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Universal impurity-induced bound state in topological superfluids

Hui Hu¹, Lei Jiang², Han Pu³, Yan Chen⁴, and Xia-Ji Liu^{1*}

¹Centre for Atom Optics and Ultrafast Spectroscopy,

Swinburne University of Technology, Melbourne 3122, Australia

 2 Joint Quantum Institute, University of Maryland and National Institute

of Standards and Technology, Gaithersburg, Maryland 20899, USA

³Department of Physics and Astronomy, and Rice Quantum Institute, Rice University, Houston, TX 77251, USA

⁴Department of Physics, State Key Laboratory of Surface Physics and

Laboratory of Advanced Materials, Fudan University, Shanghai, 200433, China

We predict a universal mid-gap 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 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 are a number of proposals for practical realizations of topological superfluids, including p + ip superconductors [6, 7], surfaces of three-dimensional (3D) 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 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 topological properties of the nanowires are still missing.

In this Letter, we propose that a *universal* mid-gap bound state, induced by strong non-magnetic or magnetic impurity scattering, could provide a clear signature for the existence of topological superfluids. In 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 used to determine the superconducting pairing symmetry of unconventional non-s-wave superconductors [22] and to demonstrate Friedel oscillations on 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 sufficiently strong scattering strength can create a universal mid-gap 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 universal impurityinduced 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 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]. Benefited from the high controllability in 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 solid state. We propose a realistic scenario of creating universal bound state in ⁴⁰K 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 spinorbit 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, $\mathcal{H} = \int d\mathbf{r} [\mathcal{H}_0(\mathbf{r}) + \mathcal{H}_I(\mathbf{r}) + \mathcal{H}_{imp}(\mathbf{r})]$, where

$$\mathcal{H}_{0}(\mathbf{r}) = \sum_{\sigma=\uparrow,\downarrow} \psi_{\sigma}^{\dagger} \mathcal{H}_{\sigma}^{S}(\mathbf{r}) \psi_{\sigma} + \left[\psi_{\uparrow}^{\dagger} V_{SO}(\mathbf{r}) \psi_{\downarrow} + \text{H.c.} \right]$$
(1)

is the single-particle Hamiltonian density in the presence of Rashba spin-orbit coupling $V_{SO}(\mathbf{r}) = -i\lambda(\partial_y + i\partial_x)$, $\mathcal{H}_{I}(\mathbf{r}) = U_{0}\psi_{\uparrow}^{\dagger}(\mathbf{r})\psi_{\downarrow}^{\dagger}(\mathbf{r})\psi_{\uparrow}(\mathbf{r})$ represents the interaction, and $\mathcal{H}_{imp}(\mathbf{r}) = \sum_{\sigma=\uparrow,\downarrow} \psi_{\sigma}^{\dagger} V_{imp}^{\sigma}(\mathbf{r})\psi_{\sigma}$ describes the potential scattering due to the impurity. Here, $\psi_{\uparrow,\downarrow}^{\dagger}$ are respectively the creation field operators for the spinup and spin-down atoms and, $\mathcal{H}_{\sigma}^{S}(\mathbf{r}) \equiv -\hbar^{2}\nabla^{2}/(2M) + M\omega^{2}r^{2}/2 - \mu - h\sigma_{z}$ is the single-particle Hamiltonian in a 2D harmonic trapping potential $M\omega^{2}r^{2}/2$, 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 origin and consider either a delta-like scattering potential, $V_{\rm imp}^{\sigma}(\mathbf{r}) = V_{\rm imp}^{\sigma}\delta(r)$, or a gaussian-shape potential with width d, $V_{\rm imp}^{\sigma}(\mathbf{r}) = [V_{\rm imp}^{\sigma}/(\pi d^2)] \exp[-r^2/d^2]$. In the case of magnetic impurity, we take the potential strength $V_{\rm imp}^{\uparrow} = -V_{\rm imp}^{\downarrow} = -V_{\rm imp}$; while for non-magnetic impurity, $V_{\rm imp}^{\uparrow} = V_{\rm imp}^{\downarrow} = -V_{\rm imp}$. We have checked both positive and negative values of $V_{\rm imp}$ and have observed very similar results at large $|V_{\rm imp}|$. Hereafter, we focus on the case with $V_{\rm imp} > 0$.

