Impurity probe of topological superfluids in one-dimensional spin-orbit-coupled atomic Fermi gases

Xia-Ji Liu*

ARC Centre of Excellence for Quantum-Atom Optics, Centre for Atom Optics and Ultrafast Spectroscopy, Swinburne University of Technology, Melbourne 3122, Australia

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We investigate theoretically nonmagnetic impurity scattering in a one-dimensional atomic topological superfluid in harmonic traps by solving self-consistently the microscopic Bogoliubov-de Gennes equation. In sharp contrast to topologically trivial Bardeen-Cooper-Schrieffer s-wave superfluid, topological superfluid can host a midgap state that is bound to localized nonmagnetic impurity. For strong impurity scattering, the bound state becomes universal, with nearly zero energy and a wave function that closely follows the symmetry of that of Majorana fermions. We propose that the observation of such a universal bound state could be useful evidence for characterizing the topological nature of topological superfluids. Our prediction is applicable to an ultracold, resonantly interacting Fermi gas of $^{40}$K atoms with spin-orbit coupling confined in a two-dimensional optical lattice.

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I. INTRODUCTION

Impurity scattering plays an important role in understanding the quantum state of hosting systems [1]. This is particularly significant in solid-state systems, where impurity scattering and disorder are intrinsic. In superconductors, the study of impurity effects has the potential to uncover the nature and origin of the superconducting state [2]. In strongly correlated electronic systems near quantum critical points, where several types of ordering compete in a delicate balance, the study of impurity scatterings has the power to underpin in favor of one of the orders [3]. In this work, we aim to investigate theoretically impurity scattering in one-dimensional (1D) topological superfluids. We show that an impurity-induced bound state will provide a sensitive probe for the topological order in such systems.

Topological superfluid is a novel state of quantum matter [4], which is gapped in the bulk but hosts nontrivial zero-energy surface states—the so-called Majorana fermions [5,6]—near its boundary. It has attracted great attention in recent years because of its potential application in topological quantum computation and quantum information [7,8]. The realization of topological superfluids and the manipulation of Majorana fermions are currently the most popular research topics in a variety of fields in physics, ranging from condensed-matter physics to ultracold-atomic systems. Until now, indirect evidence of the existence of topological superfluids in hybrid superconductor-semiconductor InSb or InAs nanowires has been reported [9–11]. Theoretical schemes of processing topological quantum information in such nanowire devices have also been proposed [12,13].

Our investigation of impurity scattering in 1D topological superfluids is strongly motivated by the rapid experimental progress [9–11]. On one hand, impurity scattering is unavoidable in InSb or InAs nanowires. A realistic simulation of impurity scattering may, therefore, be useful for future solid-state experiments. On the other hand, we anticipate that impurity may induce a new exotic bound state, thus providing a clear local probe of the topological nature of the systems that we consider.

In this paper, we use a 1D spin-orbit-coupled atomic Fermi gas to model 1D topological superfluids [14–16], instead of considering nanowire devices used in the solid state [9–11]. This is because we have unprecedented controllability with ultracold-atomic gases [17]. By using magnetic Feshbach resonances, the interatomic interactions can be precisely tuned [18]. Using the technique of optical lattices, artificial 1D and 2D environments can be easily created [19,20]. The spin-orbit coupling, which is the necessary ingredient of a realistic topological superfluid, can also be engineered with arbitrary strength [21,22]. Thus, ultracold spin-orbit-coupled atomic Fermi gas is arguably the best candidate to simulate the desired topological superfluids. Furthermore, even though cold-atom systems are intrinsically clean, individual impurities can be realized using off-resonant dimple laser light or another species of atoms or ions [23]. The disorder effect of many randomly distributed impurities can also be created by employing quasiperiodic bichromatic lattices or laser speckles [24].

We investigate the impurity effect in 1D spin-orbit-coupled atomic Fermi gas of $^{40}$K atoms by solving self-consistently the microscopic Bogoliubov-de Gennes (BdG) equation with realistic experimental parameters. We observe the existence of a midgap state that is bound to localized nonmagnetic impurity. For strong impurity scattering, the bound state tends to be universal, with nearly zero energy and a wave function that closely follows the symmetry of that of Majorana fermions. This feature is clearly absent in topologically trivial superfluids. Therefore, we argue that the observation of such a universal bound state would be useful evidence for characterizing the topological nature of topological superfluids. We note that a midgap bound state induced by nonmagnetic impurity has also been predicted in 1D spin-orbit-coupled superconductors by using non-self-consistent T-matrix theory [25]. The effect of magnetic impurity in 2D spin-orbit-coupled Fermi gases has also been studied analytically using T-matrix formalism [26].

Our paper is arranged as follows. In the next section (Sec. II), we introduce briefly the model Hamiltonian and the solution of BdG equations and then present a phase diagram for a given set of experimental parameters. In Sec. III, we study nonmagnetic impurity scatterings and show the emergence
of a universal bound state in the strong scattering limit. The properties of such a universal bound state are analyzed in greater detail. To better simulate the realistic experimental setup, we also consider an extended impurity with Gaussian-shaped scattering potential. Finally, we summarize in Sec. IV. The detailed numerical procedure of solving BdG equations is listed in the Appendix, together with a careful check of numerical accuracy.

