Heavy polarons in ultracold atomic Fermi superfluids at the BEC-BCS crossover: formalism and applications

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We investigate the system of a heavy impurity embedded in a paired two-component Fermi gas at the crossover from a Bose-Einstein condensate (BEC) to a Bardeen-Cooper-Schrieffer (BCS) superfluid via an extension of the functional determinant approach (FDA). FDA is an exact numerical approach applied to study manifestations of Anderson’s orthogonality catastrophe (OC) in the system of a static impurity immersed in an ideal Fermi gas. Here, we extend the FDA to a strongly correlated superfluid background described by a BCS mean-field wavefunction. In contrast to the ideal Fermi gas case, the pairing gap in the BCS superfluid prevents the OC and leads to genuine polaron signals in the spectrum. Thus, our exactly solvable model can provide a deeper understanding of polaron physics. In addition, we find that the polaron spectrum can be used to measure the superfluid pairing gap, and in the case of a magnetic impurity, the energy of the sub-gap Yu-Shiba-Rusinov (YSR) bound state. Our theoretical predictions can be examined with state-of-art cold-atom experiments.

I. INTRODUCTION

The dynamics of an impurity interacting with a bath of quantum-mechanical particles are unique and fundamental in understanding many-body quantum physics [1–3]. On the one hand, the system’s simplicity allows us to develop insightful theoretical models and, in some cases, access exact solutions to make quantitative comparisons with experiments [4, 5]. On the other hand, since a single impurity barely affects the background, we can apply the impurity as a sensitive probe of the surrounding many-particle medium [1]. Two important and related theoretical concepts have been developed to study the impurity-medium problems: polarons [2, 3] and orthogonality catastrophe (OC) [4, 5].

In 1933, Landau [8] introduced the general concept of polarons to describe impurity-medium systems as quasiparticles formed by dressing the impurity with elementary excitations of the medium. Polarons have become some of the most celebrated “quasiparticles” in condensed matter physics and can be commonly found in various crystalline solids [9, 10]. In recent years, polaron physics in experiment [11, 21] and theory [22, 50] has progressed rapidly in the new platform of ultracold quantum gases, which provides unprecedented controllability over many-body physics and is exactly solvable [42, 43] via the functional determinant approach (FDA) [44–47]. Unfortunately, OC leads to vanishing quasiparticle residues [3], where polaron does not technically exist. Consequently, this exactly solvable model may not be directly applied to understand polarons.

The present study, which accompanies the Letter Ref. [48], investigates a heavy impurity immersed in a two-component Fermi superfluid medium described by the standard Bardeen-Cooper-Schrieffer (BCS) pairing theory. The purpose is twofold.

First, we aim to construct an exactly solvable model for polaron with finite residue. As shown in this study, our system is suitable for an exact approach — an extended FDA, and the presence of a pairing gap can efficiently suppress multiple particle-hole excitations and prevent Anderson’s OC. Therefore, our model provides a benchmark calculation of the polaron spectrum and rigorously examine all the speculated polaron features. We name our system “heavy crossover polaron” since the background Fermi gas can undergo a crossover from a Bose-Einstein condensation (BEC) to a BCS superfluid. Second, our prediction can be applied to investigate the background Fermi superfluid excitations, a long-standing topic in ultracold atoms. Polarons have already been realized in BEC and ideal Fermi gas experimentally, but
the physics of these weakly interacting background gas are well understood. More recently, it has also been shown that polarons in BEC with a synthetic spin-orbit-coupling can reveal the nature of the background roton excitations. Investigating polaron physics in a strongly correlated Fermi superfluid at the BEC-BCS crossover, namely crossover polaron, has also been proposed in several pioneering works with approximated approaches. Our exact method in the heavy impurity limit allows us to apply the polaron spectrum to measure the Fermi superfluid excitation features such as the pairing gap and sub-gap Yu-Shiba-Rusinov (YSR) bound states, which is highly experimentally relevant. Nowadays, it is standard to use Feshbach resonance at the BEC-BCS crossover to realize a BCS Fermi superfluid. Recent experiments have already demonstrated the coexistence of Bose and Fermi superfluids in several realizable systems, $^6$Li-$^7$Li, $^6$Li-$^{41}$K, and $^6$Li-$^{174}$Yb mixtures, where the heavy species can serve as the impurity at will. The combinations $^6$Li-$^{133}$Cs, $^6$Li-$^{168}$Er, and $^6$Li-$^{168}$Er are also promising candidates, where the interspecies Feshbach resonances have been characterized.

The rest of this paper is organized as follows. In the following section, we establish our general formalism and show how to extend the exact FDA approach to the case of a BCS superfluid as a background system. Section III is devoted to presenting our numerical results, and Section IV is given to the discussion of possible experimental realizations. Finally, we conclude our paper by discussing the physics and proposing applications in section V.