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

$$\mathcal{H}_{BdG} = \begin{bmatrix} \mathcal{H}^{S}_{\uparrow}(\mathbf{r}) + V^{\uparrow}_{imp}(\mathbf{r}) & V_{SO}(\mathbf{r}) & 0 & -\Delta(\mathbf{r}) \\ V^{\dagger}_{SO}(\mathbf{r}) & \mathcal{H}^{S}_{\downarrow}(\mathbf{r}) + V^{\downarrow}_{imp}(\mathbf{r}) & \Delta(\mathbf{r}) & 0 \\ 0 & \Delta^{*}(\mathbf{r}) & -\mathcal{H}^{S}_{\uparrow}(\mathbf{r}) - V^{\uparrow}_{imp}(\mathbf{r}) & V^{\dagger}_{SO}(\mathbf{r}) \\ -\Delta^{*}(\mathbf{r}) & 0 & V_{SO}(\mathbf{r}) & -\mathcal{H}^{S}_{\downarrow}(\mathbf{r}) - V^{\downarrow}_{imp}(\mathbf{r}) \end{bmatrix}$$
(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 meanfield, 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, $n_{\sigma}(\mathbf{r}) = (1/2) \sum_{n} [|u_{\sigma\eta}|^2 f(E_{\eta}) + |v_{\sigma\eta}|^2 f(-E_{\eta})].$ Here $f(x) \equiv 1/(e^{x/k_BT}+1)$ is the Fermi distribution function at temperature T. The chemical potential μ , implicit in $\mathcal{H}^{S}_{\sigma}(\mathbf{r})$, 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 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 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 cut-off 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 $E_F = \hbar^2 k_F^2/(2M) = \sqrt{N}\hbar\omega$ as the units for length and energy, respectively. The strength of impurity scattering potential $V_{\rm imp}^{\sigma}$ will be measured in units of $r_F^2 E_F$. 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 delta-like scattering potential $V_{\rm imp}^{\sigma}\delta(r)$.

Emergence of universal impurity bound state. — According to Anderson's theorem [30], a conventional swave superfluid can barely be affected by non-magnetic impurities. In contrast, magnetic impurities can break time-reversal symmetry of superfluid and act as pair breakers, leading to the appearance of mid-gap state the so-called Yu-Shiba state - which is bound to localized impurities inside the pairing gap [31, 32]. The energy of such a mid-gap bound state is determined by the strength of the impurity scattering potential $V_{\rm imp}$. As $V_{\rm imp}$ 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 increasing the strength of 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 superfluid, we observe entirely different behavior, as revealed in Fig. 1. For non-magnetic impurities, an

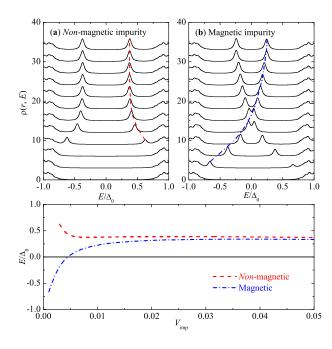


FIG. 1: (color online) Bound states induced by a nonmagnetic delta-like impurity (a) and by a magnetic deltalike impurity (b), $V_{imp}^{\sigma}(\mathbf{r}) = V_{imp}^{\sigma}\delta(r)$, in a topological superfluid at $h = 0.7E_F$, as shown by the peaks in the total local density of state (LDOS) $\rho(r, E)$ 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 $V_{imp} = 0$ to $V_{imp} = 0.011r_F^2 E_F$, in steps of $0.001r_F^2 E_F$. The curves are offset for clarity, except for the lowest curve at $V_{imp} = 0$. (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, $\Delta_0 \simeq 0.307 E_F$.

unexpected bound state appears from one gap edge as the impurity strength is larger than a critical strength $V_{\rm imp} \gtrsim 0.004 r_F^2 E_F$. As $V_{\rm imp}$ increases, the bound state moves towards, but never reaches zero energy. In fact, its energy saturates quickly to $E \simeq 0.11 E_F \simeq \Delta_0^2/E_F$, where $\Delta_0 \simeq 0.307 E_F$ is the gap parameter at the trap center in the absence of 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 non-magnetic 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 order parameter near the impurity. For a weak non-magnetic impurity, as shown in Fig. 2(a), the gap parameter is already strongly modi-