II. MODEL HAMILTONIAN AND BdG EQUATIONS

The framework of our theoretical approach has been briefly described in our previous work [15]. Here, we emphasize the experimental origin of the model Hamiltonian and generalize the theoretical approach to include a classical nonmagnetic impurity. A detailed discussion of the numerical procedure is given in the Appendix.

A. 1D spin-orbit-coupled Fermi gas

Let us consider a spin-orbit-coupled Fermi gas of $^{40}$K atoms in harmonic traps, realized recently at Shansi University [21]. We assume additional confinement due to a very deep 2D optical lattice in the transverse $y$-$z$ plane, which restricts the motion of atoms to the $x$ axis. The spin-orbit coupling is created by two counterpropagating Raman laser beams that couple the two spin states of the system along the $x$ axis [21]. Near the Feshbach resonance $B_0 \approx 202.20$ G, the quasi-1D Fermi system may be described by a single-channel model Hamiltonian $H = H_0 + H_{\text{int}}$, where

$$H_0 = \sum_{\sigma=\uparrow,\downarrow} \int dx \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \mu + V_T \right] \Psi_{\sigma}(x)$$

$$- \frac{\Omega_R}{2} \int dx \left[ \Psi_{\uparrow}(x) e^{i2k_x x} \Psi_{\downarrow}(x) + \text{H.c.} \right]$$

(1)

is the single-particle Hamiltonian in the presence of the Raman process, and

$$H_{\text{int}} = g_{1D} \int dx \Psi_{\uparrow}^\dagger(x) \Psi_{\downarrow}^\dagger(x) \Psi_{\downarrow}(x) \Psi_{\uparrow}(x)$$

(2)

is the interaction Hamiltonian describing the contact interaction between two spin states. Here, the pseudospins $\sigma = \uparrow, \downarrow$ denote the two hyperfine states, and $\Psi_{\sigma}(x)$ is the Fermi field operator that annihilates an atom with mass $m$ at position $x$ in the spin $\sigma$ state. The chemical potential $\mu$ is determined by the total number of atoms $N$ in the system. For the two-photon Raman process, $\Omega_R$ is the coupling strength of Raman beams, $k_R = 2\pi / \lambda_R$ is determined by the wavelength $\lambda_R$ of two lasers, and, therefore, $2\hbar k_R$ is the momentum transfer during the process. The trapping potential $V_T(x) \equiv m \omega^2 x^2 / 2$ refers to the harmonic trap with an oscillation frequency $\omega = \omega_x$ in the axial direction. In such a quasi-one-dimensional geometry, it is shown by Bergeman et al. [27] that the scattering properties of the atoms can be well described using a contact potential $g_{1D} \delta(x)$, where the 1D effective coupling constant $g_{1D} < 0$ may be expressed through the 3D scattering length $a_{3D}$,

$$g_{1D} = \frac{2\hbar^2 a_{3D}}{ma^2} \frac{1}{(1 - A a_{3D} / a_{\perp})},$$

(3)

where $a_{\perp} \equiv \sqrt{\hbar/(m \omega_{\perp})}$ is the characteristic oscillator length in the transverse axis, for a given transverse trapping frequency $\omega_{\perp}$ set by the deep 2D optical lattice. The constant $A = -\xi(1/2)/\sqrt{2} \approx 1.0326$ is responsible for the confinement-induced Feshbach resonance [27], which changes the scattering properties dramatically when the 3D scattering length is comparable to the transverse oscillator length. It is also convenient to express $g_{1D}$ in terms of an effective 1D scattering length, $g_{1D} = -2\hbar^2 / (ma_{1D})$, where $a_{1D} = (a_{\perp}^2 / a_{3D})(1 - A a_{3D} / a_{\perp}) > 0$. The interatomic interaction can then be described by a dimensionless interaction parameter $\gamma \equiv a / \sqrt{N a_{1D}}$, where $a \equiv \sqrt{\hbar/(m \omega)}$ is the oscillator length in the $x$ axis. Near the Feshbach resonance, the typical value of the interaction parameter $\gamma$ is about 5 [20,28,29].

To illustrate how the spin-orbit coupling is induced by the two-photon Raman process, it is useful to remove the spatial dependence of the Raman coupling term by taking the following local gauge transformation:

$$\Psi_{\uparrow}(x) = e^{i\lambda_\uparrow x} \tilde{\Psi}_{\uparrow}(x),$$

(4)

$$\Psi_{\downarrow}(x) = e^{-i\lambda_\downarrow x} \tilde{\Psi}_{\downarrow}(x).$$

(5)

Using the new field operators $\tilde{\Psi}_{\uparrow}(x)$ and $\tilde{\Psi}_{\downarrow}(x)$, we can recast the single-particle Hamiltonian as

$$H_0 = \int dx \left[ \tilde{\Psi}_{\uparrow}^\dagger(x) \tilde{\Psi}_{\downarrow}^\dagger(x) H_0 \left[ \tilde{\Psi}_{\downarrow}(x) \tilde{\Psi}_{\uparrow}(x) \right] \right],$$

(6)

$$H_{0} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \mu + V_T(x) - h \sigma_z + \lambda \hat{k}_x \sigma_x,$$