II. FORMALISM

A. Heavy impurity in a BCS superfluid

Our system consists of a static impurity atom, that either is localized by a deep optical lattice or has infinitely heavy mass, and a two-component Fermi superfluid with equal mass $m_{\uparrow} = m_{\downarrow} = m$. We assume the impurity can be in either a non-interacting or an interacting hyperfine state with the background fermions, where the many-body Hamiltonian is given by $\hat{H}_i$ and $\hat{H}_f$ correspondingly. The energy difference of these two hyperfine states only leads to trivial effects and is neglected in this work. The interaction between unlike atoms in the two-component Fermi gas can be tuned by a broad Feshbach resonance, and characterized by the s-wave scattering length $a$. At low temperature $T$, these strongly interacting fermions undergo a crossover from a BEC to a BCS superfluid, which can be described by the celebrated BCS theory at a mean-field level and is briefly reviewed here and in Appendix A.

Using the units $\hbar = 1$ hereafter, the BCS Hamiltonian is given by

$$\hat{H}_i = K_0 + \sum_k \hat{\psi}_k^\dagger h_i(k) \hat{\psi}_k,$$

where $\hat{\psi}_k \equiv (c_{k\uparrow}, c_{-k\downarrow})$ is the Nambu spinor representation with $c_{k\sigma} (c_{k\sigma}^\dagger)$ being the creation (annihilation) operator for a $\sigma$-component fermion with momentum $k$. Here, $K_0 \equiv -V\Delta^2/g + \sum_k (\epsilon_k - \mu)$ with $V$ denoting the system volume and $\Delta$ being the pairing gap parameter. $\epsilon_k \equiv \hbar^2 k^2/2m$ is the single-particle dispersion relation and $\mu$ is the chemical potential. The bare coupling constant $g$ should be renormalized by the s-wave scattering length $a$ between the two components via

$$g^{-1} = \frac{m}{4\pi\hbar^2 a} - \frac{\Lambda}{2\varepsilon_k},$$

where $\Lambda$ is an ultraviolet cut-off. $h_i(k)$ can be regarded as a single-particle Hamiltonian in momentum space and has a matrix form:

$$h_i(k) = \begin{bmatrix} \xi_k & \Delta \\ \Delta & -\xi_k \end{bmatrix},$$

where $\xi_k \equiv \epsilon_k - \mu$. For a given scattering length $a$ and temperature $T$, $\Delta$ and $\mu$ are determined by a set of the mean-field number and gap equations (see Appendix A).

When the static impurity is in the interacting hyperfine state, the many-particle Hamiltonian is given by

$$\hat{H}_f = \hat{H}_i + \hat{V} \equiv \hat{H}_i + \sum_{\sigma} \hat{V}_{\sigma}(k - q) c_{k\sigma}^\dagger c_{q\sigma},$$

where $\hat{V}_{\sigma}(k)$ is Fourier transformation of $V_{\sigma}(r)$, the potential between impurity and $\sigma$-component fermion. For a reason which will become clear soon, we would like to express $\hat{H}_i$ and $\hat{H}_f$ in a bilinear form. Defining $\hat{\psi}_k(q) = (c_{k\uparrow}, c_{-k\downarrow}) \equiv (c_{k\downarrow}, h_k^\dagger)$ and rewriting $\hat{V}$ as

$$\hat{V} = \sum_{kq} \left[ \hat{V}_\uparrow(k - q) c_{k\uparrow}^\dagger c_{q\uparrow} - \hat{V}_\downarrow(q - k) h_k^\dagger h_q \right] + \sum_k \hat{V}_\downarrow(0),$$

make the bilinear form apparent. We can write the bilinear form of $\hat{H}_f$ explicitly,

$$\hat{H}_f = K_0 + \omega_0 + \sum_{kq} \hat{\psi}_k^\dagger h_f(k, q) \hat{\psi}_q,$$

where $\omega_0 = \sum_k \hat{V}_\downarrow(0)$ and

$$h_f(k, q) = h_i(k) \delta_{kq} + \begin{bmatrix} \hat{V}_\uparrow(k - q) & 0 \\ 0 & -\hat{V}_\downarrow(q - k) \end{bmatrix}$$

can be regarded as a single-particle Hamiltonian $\hat{h}_f$ in momentum space and in a matrix form. We can see that,
\( \hat{h}_i \) and \( \hat{h}_f \) are the single-particle representative of \( \hat{H}_i \) and \( \hat{H}_f \) up to some constants, respectively.

