaard, and F. Besenbacher, Science **275**, 1764 (1997).
[24] A. J. Millis, Solid State Commun. **126**, 3 (2003).
[25] C. Caroli, P. G. de Gennes, and J. Matricon, Phys. Lett. **9**, 307 (1964).
[26] P. Wang, Z.-Q. Yu, Z. Fu, J. Miao, L. Huang, S. Chai, H. Zhai, and J. Zhang, Phys. Rev. Lett. **109**, 095301 (2012).
[27] L. W. Cheuk, A. T. Sommer, Z. Hadzibabic, T. Yefsah, W. S. Bakr, and M. W. Zwierlein, Phys. Rev. Lett. **109**, 095302 (2012).
[28] M. Randeria, J.-M. Duan, and L.-Y. Shieh, Phys. Rev. Lett. **62**, 981 (1989).
[29] X.-J. Liu, H. Hu, and P. D. Drummond, Phys. Rev. A **75**, 023614 (2007).
[30] P. W. Anderson, J. Phys. Chem. Solids **11**, 26 (1959).
[31] L. Yu, Acta Phys. Sin. **21**, 75 (1965).
[32] H. Shiba, Prog. Theor. Phys. **40**, 435 (1968).
[33] W.-Y. Shan, J. Lu, H.-Z. Lu, and S.-Q. Shen, Phys. Rev. B **84**, 035307 (2011); J. Lu, W.-Y. Shan, H.-Z. Lu, and S.-Q. Shen, New J. Phys. **13**, 103016 (2011).
[34] J. Alicea, Rep. Prog. Phys. **75**, 076501 (2012).
[35] M. Stone and R. Roy, Phys. Rev. B **69**, 184511 (2004).
[36] Y. Shin, C. H. Schunck, A. Schirotzek, and W. Ketterle, Phys. Rev. Lett. **99**, 090403 (2007).
[37] L. Jiang, L. O. Baksmaty, H. Hu, Y. Chen, and H. Pu, Phys. Rev. A **83**, 061604 (2011).
[38] P. Dyke, E. D. Kuhnle, S. Whitlock, H. Hu, M. Mark, S. Hoinka, M. Lingham, P. Hannaford, and C. J. Vale, Phys. Rev. Lett. **106**, 105304 (2011).
[39] B. Fröhlich, M. Feld, E. Vogt, M. Koschorreck, W. Zwerger, and M. Köhl, Phys. Rev. Lett. **106**, 105301 (2011).
[40] D. M. Stamper-Kurn, H.-J. Miesner, A. P. Chikkatur, S. Inouye, J. Stenger, and W. Ketterle, Phys. Rev. Lett. **81**, 2194 (1998).
[41] J. D. Sau and E. Demler, arXiv:1204.2537.