(7)

where we have absorbed a constant energy shift $E_R \equiv \hbar^2 k_R^2 / (2m)$ (the recoil energy) in the chemical potential $\mu$, and have defined the momentum operator $\hat{k}_x \equiv -i \partial / \partial x$, the spin-orbit-coupling constant $\lambda \equiv \hbar^2 k_R / m$, and an effective Zeeman field $h \equiv \Omega_R / 2$, $\sigma_z$, and $\sigma_x$ are Pauli’s matrices. The spin-orbit coupling in the Hamiltonian $H_0$ can be regarded as an equal-weight combination of Rashba and Dresselhaus spin-orbit coupling (i.e., $\lambda \hat{k}_x \sigma_z$. This is evident after we take the second local gauge transformation,

$$\tilde{\Psi}_{\uparrow}(x) = \frac{1}{\sqrt{2}} \left[ \Psi_{\uparrow}(x) - i \Psi_{\downarrow}(x) \right],$$

(8)

$$\tilde{\Psi}_{\downarrow}(x) = \frac{1}{\sqrt{2}} \left[ \Psi_{\uparrow}(x) + i \Psi_{\downarrow}(x) \right],$$

(9)

with which the single-particle Hamiltonian becomes

$$H_0 = \int dx \left[ \tilde{\Psi}_{\uparrow}^\dagger(x) \tilde{\Psi}_{\uparrow}^\dagger(x) H_0 \left[ \tilde{\Psi}_{\downarrow}(x) \tilde{\Psi}_{\downarrow}(x) \right] \right],$$

(10)

$$H_{0} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_T(x) - h \sigma_z + \lambda \hat{k}_x \sigma_z,$$

(11)

The form of the interaction Hamiltonian is invariant after two gauge transformations, i.e.,

$$H_{\text{int}} = g_{1D} \int dx \tilde{\Psi}_{\uparrow}^\dagger(x) \tilde{\Psi}_{\downarrow}^\dagger(x) \tilde{\Psi}_{\downarrow}(x) \tilde{\Psi}_{\uparrow}(x).$$

(12)

We note that the operator of total density $\hat{n}(x) \equiv \sum_\sigma \tilde{\Psi}_{\sigma}(x)^\dagger \tilde{\Psi}_{\sigma}(x)$ is also invariant in the gauge transformation.
B. Impurity scattering Hamilton

Now we add the nonmagnetic impurity scattering term,

$$H_{\text{imp}} = \int dx V_{\text{imp}}(x) \sum \sigma \psi_\sigma^\dagger(x) \psi_\sigma(x),$$

(13)

to the total Hamiltonian. The nonmagnetic scattering can be realized experimentally by using an off-resonant dimple laser light. We consider either a localized scattering potential at position $x_0$,

$$V_{\text{imp}}(x) = V_{\text{imp}} \delta(x - x_0),$$

(14)
or an extend potential with a width $d$ in the Gaussian line shape,

$$V_{\text{imp}}(x) = \frac{V_{\text{imp}}}{\sqrt{2\pi d}} \exp \left[-\frac{(x-x_0)^2}{2d^2}\right].$$

(15)

The strength of the impurity scattering is given by $V_{\text{imp}}$. In the narrow-width limit $d \to 0$, the Gaussian potential returns back to the $\delta$-like potential. We may place the impurity at an arbitrary position, as long as the Fermi system is locally in the topological superfluid state. To be concrete, we shall set $x_0 = 0$.

We may also consider a magnetic impurity scattering in the form $H_{\text{imp}} = \int dx V_{\text{imp}}(x) [\psi^\dagger_\sigma(x) \psi^\dagger_\tau(x) - \psi^\dagger_\tau(x) \psi^\dagger_\sigma(x)]$. However, it is of theoretical interest only. The field operator of the density difference is not invariant in the second local gauge transformation. Thus, experimentally, the magnetic impurity scattering potential is more difficult to realize.

C. Bogoliubov-de Gennes equation

We use the standard mean-field theory to solve the model Hamiltonian. By introducing a real order parameter $\Delta(x) \equiv -\sigma_{1D} \langle \psi_\uparrow(x) \psi_\downarrow(x) \rangle$, the interaction Hamiltonian is decoupled as

$$H_{\text{int}} \simeq -\int dx \left[ \Delta(x) \psi^\dagger_\uparrow(x) \psi^\dagger_\downarrow(x) + \text{H.c.} + \frac{|\Delta(x)|^2}{\sigma_{1D}} \right].$$

(16)

It is then convenient to introduce a Nambu spinor $\Psi(x) \equiv [\psi^\dagger_\uparrow(x), \psi_\downarrow(x), \psi^\dagger_\downarrow(x), \psi_\uparrow(x)]^T$ and rewrite the mean-field Hamiltonian in a compact form

$$H_{\text{mf}} = \frac{1}{2} \int dx \left[ \Psi \mathcal{H}_{\text{BdG}} \Psi + \text{Tr} \mathcal{H}_S - \int dx \frac{|\Delta(x)|^2}{\sigma_{1D}} \right],$$