It is worth noting that, in the many-body Hamiltonian \( \hat{H}_f \) we have assumed that the pairing order parameter \( \Delta \) remains unchanged by introducing the interaction potential \( V(r) \). For a non-magnetic potential \( (V_\uparrow = V_\downarrow) \) that respects time-reversal symmetry, this is a reasonable assumption, according to Anderson's theorem [1]. For a magnetic potential \( (V_\uparrow \neq V_\downarrow) \), the local pairing gap near the impurity will be affected, as indicated by the presence of the YSR bound state. We will follow the typical non-self-consistent treatment of the magnetic potential in condensed matter physics [1, 54] and assume a constant pairing gap as the first approximation for simplicity. We leave a more rigorous self-consistent calculation of a pairing gap to future studies.

**B. Functional determinant approach**

We are interested in a situation where the impurity is driven from a non-interacting hyperfine state to an interacting hyperfine state at \( t = 0 \), as sketched in Fig. 1. The most basic quantity to describe the response to this process is the time-overlapping function

\[
S(t) = \left\langle e^{i \hat{H}_i t} e^{-i \hat{H}_f t} \right\rangle \equiv \text{Tr} \left[ e^{i \hat{H}_i t} e^{-i \hat{H}_f t} \hat{\rho}_0 \right],
\]

where \( \hat{\rho}_0 \) is the initial thermal density matrix, and \( \hat{H}_i \) and \( \hat{H}_f \) are the many-body Hamiltonian with the impurity in non-interacting and interacting hyperfine state, respectively. The response in frequency domain can be obtained via a Fourier transformation

\[
A(\omega) = \frac{1}{\pi} \text{Re} \int_0^\infty e^{i \omega t} S(t) dt,
\]

which is also called spectral function.

We review our main theoretical tool, FDA, and show how to extend this method to the case of an ultracold BCS superfluid as the background medium. An exact calculation of Eq. [3] is usually not accessible due to the exponentially growing complexity of the many-body Hamiltonian with respect to particle number \( N \). However, one can prove that Eq. [3] can reduce to a determinant in a single-particle Hilbert space that grows only linearly to \( N \), if \( \hat{H}_i \) and \( \hat{H}_f \) are both fermionic, bilinear many-body operators, such as Eq. [1] and Eq. [3] shown in the previous subsection. In that case, we have,

\[
S(t) = e^{-i \omega_0 t} \text{det} \left[ 1 - \hat{n} + e^{i \hat{h}_i t / \hbar} e^{-i \hat{h}_f t / \hbar} \hat{n} \right]
\]

where \( \hat{n} \) is the occupation number operator.

It would be more convenient to carry out numerical calculations in the coordinate space in a finite system confined in a sphere of radius \( R \). We then take the system size towards infinity, while keeping the density constant, until numerical results are converged. The bilinear form of the many-body Hamiltonians in coordinate space are given by

\[
\hat{H}_i = K_0 + \int d\mathbf{r} \bar{\phi}^\dagger (\mathbf{r}) \mathbf{h}_i (\mathbf{r}) \phi (\mathbf{r}),
\]

\[
\hat{H}_f = K_0 + \omega_0 + \int d\mathbf{r} \bar{\phi}^\dagger (\mathbf{r}) \mathbf{h}_f (\mathbf{r}) \phi (\mathbf{r}),
\]
with \( K_0 = -\mathcal{V} \Delta^2/g + \sum_k (\epsilon_k - \mu) \) being an unimportant constant that cancels out in Eq. (10). Here, \( \hat{c}^\dagger (r) = [c_\uparrow^\dagger (r), c_\downarrow^\dagger (r)] \equiv [c^\dagger (r), h^\dagger (r)] \) are creation operators in the coordinate space. Since higher partial wave interaction is negligible at low temperature, we focus on the s-wave channel. We also assume \( V_\sigma (r) = V_\uparrow (r) \) is spherically symmetric and short-range. The single-particle representative of Hamiltonians in coordinate space, therefore, are given by

\[
h_f (r) = h_\uparrow (r) + \begin{pmatrix} V_\uparrow (r) & 0 \\ 0 & -V_\downarrow (r) \end{pmatrix} \equiv \begin{pmatrix} -\frac{1}{2m} \frac{d^2}{dr^2} + V_\uparrow (r) - \mu & \Delta \\ \Delta & \frac{1}{2m} \frac{d^2}{dr^2} - V_\downarrow (r) + \mu \end{pmatrix}.
\]

