Universal Impurity-Induced Bound State in Topological Superfluids

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(Received 21 September 2012; published 10 January 2013)

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 40K atoms is proposed.

DOI: 10.1103/PhysRevLett.110.020401 PACS numbers: 03.75.Ss, 03.75.Hh, 05.30.Fk, 67.85.-d

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 bound state 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 $\mathbf{h}$, which is believed to be a topological superfluid when the Zeeman field exceeds a threshold $h_0$ [16]. The model Hamiltonian of the system is given by $\hat{H} = \int d\mathbf{r} [\hat{H}_0(\mathbf{r}) + \hat{H}_J(\mathbf{r}) + \hat{H}_{\text{imp}}(\mathbf{r})]$, where

\[ \mathcal{H}_0(r) = \sum_{\sigma \rightarrow 1} \psi^\dagger \mathcal{H}_{\sigma}^0(r) \psi_{\sigma} + \left[ \psi^\dagger \mathcal{V}_{SO}(r) \psi_{\uparrow} + \text{H.c.} \right] \]  

(1)

is the single-particle Hamiltonian density in the presence of Rashba spin-orbit coupling \( \mathcal{V}_{SO}(r) = -i\lambda (\partial_x + i\partial_y) \). \( \mathcal{H}_I(r) = U_0 \psi^\dagger \uparrow(r) \psi_{\uparrow}(r) \psi_{\downarrow}(r) \psi^\dagger \downarrow(r) \) represents the interaction, and \( \mathcal{H}_{\text{imp}}(r) = \sum_{\sigma \rightarrow 1} \psi^\dagger \mathcal{V}_{\sigma}(r) \psi_{\sigma} \) describes the potential scattering due to the impurity. Here, \( \psi_{\uparrow\downarrow}(r) \) are respectively the creation field operators for the spin-up and spin-down atoms and \( \mathcal{H}_{\sigma}^0(r) = -\hbar^2\nabla^2/(2M) + M\omega^2r^2/2 - \mu - \hbar \sigma \). is the single-particle Hamiltonian in a 2D harmonic trapping potential \( M\omega^2r^2/2 \), in reference to the chemical potential \( \mu \). 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

\[ \mathcal{H}_{\text{BdG}} = \begin{bmatrix} \mathcal{H}_{\uparrow}(r) + \mathcal{V}_{\text{imp}}(r) & \mathcal{V}_{SO}(r) \\ \mathcal{V}_{SO}(r) & \mathcal{H}_{\downarrow}(r) + \mathcal{V}_{\text{imp}}(r) \end{bmatrix} \begin{bmatrix} 0 & -\Delta(r) \\ \Delta^*(r) & 0 \end{bmatrix} \begin{bmatrix} \mathcal{H}_{\uparrow}(r) - \mathcal{V}_{\text{imp}}(r) & \mathcal{V}_{SO}(r) \\ -\mathcal{V}_{SO}(r) & \mathcal{H}_{\downarrow}(r) - \mathcal{V}_{\text{imp}}(r) \end{bmatrix} \]  

(2)

is the BdG Hamiltonian, \( \Psi_{\eta}(r) = [u_{\eta\uparrow}, u_{\eta\downarrow}, v_{\eta\uparrow}, v_{\eta\downarrow}]^T \), and \( E_\eta \) are the Nambu spinor wave functions and energies for quasiparticles, respectively. Within the mean field, the order parameter takes the form \( \Delta(r) = -(U_0/2)\sum_{\eta} [u_{\eta\uparrow}^* v_{\eta\uparrow} f(E_\eta) + u_{\eta\downarrow}^* v_{\eta\downarrow} f(-E_\eta)] \) and, to be solved self-consistently together with the atomic densities, \( n_\sigma(r) = (1/2)\sum_{\eta} |u_{\eta\sigma}(r)|^2 f(E_\eta) + |v_{\eta\sigma}(r)|^2 f(-E_\eta). \) Here \( f(x) \equiv 1/(e^{x/\hbar} + 1) \) is the Fermi distribution function at temperature \( T \). The chemical potential \( \mu \), implicit in \( \mathcal{H}_{\sigma}^0(r) \), can be determined by the total number of atoms \( N \) using the number equation \( \int dr [n_{\uparrow}(r) + n_{\downarrow}(r)] = N \). As the impurity is placed at the origin \( r = 0 \), the BdG Hamiltonian preserves rotational symmetry. Therefore, we take \( \Delta(r) = \Delta(r) \) and decouple the BdG equation into different angular momentum channels indexed by an integer \( m \), with which the quasiparticle wave functions become \([u_{\eta\uparrow}(r), u_{\eta\downarrow}(r)e^{\lambda}, v_{\eta\uparrow}(r)e^{\lambda}, v_{\eta\downarrow}(r)e^{\lambda}]^T \). By expanding \( u_{\eta\sigma}(r) \) and \( v_{\eta\sigma}(r) \) 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 \( \eta \). 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 \( r_F = (4N)^{1/3}\sqrt{\hbar/(M\omega)} \) 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 \( V_{\text{imp}} \) will be measured in units of \( r_F^2E_F \). We have taken an interaction parameter \( E_u = 0.2E_F \) 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 \( h_c \approx 0.57E_F \) [16]. Let us first consider the localized impurities with a deltallike scattering potential \( V_{\sigma}(r) \).