(17)

where

$$\mathcal{H}_{\text{BdG}} = \begin{bmatrix} \mathcal{H}_S - \hbar \frac{\partial}{\partial x} & -\lambda \frac{\partial}{\partial x} & 0 & -\Delta(x) \\ \lambda \frac{\partial}{\partial x} & \mathcal{H}_S + \hbar \frac{\partial}{\partial x} & \Delta(x) & 0 \\ 0 & -\Delta^*(x) & -\mathcal{H}_S + \hbar \lambda \frac{\partial}{\partial x} \\ -\Delta^*(x) & 0 & -\lambda \frac{\partial}{\partial x} & -\mathcal{H}_S - \hbar \lambda \frac{\partial}{\partial x} \end{bmatrix}$$

(18)

and

$$\mathcal{H}_S(x) \equiv -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \mu + \frac{\hbar^2}{2} \lambda^2 x^2 + V_{\text{imp}}(x).$$

(19)

The term $\text{Tr} \mathcal{H}_S$ in $H_{\text{mf}}$ results from the anticommutativity of Fermi field operators.

The mean-field Hamiltonian given by Eq. (17) can be diagonalized by the standard Bogoliubov transformation. By defining the field operators $a_\eta$ for Bogoliubov quasiparticles,

$$a_\eta = \int dx \sum \sigma \left[ u^\alpha_\eta(x) \psi^\dagger_\sigma(x) + v^\alpha_\eta(x) \psi_\sigma(x) \right],$$

(20)

we obtain

$$H_{\text{mf}} = \frac{1}{2} \sum \eta E_\eta a_\eta^\dagger a_\eta + \text{Tr} \mathcal{H}_S - \int dx \frac{|\Delta(x)|^2}{\sigma_{1D}}.$$

(21)

Here, $\Phi_\eta(x) \equiv [u^\alpha_\eta(x),u_\eta^\dagger(x),v^\beta_\eta(x),v_\eta^\dagger(x)]^T$ and $E_\eta$ are, respectively, the wave function and energy of Bogoliubov quasiparticles, satisfying the BdG equation

$$\mathcal{H}_{\text{BdG}} \Phi_\eta(x) = E_\eta \Phi_\eta(x).$$

(22)

The BdG Hamiltonian given by Eq. (18) includes the pairing gap function $\Delta(x)$ that should be determined self-consistently. For this purpose, we take the inverse Bogoliubov transformation and obtain

$$\psi_\sigma(x) = \sum_\eta \left[ u^\alpha_\eta(x) a_\eta + v^\alpha_\eta(x) a^\dagger_\eta \right].$$

(23)

Here the summation is restricted to the postive energy level, $E_\eta \geq 0$. The gap function is then given by

$$\Delta(x) = \frac{\sigma_{1D}}{2} \sum \eta \left[ u^\alpha_\eta(x) v^\beta_\eta(x) f(E_\eta) + u^\beta_\eta(x) v^\alpha_\eta(x) f(-E_\eta) \right],$$

(24)

where $f(E) \equiv 1/\left[ e^{E/k_BT} + 1 \right]$ is the Fermi distribution function at temperature $T$. Accordingly, the total density takes the form

$$n(x) = \frac{1}{2} \sum_{\sigma \eta} \left[ |u^\alpha_\eta(x)|^2 f(E_\eta) + |v^\alpha_\eta(x)|^2 f(-E_\eta) \right].$$

(25)

The chemical potential $\mu$ can be determined using the number equation $N = \int dx n(x)$.

It is important to note that the use of Nambu spinor representation enlarges the Hilbert space of the system. As a result, there is an intrinsic particle-hole symmetry in the Bogoliubov solutions [28,29]: for any “particle” solution with the wave function $\Phi_\eta^{\text{(p)}}(x) = [u^\alpha_\eta(x),u^\beta_\eta(x),v^\beta_\eta(x),v^\alpha_\eta(x)]^T$ and energy $E^{\text{(p)}}_\eta \geq 0$, we can always find another partner “hole” solution with the wave function $\Phi_\eta^{\text{(h)}}(x) = [v^\alpha_\eta(x),v^\beta_\eta(x),u^\beta_\eta(x),u^\alpha_\eta(x)]^T$ and energy $E^{\text{(h)}}_\eta = -E^{\text{(p)}}_\eta \leq 0$. In general, these two solutions correspond to the same physical state. To remove this redundancy, we have added an extra factor of $1/2$ in the expressions for the pairing gap function (24) and total density (25).

The Bogoliubov equation (18) can be solved iteratively with Eqs. (24) and (25) by using a basis expansion method, together with a hybrid strategy that takes care of the high-lying energy states [15,28,29]. A detailed discussion of the numerical procedure and a self-consistent check on the numerical accuracy are outlined in the Appendix.