In our numerical calculation, we choose a soft-core van-der-Waals potential

\[
V_\sigma (r) = -\frac{C_0}{r^6} \exp \left[ -\frac{r^6}{r_0^6} \right],
\]

where \( C_0 \) is the dispersion coefficient describing the long-range behavior of the impurity-fermion interaction and determines the van-der-Waals length \( l_{vdW} = (2mC_0)^{1/4}/2 \). The short-range parameter \( r_\sigma \) are tuned to give the desired energy-dependent scattering length

\[
a_\sigma (E_F) = -\frac{\tan \eta_\sigma (k_F)}{k_F},
\]

where \( \eta_\sigma (k_F) \) is the s-wave scattering length between the impurity and \( \sigma \)-component fermions at the Fermi energy \( E_F = k_F^2/2m \). We find our calculations are insensitive to other details of \( V_\sigma (r) \) (such as the value of \( l_{vdW} \) and the number of short-range bound states the potential supported) as long as \( k_F l_{vdW} \ll 1 \). Therefore, we denote \( a_\sigma (E_F) \equiv a_\sigma \) hereafter for the simplicity of notation. In the calculations here, we choose \( k_F l_{vdW} = 0.01 \) unless otherwise stated. To calculate Eq. (10), we need to find the eigenpairs \( E_{\nu_\uparrow}, \phi_\uparrow \equiv [\phi_{\nu_\uparrow}^\dagger(\nu), \phi_{\nu_\uparrow}^\dagger(\nu)] \) for \( h_\uparrow (r) \) and \( \tilde{E}_{\nu_\downarrow}, \tilde{\phi}_\downarrow \) for \( h_\downarrow (r) \), and express the occupation operator \( \hat{n} \) as a diagonal matrix with elements

\[
n_{\nu_\nu} = \begin{cases} 1, & \text{if } \nu = \nu_\nu \\ 0, & \text{otherwise} \end{cases}
\]

We also need to take care of \( \omega_0 \) if \( V_\downarrow \neq 0 \). Noticing that the original definition \( \omega_0 = \sum_k V_i (0) = \sum_k (k|V(r)|r|k\rangle \) equivalent to taking the trace of the matrix representative of \( \hat{V}_\downarrow \) in momentum state basis. Therefore, \( \omega_0 \) can also be obtained via tracing \( \hat{V}_\downarrow \), the matrix format of \( \hat{V}_\downarrow \) in an arbitrary complete orthogonal set of basis, i.e., \( \omega_0 = \text{Tr} \hat{V}_\downarrow \). In practical calculations, we use the same discretization basis set in coordinate space as the one applied to diagonalize \( h_\uparrow (r) \) and \( h_\downarrow (r) \).

We give a few further remarks on some possible extensions of our methods. As already noticed in Ref. [7], generalization of FDA to other geometries and confinement can be easily implemented to the single-particle Hamiltonian. Our single-channel soft-core van-der-Waals potential have been proved to mimic the interatomic interaction near broad Feshbach resonances very well [64], and can be replaced by multi-channel interactions to describe closed-channel dominated Feshbach resonances.

III. RESULTS

A. Single particle spectrum

It is illustrative to first see the structure of single particle spectrum, as sketched in Fig. [1]. When the impurity interaction is absent, diagonalizing \( h_\uparrow (r) \) gives the well-known BCS dispersion relation

\[
E_\nu = \pm \xi_a = \pm \sqrt{\xi_a^2 + \Delta^2},
\]

where \( \xi_a = n_{\nu} \pi \) with integer \( n_{\nu} \). The positive and negative branches of the spectrum are separated by an energy gap

\[
2\Delta = \begin{cases} \frac{2\Delta}{2\sqrt{\Delta^2 + \mu^2} - \mu} & \mu \geq 0 \\ \frac{2\Delta}{2\sqrt{\Delta^2 + \mu^2} - \mu} & \mu < 0 \end{cases}
\]

which represents the minimum energy required to break a Cooper-pair into a particle-hole excitation. At zero temperature, the many-body ground state can be regarded as a fully filled Fermi sea of the lower branch, and a
completely empty Fermi sea of the upper branch. Notice that the $E_\nu$ are measured with respect to chemical potential $\mu$, which leads to the occupation $f(E_\nu) = 1/(e^{-E_\nu/\beta} + 1)$.

In the presence of impurity interaction, our numerical calculations show that $\tilde{E}_\nu$ still consists of two branches separated by $2\Delta$, with each individual energy level shifted as shown in Fig. 1. Moreover, when the impurity scattering is magnetic ($a_\uparrow \neq a_\downarrow$), a sub-gap YSR bound state exists. Figure 2 shows the YSR bound state energy as a function of $1/(k_F a_\uparrow)$ for the case $k_F a_\uparrow = -2$ and $k_F a_\downarrow = 0$ at zero temperature. The decreasing bound state energy with increasing $1/(k_F a_\uparrow)$ can be qualitatively understood from the analytic expression

$$E_{YSR} \simeq \Delta \cos \left[ \eta_\uparrow(E_F) - \eta_\downarrow(E_F) \right], \quad (19)$$

which holds in the weak-coupling limit ($a \to 0^+$). Here, $\eta_\uparrow(E_F)$ and $\eta_\downarrow(E_F) = 0$ are the impurity scattering phase shifts of the potentials $V_\uparrow(r)$ and $V_\downarrow(r)$ at Fermi energy $E_F$. The inset of Fig. 2 shows the YSR wave-function at $k_F a_\uparrow = -2$, where one can see that the YSR bound state has a relatively large size (about 30$\ell_F^{-1}$ in this case) and shows an oscillation behavior at large distances.