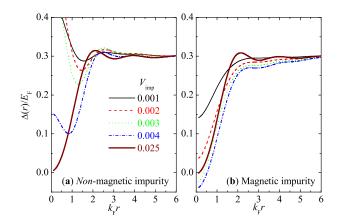


FIG. 2: (color online) Gap parameter as a function of impurity strength $V_{\rm imp}$ (in units of $r_F^2 E_F$), for a non-magnetic impurity (a) and for a magnetic impurity. In the limit of strong impurity scattering, the gap parameter has the same spatial distribution, no matter the impurity is non-magnetic or magnetic.

fied at $V_{\rm imp} \gtrsim 0.004 r_F^2 E_F$. Being regarded 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 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 wellknown CdGM vortex-core bound states [25]. Indeed, the energy of the universal impurity state, $E \simeq \Delta_0^2/E_F$, is at the same order as that of 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 non-topological 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.

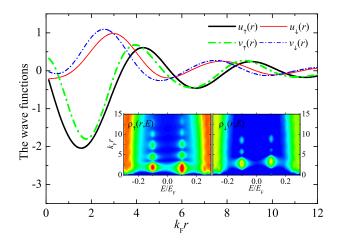


FIG. 3: (color online) The wave-function of the universal bound state, induced by either non-magnetic or magnetic impurity in the strong scattering limit. The inset shows the linear contour of LDOS for spin-up and spin-down atoms near the impurity site.

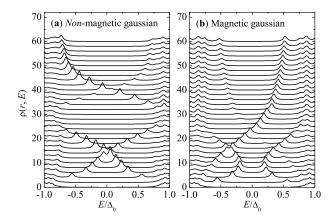


FIG. 4: Loss of the universal bound state for an extended impurity. Here, we take a gaussian-shape scattering potential, $V_{\rm imp}^{\sigma}(\mathbf{r}) = [V_{\rm imp}^{\sigma}/(\pi d^2)] \exp[-r^2/d^2]$, with width $k_F d = 0.5$. From bottom to top, the impurity strength increases from $V_{\rm imp} = 0$ to $V_{\rm imp} = 0.06r_F^2 E_F$, in steps of $0.002r_F^2 E_F$. Other parameters are the same as in Fig. 1.

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 solid state [37]. The wave-function of the universal bound state can therefore be determined from the real-space structure of LDOS within the gap.

Loss of university. — The universality of the impurityinduced bound state can be lost if the impurity scattering has a finite width. In this case, a hole will be created in the strong impurity scattering limit, instead of a point defect. Therefore, there are a series of edge states. The wave-function and energy of these edge states would depend critically on the shape and strength of the impurity potential. In Fig. 4, we show the bound states induced by a non-magnetic (a) and a magnetic (b) gaussian impurity, with a finite width $k_F d = 0.5$. It is readily seen that with increasing the impurity strength the bound state never approaches to 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 ⁴⁰K atoms is a potential candidate for observing the predicted universal impurity-induced bound state. A 3D spin-orbit coupled ⁴⁰K Fermi gas was recently realized at Shanxi university [26]. By loading a pancake-like optical trap $V(\mathbf{r}, z) = M[\omega^2 r^2 + \omega_z^2 z^2]/2$ with trapping frequencies $\omega_z \gg \omega$ [38] or using a deep 1D optical lattice [39], a 2D topological superfluid with number of atoms $N \sim 1000$ and size $r_F \sim 100 \mu m$ may be prepared at the temperature about 10nK. 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 non-magnetic 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 Sr_2RuO_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 zeroenergy. 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 non-magnetic and magnetic impurity scattering in an atomic topological superfluid and have predicted the existence of 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 Sr_2RuO_4 and 1D topological superconductor of InSb nanowires.

Note added. — After completing this work, we were aware a related non-self-consistent T-matrix calculation

in 1D topological superconductors, which predicted a bound state induced by non-magnetic impurities [41].

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- * Electronic address: xiajiliu@swin.edu.au
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