D. Phase diagram in the absence of impurity

In our previous study [15], we discussed the phase diagram of a weakly interacting spin-orbit-coupled Fermi gas, with an
Figure 1 shows the energy spectrum at the transition point is slightly affected by finite temperature. The inset demonstrates the transition from BCS superfluid to a topologically nontrivial superfluid. The phase is characterized by the lowest energy of Bogoliubov quasiparticles, \( \Delta_1 \). With increasing Zeeman field, the Fermi cloud changes from a standard Bardeen-Cooper-Schrieffer (BCS) superfluid to a topologically nontrivial superfluid. The phase transition point is slightly affected by finite temperature. The inset shows the energy spectrum at \( h = 1.2E_F \) as a function of the position of quasiparticles. A zero-energy quasiparticle (i.e., Majorana fermion) at the trap edge has been highlighted by a big dark circle. Here, we characterize the position of a quasiparticle by using its wave function: 

\[
\langle x \rangle = \int dx x^2 \sum_{\sigma} [u_{1, \sigma}(x) + v_{1, \sigma}(x)].
\]

The real experiment, however, would be carried out near Feshbach resonances, where the typical interaction parameter is \( \gamma = 3.2 \) [20,28,29]. In this work, we take a realistic interaction parameter \( \gamma = \pi/2 \approx 1.6 \). The lowest energy in the spectrum is fairly evident in the quasiparticle spectrum. This is well known for homogeneous spin-orbit-coupled Fermi gases, it is given by [30,31]

\[
h_c = \sqrt{\mu^2 + \Delta^2}. \tag{26}
\]

In harmonic traps, as we consider here, the critical Zeeman field becomes position dependent. The local critical Zeeman field, calculated using \( h_c(x) = \sqrt{\mu^2(x) + \Delta^2(x)} \), with the local chemical potential \( \mu(x) = \mu - \hbar \omega x^2/2 \) and the local pairing gap \( \Delta(x) \), increases monotonically towards the trap edge [34]. The Fermi cloud at position \( x \) will locally be in a topological state if the Zeeman field \( h > h_c(x) \). For the parameters given above, this first happens at \( \hbar \omega \sim 1.05E_F \), for which the local phase at the trap center \( (x = 0) \) starts to become topologically nontrivial. In Fig. 2(a), we show the local pairing gap \( \Delta(x) \) and the criterion for a local topological state, \( h > h_c(x) \), at the Zeeman field \( h = 1.2E_F \). At this field, the topological area is extended to the edge of the trap, as highlighted by a shaded crosshatching. The appearance of Majorana fermion modes may be probed by measuring the local density of state through spatially resolved radio-frequency (rf) spectroscopy [15,23]. In Fig. 2(b), we present the local density of state at \( h = 1.2E_F \),

\[
\rho(x, \omega) = \frac{1}{2} \sum_{\sigma, \eta} [\langle u_{\sigma \eta}(x) \rangle^2 \delta(\omega - \Delta_1) + \langle v_{\sigma \eta}(x) \rangle^2 \delta(\omega + \Delta_1)].
\]

At each of the two trap edges, we observe a series of edge states, including the zero-energy Majorana fermion mode, which is clearly visible.
III. UNIVERSAL IMPURITY-INDUCED BOUND STATE

We are now ready to investigate how Bogoliubov quasiparticles are affected by a nonmagnetic impurity. Hereafter, we focus on the topological state at \( h = 1.2E_F \). For a topologically trivial state at \( h < 1.05E_F \), we have checked numerically that quasiparticles are essentially not affected by the nonmagnetic impurity scattering. This is in accord with the well-known Anderson’s theorem that potential scattering impurities are not pair breakers in \( s \)-wave superconductors [1,32].

A. Impurity-induced midgap state

In Fig. 3, we report the density profile and pairing gap distribution in the presence of a strong nonmagnetic impurity with scattering potential strength \( V_{\text{imp}} = -0.30x_F E_F \). Both of them are completely depleted at the impurity site \( x = 0 \). Accordingly, we observe the appearance of a new midgap state that is bound to the impurity, as shown in the inset for the spatial distribution of Bogoliubov quasiparticles. This is clearly seen when we compare the quasiparticle spectrum without and with the nonmagnetic impurity, i.e., the inset in Figs. 1 and 3, respectively. Away from the impurity site, the distribution of Bogoliubov quasiparticles is also disturbed by the impurity. However, the series of edge states at the trap edge seems to be very robust against the impurity scattering.

In Fig. 4, we show the local density of state \( \rho(x,\omega) \).

The midgap bound state can be easily identified in spatially resolved rf spectroscopy, which is a cold-atom analog of scanning tunneling microscopy (STM). If such a bound state exists, then one would observe a strong rf signal at around origin and zero energy, which decays exponentially in space and energy. The maximum rf signal, however, is located slightly away from the origin, as the total density is completely depleted right at the impurity site.

The existence of a midgap state in the topological superfluid phase is certainly not consistent with Anderson’s theorem [32] for potential scattering in \( s \)-wave superconductors. However, it can be understood from the combined effect of the spin-orbit coupling and effective Zeeman field. Beyond the critical Zeeman field \( h_c \), the Fermi cloud is actually a \( p \)-wave-like superfluid (see, for example, the discussion in Sec. II A of Ref. [16]). This is also the underlying reason why the cloud is in a topological state. For superfluids with a nonzero angular momentum order parameter, nonmagnetic impurity is a pair breaker and would lead to a midgap bound state.