We give some further remarks here on the two-body bound states supported solely by the short-range potential $V_\nu(r)$, when the other component of fermions are absent. In general, there are multiple such bound states, and almost all of them are deeply bound with large binding energy $E_b \gg \Delta$ and highly localized to the impurity. As a result, the overlapping between these deeply bound states and BCS scattering waves are vanishingly small. Therefore, these deeply bound states are almost unaffected by the presence of the other component and give negligible effects on the response functions. The only exception is the shallowest bound state with $a_\sigma > 0$. This shallow bound state can strongly couple to the scattering states of the other component, and hence can no longer be distinguished from the eigenstates $\phi_\nu$.

**B. Magnetic impurity**

We first focus on the simplest case, where the impurity only interacts with the spin-up component, i.e. $a_\downarrow = 0$.

When $\Delta = 0$ and $a_\downarrow = 0$, our system reduces back to an ideal Fermi gas (consisting of spin-up fermions), and the asymptotic behavior of the Ramsey response at $t \to \infty$ is given by

$$S(t) \simeq C e^{-i\Delta E_\nu t/\hbar} \left( \frac{1}{iE_F t/\hbar + 0^+} \right)^\alpha + C_b e^{-i(\Delta E - E_F + E_b)t/\hbar} \left( \frac{1}{iE_F t/\hbar + 0^+} \right)^{\alpha_b}, \quad (20)$$

where $C$ and $C_b$ are both numerical constants independent with respect to $k_F a$ and $C_b = 0$ for $a_\uparrow < 0$. Here,

$$\alpha = \frac{\eta_\uparrow(E_F)^2}{\pi^2} \quad (21)$$

and

$$\alpha_b = \left[ 1 + \frac{\eta_\uparrow(E_F)^2}{\pi^2} \right]$$. \quad (22)

are determined by the scattering phase shifts $\eta_\uparrow(E_F)$ at Fermi energy. $E_b$ is the binding energy of the shallowest bound state consisting of the impurity and a spin-up fermion for $a_\uparrow > 0$ and $\Delta = 0$. Furthermore, the change in energy is given by

$$\Delta E = \sum_{E_\nu < E_b} (E_\nu - \tilde{E_\nu}), \quad (23)$$

where deeply bound states are excluded from $\tilde{E_\nu}$. Notice that the power-law decaying behavior of $|S(t)|$ at $\Delta = 0$ is evident in Fig. 3 (see the blue lines).
In sharp contrast, for cases with nonzero pairing gap, the asymptotic behavior in the long-time limit shows that $|S(t \to \infty)| \propto t^0$ approach to some constants. These asymptotic constants are larger for larger $\Delta$. Further details can be obtained by an asymptotic form that fits our numerical calculations perfectly well, as reported in Fig. 4.

$$S(t) \simeq D_a e^{-iE_a t} + D_r e^{-iE_r t}, \quad (24)$$

where $D_r = 0$ for $a_\uparrow < 0$. We obtain $D_a$, $D_r$, $E_a$ and $E_r$ from fitting, and find that $E_r = \text{Re}E_r + i\text{Im}E_r$ is in general complex. In contrast, $E_a = \sum_{E_v < 0}(E_v - \bar{E}_v)$ (where $\bar{E}_v$ excludes the two-body deeply bound states) is purely real, and can be explained as a renormalization of the filled Fermi sea, as indicated by the grey arrows in Fig. 1(a).

The long-time asymptotic behavior of $S(t)$ manifests itself as some characterized lineshape in the spectral function

$$A(\omega) \propto \begin{cases} Z_a \delta(\omega - E_a) & \omega \approx E_a \\ Z_r \frac{\text{Re}E_r}{(\omega - \text{Re}E_r)^2 + (\text{Im}E_r)^2} & \omega \approx \text{Re}E_r \end{cases}, \quad (25)$$