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 \( V_{\text{imp}} \). As \( V_{\text{imp}} \) 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
the spatial profile of the order parameter near the impurity.

In Fig. 2, we examine the lowest curve at \( 0 \) in the limit of strong impurity scattering. In topological superfluids a universal bound state emerges due to strong nonmagnetic impurities. This coincides 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 \( V_{\text{imp}} \approx 0.004 r_F^2 E_F \). 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, \( E \approx \Delta^2_0 / E_F \), 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 \( \ell \) is given by \( E(m) = -(m + 1) \Delta_0 / (k_F \xi) \). 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 \( E \sim \Delta^2_0 / E_F \), in good agreement with the observed energy of the universal bound state.

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**FIG. 1** (color online). Bound states induced by a nonmagnetic deltaliike impurity (a) and by a magnetic deltaliike impurity (b), \( V_{\text{imp}}(r) = V_{\text{imp}}^* \delta(r) \), in a topological superfluid at \( h = 0.7 E_F \), as shown by the peaks in the total local density of states (LDOS) \( \rho(r, E) \) at \( k_F r = 2 \). Here, \( \rho(r, E) = \sum_{\alpha} |\psi_{\alpha}(r)|^2 \delta(E - E_{\psi_{\alpha}}) \). 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 \( V_{\text{imp}} = 0 \) to \( 0.011 r_F^2 E_F \), in steps of \( 0.001 r_F^2 E_F \). The curves are offset for clarity, except for the lowest curve at \( V_{\text{imp}} = 0 \). (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, \( \Delta_0 \approx 0.307 E_F \).

For a magnetic impurity, 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, \( E \approx \Delta^2_0 / E_F \), is of the same order as that of the CdGM bound states.
In Fig. 3, we examine the wave function of the universal bound state. Indeed, it satisfies approximately the symmetry \( u_\sigma (\mathbf{r}) = v_\sigma (\mathbf{r}) \), which should be obeyed by zero-energy Majorana fermions. In the inset, we present the LDOS close to the impurity site. The universal bound state is clearly visible within the gap. Experimentally, the LDOS may be measured through spatially resolved radio–frequency (rf) spectroscopy [36], which provides a cold-atom analog of the widely used scanning tunneling microscope in the solid state [37]. The wave function of the universal bound state can therefore be determined from the real-space structure of the LDOS within the gap.

Loss of university.—The universality of the impurity-induced bound state can be lost if the impurity scattering has a finite width. In this case, a hole will be created in the 1D topological superconductor and size \( \frac{1000}{24} \). It is readily seen that with an increase in the impurity strength the bound state never approaches a universal limit. We have checked that for larger widths, the LDOS becomes very complicated, as more and more bound states appear.

Experimental proposal.—We now show that ultracold Fermi gases of \( ^{40}\text{K} \) atoms are a potential candidate for observing the predicted universal impurity-induced bound state. A three-dimensional spin-orbit coupled \( ^{40}\text{K} \) Fermi gas was recently realized at Shaxi University [26]. By loading a pancakelike optical trap \( V(\mathbf{r}, z) = M[\omega_\perp \rho^2 + \omega_\parallel z^2]/2 \) with trapping frequencies \( \omega_\perp \gg \omega_\parallel \) [38] or using a deep 1D optical lattice [39], a 2D topological superfluid with a number of atoms \( N \sim 1000 \) and size \( r_F \sim 100 \mu m \) may be prepared at a temperature of about 10 nK. It is convenient to create the delta-like impurity potential by using a dimple laser beam that has a sufficiently narrow beam width \( d < 1 \mu m \) [40], so that \( k_F d \ll 1 \). By suitably tuning its frequency, the scattering potential caused by the laser beam can be attractive or repulsive for different spins. Thus, both nonmagnetic and magnetic impurities can be simulated. The resulting universal bound state may be visualized by using the standard tool of spatially resolved rf spectroscopy. All the techniques required to observe the predicted universal state are therefore within the reach of current experiments.

Application to other solid-state systems.—Our results are apparently applicable to the triplet superconductor \( \text{Sr}_2\text{RuO}_4 \). For the possible 1D topological superconductor reported recently in InSb nanowires [20], a strong impurity potential would split the 1D topological superconductor into two. Therefore, at the impurity site we anticipate two universal bound states, with precise zero energy. The observation of such a pair of zero-energy Majorana fermions is an unambiguous identification of the topological nature of InSb nanowires.

Conclusion.—We have investigated the nonmagnetic and magnetic impurity scattering in an atomic topological superfluid and have predicted the existence of a universal bound state for strong impurity scatterings. The observation of such a universal bound state—via spatially resolved radio-frequency spectroscopy—is a smoking-gun proof of atomic topological superfluidity. Our prediction seems within experimental reach and opens the way to unambiguously characterizing the topological properties of other solid-state systems, such as the unconventional superconductor \( \text{Sr}_2\text{RuO}_4 \) and the 1D topological superconductor in InSb nanowires.
L. J. acknowledges stimulating discussions with Eite Tiesinga. H. H. and X.-J. L. are supported by the ARC DP0984522 and DP0984637 and the NFRP-China 2011CB921502. H. P. acknowledges the support from the NSF, the Welch Foundation (Grant No. C-1669) and the DARPA OLE program. Y. C. is supported by the NSFC-China and the State Key Programs of China.

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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