B. Universal midgap state

An impurity-induced bound state is not a unique feature of topological superfluids, as it can also exist in superfluids with an even-parity angular momentum order parameter, such as \( d \)-wave and \( g \)-wave superfluids. Here, however, we argue that the existence of a deep, universal, in-gap bound state in the limit of strong impurity scattering would be a robust feature of topological superfluids. Despite the details of impurity scattering (i.e., nonmagnetic or magnetic impurity, positive or attractive scattering potential), we would observe exactly the same bound state when the impurity scattering strength is strong enough. This argument is based on the consideration that a strong impurity will always deplete the atoms at the impurity site and hence create a vacuum area that is topologically trivial. Thus, at the interface between the topologically nontrivial and trivial areas, we would observe a pair of Majorana edge states [25]—the precursor of the universal bound state. Ideally, the energy of the universal bound state will be zero.

FIG. 3. (Color online) Density profile and pairing gap distribution in the presence of a strong attractive nonmagnetic impurity with scattering potential strength \( V_{\text{imp}} = -0.30x_F E_F \). The inset shows the spatial distribution of the Bogoliubov quasiparticle energy spectrum. The midgap bound state near the impurity site \( x = 0 \) is highlighted by big blue circles.

FIG. 4. (Color online) (a) Density of state for a topological superfluid \( (h = 1.2E_F) \) at \( x = 0, 0.05x_F \), and \( 0.1x_F \) (from bottom to top). For better illustration, the curves have been offset. The magnitude of the local density of state at \( x = 0 \) and \( 0.1x_F \) has been enlarged by a factor of 10. (b) Linear contour plot of the local density of state. The impurity-induced bound state is clearly visible near \( x = 0 \) and \( \omega = 0 \).
In Fig. 5, we plot the energy of the midgap bound state as a function of the impurity scattering strength at $h = 1.2E_F$. Indeed, when the absolute value of the scattering strength $V_{\text{imp}}$ is sufficiently large, the energy of the bound state converges to a single value, $E \simeq 0.113\Delta_0$, where $\Delta_0 \simeq 0.464E_F$ is the pairing gap at the trap center without impurity.

We note, however, that the bound-state energy is not precisely zero as we may anticipate from the Majorana edge-state picture, as mentioned above. This is due to the fact that a pair of zero-energy Majorana fermions, localized at the same position (i.e., impurity site), could interfere with each other, leading to a small energy splitting whose magnitude would depend on the detailed configuration of the Fermi cloud. In Fig. 6, we present the wave function of the universal impurity-induced bound state. Indeed, the wave function of the universal bound state can be viewed as the bond and antibond superposition of the wave functions of two Majorana fermions, which satisfy the symmetry $u_\sigma(x) = v_\sigma^*(x)$ or $u_\sigma(x) = -v_\sigma^*(x)$, respectively.

We note also that the midgap state induced by nonmagnetic impurities in topological superconducting nanowires has recently been predicted by Sau and Demler, based on a non-self-consistent $T$-matrix and Green’s-function method [25]. By increasing the impurity strength, it was reported that the bound-state energy saturates to zero energy, instead of converging to a nonzero value. In addition, a shallow bound state was predicted in the nontopological superconducting phase with spin-orbit coupling. These predictions are different from our numerical results. We ascribe these discrepancies to the lack of self-consistency in the $T$-matrix approach.

**FIG. 5.** (Color online) The dependence of the bound-state energy on the impurity strength for a topological superfluid at $h = 1.2E_F$. The solid and empty circles show the results for attractive and repulsive potential scattering, respectively. The dashed lines give the bound-state energy at the infinitely large impurity strength, $E \simeq \pm0.113\Delta_0$, obtained by an extrapolation. Here, $\Delta_0 \simeq 0.464E_F$ is the pairing gap at the trap center without impurity.

**FIG. 6.** (Color online) Wave function of the universal bound state with energy $E \simeq \pm0.113\Delta_0$ for a topological superfluid at $h = 1.2E_F$. The wave function at $\pm E$ may be regarded as the bond and antibond superposition of two Majorana wave functions, which satisfy, respectively, the symmetry $u_\sigma(x) = v_\sigma^*(x)$ (on the left side with $x < 0$) and $u_\sigma(x) = -v_\sigma^*(x)$ (on the right side with $x > 0$).

### C. Realistic Gaussian-shaped impurity

We consider so far a $\delta$-like impurity scattering potential. In real experiments, the nonmagnetic impurity would be simulated by an off-resonant dimple laser light, which has a finite width in space. Thus, it is more reasonable to simulate the impurity by using a Gaussian-shaped scattering potential.

Figure 7 reports the linear contour plot of the local density of state at $h = 1.2E_F$ for a (a) strong attractive and (b) repulsive Gaussian-shaped impurity potential. With a finite width $d = 0.1x_F$, we observe a series of bound states in the vicinity of the impurity site. The lowest-energy bound state is close to the universal bound state that we found earlier with a $\delta$-like impurity potential.