i.e., a $\delta$-function around $E_a$ and a Lorenzian around $\text{Re}E_r$. The existence of $\delta$-function peak unambiguously confirms the existence of a well-defined quasiparticle – the attractive polaron with energy $E_a$. The Lorenzian, on the other hand, can be recognized as a repulsive polaron with finite width and hence finite life-time. Here, $Z_a = |D_a|$ and $Z_r = |D_r|$ are the residue of attractive and repulsive polaron, correspondingly. Numerically, we find that $Z_a \propto (\Delta/E_F)^{\alpha_a}$ and $Z_r \propto (\Delta/E_F)^{\alpha_r}$ at small $\Delta$ as shown in the insets of Figs. 5(a) and 5(b). As a result, Eq. (24) have the same form as Eq. (20), the analytic expression of $S(t)$ for a non-interacting Fermi gas medium, if we replace the low-energy cut-off $1/t \to \Delta$. However, the power-law coefficients $\alpha_a$ and $\alpha_r$ are only close to but not exactly the same as the analytical expressions of $\alpha$ and $\alpha_b$. In the inset of Fig. 5(a), our numerical fitting gives $\alpha_a \approx 0.136$, comparing with $\alpha \approx 0.124$ for ideal Fermi gases. In the inset of Fig. 5(b), $\alpha_r \approx 0.083$ and $\alpha_a \approx 0.452$, in compare with $\alpha \approx 0.124$ and $\alpha_b \approx 0.419$. These small differences are probably due to the modification of scattering phase-shifts in the presence of $\Delta$.

Next, we study the full zero-temperature polaron spectrum across the BEC-BCS crossover and show them in Fig. 5. Numerically, to obtain $A(\omega)$ accurately requires a Fourier transformation that involves an integration of $S(t)$ from $t = 0$ to $t \to \infty$. We follow the procedures adopted from Ref. [7]: we numerically integrate $S(t)$ up to some large cut-off time $t^* \sim 500/E_F$, and carry-out the integration analytically with the fitting formula Eq. (24) for $t > t^*$.
As temperature increases, we observe the expected theoretical spectrum at the deep BEC side. Near the unitary limit, the repulsive polaron width becomes larger from the BCS side towards the BCS side of the Feshbach resonance for the background purity in an ideal Fermi gas [7]. The white solid curve in Fig. 5(b) shows the repulsive polaron and the molecule-hole continuum are vanishing, which can also be inferred from the behavior of Fig. 5(b). Towards the BEC side, both the repulsive polaron and the molecule-hole continuum are vanishing, which can also be inferred from the behavior of Fig. 5(b).

The white solid curve in Fig. 5(b) shows the repulsive polaron energy. We can observe that the repulsive polaron shows up for the $k_Fa_\uparrow = 2$ case at zero temperature. As expected, Fig. 7(a) shows no YSR features at $k_Fa_\uparrow = 2$ and is quite simple. In contrast, the polaron spectra on the positive side $k_Fa_\uparrow = 2$ are much more complex as depicted in Fig. 7(b).

C. Non-magnetic impurity

In this subsection, we study the case of non-magnetic impurity scattering $a_\uparrow = a_\downarrow$, where the YSR state merges into the upper branch states as a result of Eq. (19) and ceases to exist. As expected, Fig. 7(a) shows no YSR features at $k_Fa = -2$ and is quite simple. In contrast, the polaron spectra on the positive side $k_Fa_\uparrow = 2$ are much more complex as depicted in Fig. 7(b). Interestingly, we also observe some additional features. An onset of spectral weight enhancement arises sharply at the energy

$$E_{\text{YSR}}^{(+)} = E_a - (\Delta - E_{\text{YSR}}),$$

below the attractive polaron. We explain this feature as an additional decay from the upper branch state to the sub-gap YSR state illustrated by the green arrow in Fig. 1(b). There is also another feature that associates with the repulsive polaron shows up for the $k_Fa_\uparrow = 2$ case at energy

$$E_{\text{YSR}}^{(+)} = \text{Re}(E_r) - (E_{\text{YSR}} + \Delta),$$

which implies that this feature is related to the decay from the YSR state back to the lower branch as illustrated by the purple arrow in Fig. 1(b). These two decay processes are only allowed if the upper branch has thermal occupations initially, which explains why such features only show up at finite temperature. These features can be better depicted in the comparison of the full spectra as a function of $1/(k_Fa_\uparrow)$ at zero and finite temperature in Figs. 1(c) and 1(d), respectively.
FIG. 7. Polaron spectrum of heavy non-magnetic impurity \((a_\uparrow = a_\downarrow)\) in a BCS superfluid with \(k_F a = -2\) at different temperature (see legend). The impurity scattering length is (a) \(k_F a = -2\) and (b) \(k_F a = 2\). The red dashed vertical line shows a feature at \(E_s - 2\Delta\) associated with the singularity at \(E_s\). The inset shows the residue as a function of \(1/(k_F a)\). The full spectrum as a function of \(1/(k_F a)\) are shown in (c) and (d) for zero and finite temperature, respectively. The white dashed and solid curves shows attractive and repulsive polaron energy, and the red dash-dotted curve shows the finite temperature feature.

repulsive polaron at zero temperature is also characterized by a \(\delta\)-function with infinite life-time. In addition, another singularity shows up at \(E_s\). We speculate the new long-lived repulsive polaron is related to undamped density excitations (i.e., the gapless Goldstone mode of the Fermi superfluid) excited by the non-magnetic impurity potential. As the coupling to the gapless Goldstone mode does not cost energy, the OC mechanism may lead to a power-law singularity, which is the reminiscent of the damped repulsive polaron in the case of magnetic impurity scattering. With this understanding in mind, we have checked that the asymptotic \(t \to \infty\) behavior
fits the formula
\[ S(t) \approx D_a e^{-iE_a t} + D_r e^{-iE_r t} + D_s e^{-iE_s t} \left( \frac{1}{iE_F} \right)^{\alpha_s} \]
very well, as shown in Fig. S(a). Our numerical fitting confirms \( E_a, E_r \) and \( E_s \) are all purely real. We also find that the power-law component of the singularity \( \alpha_s \approx 0.5 \), which seems to be a constant insensitive to \( a_1, a_1 \) and \( a \). The residue \( Z_a = |D_a| \) and \( Z_r = |D_r| \) as a function of impurity interaction \( 1/(k_Fa) \) are shown in the inset of Fig. (7a), which shows that the attractive polaron residue decreases and repulsive polaron becomes dominated on the positive side of impurity scattering length \( a_1 > 0 \). The dependence of \( Z_a \) and \( Z_r \) on \( \Delta \) is reported in Fig. S(b). Similar to the magnetic impurity case, we observe the power-law dependences \( Z_a \propto \Delta/E_F \) and \( Z_r \propto (\Delta/E_F)^{\alpha_r} \) at small \( \Delta \), and \( Z_a \to 1 \) and \( Z_r \to 0 \) on the deep BEC side \( \Delta \to \infty \).

Figures (7c) and (7d) show the comparison between zero and finite temperature polaron spectra as a function of \( 1/(k_Fa) \). We can observe a finite temperature feature appears at \( E_s - 2\Delta \), as shown in red dash-dotted curve in Fig. (7d) [as implied by the dashed vertical line in Fig. (7b) at \( k_Fa_1 = 2 \)]. This feature is the reminiscent of the structure at \( E_Y \) in the case of magnetic impurity scattering (see Eq. (27)), if we recall the replacement \( Re(E_r) \to E_s \) and \( E_Y \to \Delta \) as a result of the dissolution of the YSR state into the upper branch single-particle states.

Finally, we present the spectrum across the BEC-BCS crossover as a function of \( 1/(k_Fa) \) in Fig. S(c). Towards the BEC side, we observe that the spectral weight of the singularity decreases [which can be implied by the increase of \( Z_a + Z_r \), shown in Fig. S(b)]. Eventually, the singularity and the repulsive polaron merges at around \( 1/(k_Fa) \approx 0.5 \), which coincides where the chemical potential \( \mu \) is changing from positive to negative.

IV. EXPERIMENTAL REALIZATION

Our predictions could be readily examined in cold-atom experiments. Indeed, several quantum mixtures consisting of a Fermi superfluid and a Bose condensate have already been demonstrated, including \(^6\text{Li} - ^7\text{Li}\) \(^{56}\), \(^6\text{Li} - ^{41}\text{K}\) \(^{61}\), and \(^6\text{Li} - ^{174}\text{Yb}\) \(^{61}\) mixtures. Quantum mixtures such as \(^{6}\text{Li} - ^{133}\text{Cs}\) \(^{62}\), \(^{6}\text{Li} - ^{168}\text{Er}\) \(^{63}\), and \(^{6}\text{Li} - ^{168}\text{Er}\) \(^{63}\) should be available soon, since the interspecies Feshbach resonances have been characterized recently. In these mixtures, polaron physics can be explored by reducing the concentration of the bosonic component. For \(^{6}\text{Li} - ^{174}\text{Yb}\), \(^{6}\text{Li} - ^{133}\text{Cs}\), and \(^{6}\text{Li} - ^{168}\text{Er}\) systems, the minority bosonic species have different polarizability, which allows imposing a deep optical lattice to localize the impurity without affecting much the itinerant fermions. Even without the optical lattice, our calculations still give quantitatively accurate predictions due to the extremely large mass ratio. The response functions predicted here can be measured via established methods: \( S(t) \) can be accessed via an interferometric Ramsey scheme; \( A(\omega) \) can be obtained in rf-spectroscopy.