To give some realistic parameters, let us consider a spin-orbit-coupled Fermi gas of $^{40}$K atoms confined to a tight 2D optical lattice, with an axial trapping frequency $\omega = 2\pi \times 116$ Hz [21]. By assuming the number of atoms $N = 100$ in each tube, the Fermi energy or temperature is about 300 nK. We may take $k_F \simeq 2k_B$ and a Raman strength $\Omega_R \simeq 10E_R$, where $E_R$ is the recoil energy. We may anticipate a topological superfluid at temperature $T < 10$ nK. The typical size of the Fermi cloud is about $x_F \simeq 15 \mu$m. Thus, we may use an off-resonant dimple laser with width $d \simeq 1.5 \mu$m to simulate the nonmagnetic impurity. The strength of the impurity can be easily tuned by controlling the strength of the dimple laser light. With these parameters, we may be able to observe the universal impurity-induced bound state discussed above.

### IV. CONCLUSIONS

In summary, we have argued that a strong nonmagnetic impurity will induce a universal bound state in topological superfluids. This provides a unique feature to characterize the long-sought topological superfluids. We have proposed...
a realistic setup to observe such a universal impurity-induced bound state in atomic topological superfluids, which are to be realized in spin-orbit-coupled Fermi gases of $^{40}$K atoms. The necessary conditions, including the realization of spin-orbit coupling by a two-photon Raman process, the achievement of one-dimensional confinement by optical lattice, and the simulation of nonmagnetic impurities using off-resonant dimple laser light, are all within current experimental reach. Therefore, we anticipate that our proposal will be realized soon at Shanxi University in China [21] or elsewhere.

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APPENDIX: SOLVING THE BdG EQUATION IN ONE DIMENSION

We solve the BdG equation (22) by expanding the Bogoliubov wave functions $u_{\sigma}(x)$ and $v_{\sigma}(x)$ in the basis of 1D harmonic oscillators $\phi_j(x) = (1/\sqrt{\pi}^{1/2}2^{j/2})H_j(x)e^{-x^2/2}$,

$$u_{\sigma}(x) = \sum_{j=0}^{M-1} U_{\sigma j} \phi_j(x), \quad \text{(A1)}$$

$$v_{\sigma}(x) = \sum_{j=0}^{M-1} V_{\sigma j} \phi_j(x). \quad \text{(A2)}$$

Here, $H_j(x)$ is the $j$th Hermite polynomial and, for convenience, we have used the natural unit in harmonic traps, $m = \hbar = \omega = 1$, so that the oscillator length $a \equiv \sqrt{\hbar/(ma\omega)} = 1$ and the oscillator energy $\hbar \omega = 1$. On such a basis, the BdG Hamiltonian (18) is converted to a $4M \times 4M$ secular matrix,

$$\mathcal{H}_{\text{BdG}} = \begin{bmatrix}
\mathcal{H}_{\text{BdG}}^{ij} & -R_{ij} & 0 & -\Delta_{ij} \\
R_{ij} & \mathcal{H}_{\text{BdG}}^{ij} + \hbar \delta_{ij} & \Delta_{ij} & 0 \\
0 & \Delta_{ij} & -\mathcal{H}_{\text{BdG}}^{ij} + \hbar \delta_{ij} & R_{ij} \\
-\Delta_{ij} & 0 & -R_{ij} & -\mathcal{H}_{\text{BdG}}^{ij} - \hbar \delta_{ij}
\end{bmatrix}, \quad \text{(A3)}$$

where the matrix elements

$$\mathcal{H}_{\text{BdG}}^{ij} = (i + 1/2 - \mu) \delta_{ij} + V_{\text{imp}}^{ij}, \quad \text{(A4)}$$

$$R_{ij} = \lambda [\sqrt{j/2} \delta_{i,j-1} - \sqrt{(j+1)/2} \delta_{i,j+1}]. \quad \text{(A5)}$$

To calculate efficiently the matrix elements $V_{\text{imp}}^{ij} \equiv \int_{-\infty}^{+\infty} dx \phi_i(x)V_{\text{imp}}(x)\phi_j(x)$ and $\Delta_{ij} \equiv \int_{-\infty}^{+\infty} dx \phi_i(x)\Delta(x)\phi_j(x)$, we discretize space ($-L/2,L/2$) into $N_{\text{grid}}$ equally spaced points, where the simulation length $L$ and the number of grid $N_{\text{grid}}$ should be sufficiently large so that the basis function $\phi_j(x)$ ($j = 0, \ldots, M - 1$) can be accurately sampled. At the number of atoms $N = 100$, typically we take $M = 500$, $N_{\text{grid}} = 6400$, and $L = 70\sqrt{\hbar/(m\omega)}$. The Gaussian impurity potential $V_{\text{imp}}(x)$ and pairing gap function $\Delta(x)$, as well as the total density $n(x)$, will be stored as an array of length $N_{\text{grid}}$. We note that for a $\delta$-like impurity, we immediately have $V_{\text{imp}}^{ij} = V_{\text{imp}}(x_0)\phi_j(x_0)$. By diagonalizing the $4M \times 4M$ secular matrix given by Eq. (A3), we obtain the quasiparticle energy $E_\eta$ and the eigenvectors $U_{\sigma j}^\eta$ and $V_{\sigma j}^\eta$ ($j = 0, \ldots, M - 1$). The latter gives the quasiparticle wave function $u_{\sigma j}(x)$ and $v_{\sigma j}(x)$. Note that the eigenvectors $U_{\sigma j}^\eta$ and $V_{\sigma j}^\eta$ have to satisfy the condition $\sum_{\sigma j}[(U_{\sigma j}^\eta)^2 + (V_{\sigma j}^\eta)^2] = 1$, due to the normalization of the quasiparticle wave functions, i.e., $\int_{-\infty}^{+\infty} dx \sum_{\sigma j}[u_{\sigma j}^2(x) + v_{\sigma j}^2(x)] = 1$.