As a concrete example, let us focus on the \(^6\text{Li} - ^{133}\text{Cs}\) mixture. Nowadays, a two-component Fermi superfluid of \(^6\text{Li}\) atoms in the lowest two energy hyperfine states \([1,2] = |F = 1/2, m_F = \pm 1/2 \) is a typical setup to realize the BEC-BCS crossover in cold-atom laboratories, owing to a broad Feshbach resonance at \( B_0 \approx 832 \text{ G} \). The Feshbach resonances between \(^{132}\text{Cs}\) and \(^6\text{Li}\) have been accurately calibrated in 2013 \(^{62}\). Remarkably, in its lowest energy state \( |a \rangle = |F = 3, m_F = 3 \) \(^{133}\text{Cs}\) atoms have a broad Feshbach resonance near \( B_0 \) with \(^6\text{Li}\) atoms in both hyperfine states \([1,2]\). The resonances locate at \( B_{\text{F}} = 843.4(2) \text{ G} \) for \(|\text{Li} : 1 \rangle + |\text{Cs} : a \rangle \) and \( B_{\text{F}} = 889.0(2) \text{ G} \) for \(|\text{Li} : 2 \rangle + |\text{Cs} : a \rangle \). The three closely located broad Feshbach resonances mean that we can conveniently tune the magnetic field, to reach three significant scattering lengths \( a, a_1 \) and \( a_1 \) at the same time. In particular, by sweeping the magnetic field near \( B_{\text{F}} = 843.4(2) \text{ G} \), the parameter sets used in Fig. S and Fig. S can be easily realized.

V. DISCUSSIONS AND APPLICATIONS

The present work shows how to generalize FDA to the system of a heavy impurity immersed in a BCS superfluid. This formalism allows us to construct an exact model to investigate polaron physics, which gives all the universal polaron features, such as attractive and repulsive polaron, dark continuum, and molecule-hole continuum. In our model, the existence of polarons is protected from OC since the superfluid pairing gap suppresses multiple particle-hole excitations, which plays a similar role as the recoil energy of a mobile impurity in conventional Fermi polarons. In addition, we have shown in an accompanying paper \(^{48}\) that the pairing gap can also protect the polarons from thermal fluctuations, allowing experimental studies at a more accessible temperature \( k_B T \sim \Delta \). Our results for the non-magnetic impurity case also show some surprising results: the existence of a repulsive polaron with an infinite lifetime and an additional singularity. These peculiar characteristics only occur at the perfect balance of the two scattering lengths, where the impurity can only excite gapless density fluctuations. It would be interesting to find an intuitive understanding of the underlying physics in future studies.

Our predictions can also be applied to measure various exciting features of the Fermi superfluid, although the BCS description is only quantitatively reliable on the BCS side, and become only qualitatively reliable near the unitary limit and the BEC side. In the magnetic impurity case, the polaron spectrum at a finite but low temperature shows sharp features that measure the sub-gap YSR bound states. In particular, if \( E_a, \text{Re}(E_r), E^{(-)}_{Y} \) and \( E^{(+)}_{Y} \) shown in Fig. S(d) are all measured accurately,
Eqs. [26] and [27] give rise to,

\[ 2\Delta = E_a + \text{Re}(E_r) - E_{\text{YSR}}^{(-)} - E_{\text{YSR}}^{(+)} \tag{29} \]

independent on \( E_{\text{YSR}} \). We believe that this relation may only depend on the existence of a pairing gap and an ingap bound state, and therefore holds independent of the theoretical model used in this work. This allows a highly accurate measurement of the pairing gap \( \Delta \) at the whole BEC-BCS crossover. In the non-magnetic impurity case, there is also a finite temperature feature associated with the singularity \( E_a - 2\Delta \), which can be applied to measure the pairing gap \( \Delta \).

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\section*{Appendix A: The BCS-Leggett theory of the BEC-BCS crossover}

For a given scattering length \( a \) and temperature \( T \), \( \Delta \) and \( \mu \) are determined by the mean-field number and gap equations,

\[ \sum_k \left[ 1 - \frac{\xi_k}{E_k} + 2\frac{\xi_k}{E_k} f(E_k) \right] = n, \tag{A1} \]

\[ \frac{m}{4\pi\hbar^2 a} \sum_k \left[ 1 - \frac{2f(E_k)}{2E_k} - \frac{1}{2\epsilon_k} \right] = 0, \tag{A2} \]

where \( f(E_k) = [\exp(-E_k/k_BT) + 1]^{-1} \) is the Fermi–Dirac distribution, with \( k_B \) is the Boltzmann constant. Here \( E_k = \sqrt{\xi_k^2 + \Delta^2} \) are the eigenvalues of Eq. \ref{eq:A1} with the corresponding eigenvector \( [\xi_k, \epsilon_k]^T \), where \( \xi_k^2 = [1 + \xi_k/E_k]/2, \epsilon_k^2 = 1 - u_k^2 \) and \( 2u_k\epsilon_k = \Delta/E_k \).
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