In the practical calculation, due to computational limitation, we have to use a finite expansion basis. This is controlled by the cutoff $M$ for the number of 1D harmonic oscillators. Furthermore, we must impose a high-energy cutoff $E_c$ for

FIG. 7. (Color online) Linear contour plot of the density of state at $\hbar = 1.2E_F$ for an attractive or a repulsive Gaussian-shaped impurity scattering potential. Here, we take $d = 0.1x_F$ and $V_{\text{imp}} = \pm 0.30x_F E_F$. 

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the quasiparticle energy levels. To make our result cutoff independent, we adopt a hybrid approach, in which we solve the discrete BdG equation for the energy levels below the high-energy cutoff $E_c$; while above $E_c$, we use a semiclassical plane-wave approximation for the wave functions that should work very well for high-lying energy levels. For simplicity, to take the semiclassical approximation, we may neglect the spin-orbit-coupling term $R_{ij}$ in the BdG Hamiltonian given by Eq. (A3). In the end, for the pairing gap function and the total density, we shall use the semiclassical expressions listed in Sec. IV C of Ref. [28]. To summarize briefly, the contributions of discrete low-lying energy levels (labeled by an index “$n$”) and continuous high-lying energy levels to the total density are given by

$$n_d(x) = \frac{1}{2} \sum_{|E_n| < E_c} \sum_{\sigma} \left[ |u_{\sigma}(x)|^2 f(E_n) + |v_{\sigma}(x)|^2 f(-E_n) \right]$$  \hspace{1cm} (A6)

and

$$n_c(x) = \frac{\sqrt{2m}}{4\pi \hbar} \left( \int_{E_c+h}^{+\infty} + \int_{E_c-h}^{-\infty} \right) \frac{d\epsilon}{\sqrt{\epsilon^2 - \Delta^2(x)}} \left[ 1 - \frac{\epsilon}{\sqrt{\epsilon^2 - \Delta^2(x)} + \mu} \right]$$  \hspace{1cm} (A7)

respectively. For the pairing gap function, we have

$$\Delta(x) = -\frac{g_{1D}^{\text{eff}}(x)}{2} \sum_{|E_n| < E_c} \sum_{\sigma} \left[ u_{1\sigma}(x) u_{1\sigma}^*(x) f(E_n) \right]$$

$$+ u_{1\lambda}(x) u_{1\lambda}^*(x) f(-E_n)],$$  \hspace{1cm} (A8)

where the effective interaction strength $g_{1D}^{\text{eff}}(x)$ is determined by

$$\frac{1}{g_{1D}^{\text{eff}}(x)} = \frac{1}{g_{1D}} + \frac{\sqrt{2m}}{4\pi \hbar} \int_{E_c-h}^{\infty} \frac{d\epsilon}{\sqrt{\epsilon^2 - \Delta^2(x)}}.$$  \hspace{1cm} (A9)

The numerical procedure of solving the BdG equation is, therefore, as follows. For a given set of parameters ($N$, $g_{1D}$, $h$, $\lambda$, and $T$), we (i) start with an initial guess or a previously determined better estimate for $\Delta(x)$, (ii) solve Eq. (A9) for the effective coupling constant, (iii) solve Eq. (A3) for all of the quasiparticle wave functions up to the chosen energy cutoff to find $u_{\sigma}(x)$ and $v_{\sigma}(x)$, and (iv) finally determine an improved value for the order parameter from Eq. (A8). During the iteration, the total density $n(x) = n_d(x) + n_c(x)$ is updated. The chemical potentials $\mu$ are adjusted slightly in each iterative step to enforce the number-conservation condition $\int_{-\infty}^{\infty} dx n(x) = N$, until final convergence is reached.

1. Check on the numerical accuracy

We have checked carefully the numerical accuracy of our hybrid approach at different sets of parameters and at both zero temperature and finite temperatures. In Fig. 8, we check the dependence on the cutoff energy $E_c$ at $h = 1.2E_F$ in the absence of impurity scattering. The pairing gap function becomes essentially independent of $E_c$ once $E_c \geq 6E_F$, with a relative error less than 1%. The cutoff energy dependence for the total density is even weaker (not shown in the figure). Thus, we conclude that our hybrid calculation is quantitatively reliable with $E_c = 6E_F$. At this energy cutoff, each iteration in the self-consistent calculation takes approximately several minutes using a standard desktop computer. The convergence for a set of parameters is typically reached after 20–50 iterations.

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[33] The energy of the gapless excitations is not precisely zero due to the finite size of the system. It scales exponentially with the cloud size. Typically, it is about $10^{-10}E_F$.
[34] For weak attractive interactions, the local critical Zeeman field may decrease towards the trap edge. As a result, the topological phase appears first at the trap edge, leading to a phase-separation phase consisting of a topological superfluid at the edge and a BCS superfluid at the center. See, for example, Ref. [15] for more details.