Exact Quasiparticle Properties of a Heavy Polaron in BCS Fermi Superfluids

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We present the Ramsey response and radio-frequency spectroscopy of a heavy impurity immersed in an interacting Fermi superfluid, using the exact functional determinant approach. We describe the Fermi superfluid through the conventional Bardeen-Cooper-Schrieffer theory and investigate the role of the pairing gap on quasiparticle properties revealed by the two spectroscopies. The energy cost for pair breaking prevents Anderson's orthogonality catastrophe that occurs in a noninteracting Fermi gas and allows the existence of polaron quasiparticles in the exactly solvable heavy impurity limit. Hence, we rigorously confirm the remarkable features such as dark continuum, molecule-hole continuum, and repulsive polaron. For a magnetic impurity scattering at finite temperature, we predict additional resonances related to the subgap Yu-Shiba-Rusinov bound state, whose positions can be used to measure the superfluid pairing gap. For a nonmagnetic scattering at zero temperature, we surprisingly find undamped repulsive polarons. These exact results might be readily observed in quantum gas experiments with Bose-Fermi mixtures that have a large-mass ratio.

Thanks to the unprecedented controllability recently achieved in ultracold quantum gases, investigations on nonequilibrium quantum dynamics in many-body systems have progressed rapidly [1]. One such intriguing problem is how a quantum gas medium responds to a suddenly introduced impurity [2,3]. The quantum gas can be either a degenerate Fermi gas or a Bose-Einstein condensate (BEC). The impurity-medium interaction can essentially be tuned arbitrarily via Feshbach resonance [4], and a variety of impurities, such as Rydberg atoms [5–7] or quantum rotor [8], can be introduced. A unique advantage of these impurity-medium systems is that they present probably the simplest nontrivial many-particle problem, where the medium response can be directly measured (i.e., by Ramsey and radio-frequency spectroscopies) and efficiently calculated even in the nonperturbative strong-coupling regime [3,9]. Consequently, they can serve as a critical meeting point for theoretical and experimental efforts to understand the complicated quantum dynamics of interacting many-particle systems.

Historically, the first research of impurity-medium systems led Landau to introduce a general concept of polarons—quasiparticles formed by dressing the impurity with elementary excitations of the medium [10]. The new platform of ultracold quantum gases has enabled the exploration of polaron quasiparticle properties in a controllable and quantitative manner over the last decade, both experimentally [11–21] and theoretically [22–42]. In particular, a number of salient features of polarons have been predicted by approximate theories and Monte Carlo simulations, including the excited repulsive polaron with finite lifetime [26] and the dark continuum [35] and molecule-hole continuum [2] that separate the attractive and repulsive polaron branches. While the repulsive polaron has been unambiguously observed in experiments [13,14], the existence of the dark and molecule-hole continua remains elusive due to the uncertainty in theoretical calculations. The purpose of this Letter is to present an *exact* calculation of polaron quasiparticle properties in the heavy impurity limit and in the experimentally unexplored regime with a Fermi superfluid medium [43–47].

Our work naturally extends the well-known exactly solvable many-body problem of the Fermi-edge singularity of x-ray absorption spectra in metals [48,49], which is the first and most important example of nonequilibrium many-body physics [50,51]. In this impurity-medium problem, the suddenly introduced infinitely heavy impurity can excite particle-hole pairs close to Fermi surfaces without costing finite recoil energy [3,9]. The multiple particle-hole excitations completely changes the many-particle states in the limit of a large particle number. As a result, the many-particle states with and without impurity become orthogonal, i.e., Anderson's "orthogonality catastrophe" (OC) [52]. In the context of ultracold quantum gases, the Fermi-edge singularity has been quantitatively reexamined via the functional determinant approach (FDA) [53–56], providing insightful understanding of polaron physics [2,3,9].

Unfortunately, strictly speaking, due to OC the attractive and repulsive polarons do not exist, as indicated by the vanishing quasiparticle residue [3,9].

Here, we propose an exactly solvable model of a heavy impurity immersed in a Fermi superfluid medium described by the standard Bardeen-Cooper-Schrieffer (BCS) pairing theory [57–59]. As multiple particle-hole excitations can be efficiently suppressed by the energy cost of pairing breaking, Anderson's OC is avoided and polarons acquire *nonzero* quasiparticle residue. Therefore, we obtain a benchmark theoretical model with well-defined polaron quasiparticles, in which all the speculated characteristics of polarons can be rigorously examined. Our results are also highly experimentally relevant, as a BCS Fermi superfluid (of ^{6}Li or ^{40}K atoms) has now been routinely realized using Feshbach resonance at the so-called BEC-BCS crossover and a heavy atomic species such as ^{133}Cs can be manipulated at will as impurity.

In Fig. 1, we outline an injection scheme of interest in this Letter: the impurity is driven from a noninteracting hyperfine state [Fig. 1(a)] into an interacting state [Fig. 1(b)] at time $t = 0$. The dynamical evolution at later time, namely the Ramsey response, is then exactly calculated via an extension of the FDA, from which we extract the spectral function. The existence of pairing gap prevents the OC and preserves well-defined polaron quasiparticle features in the spectral function. In addition to rigorously confirming the remarkable characteristics of polarons, our exact results also reveal two novel unique features related to the Fermi superfluid medium: the resonances related to the subgap Yu-Shiba-Rusinov (YSR) state bound to a magnetic impurity [60–64] and repulsive polarons with infinitely long lifetime in the case of a nonmagnetic impurity scattering.

Theory.—The fundamental Ramsey response is the real-time overlap function between the many-body state with and without the impurity, $S(t) = \langle e^{i\hat{\mathcal{H}}_i t} e^{-i\hat{\mathcal{H}}_f t} \rangle \equiv \mathrm{Tr}[e^{i\hat{\mathcal{H}}_i t} e^{-i\hat{\mathcal{H}}_f t} \hat{\rho}_0]$, where $\mathcal{H}_i$ ($\mathcal{H}_f$) is the many-body
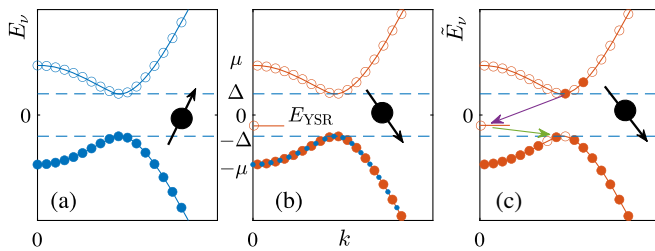

FIG. 1. A sketch of the occupation and structure of the single-particle dispersion spectrum of a two-component superfluid Fermi gas with a positive chemical potential $\mu > 0$ and the presence of a static impurity (black dot). (a) shows the spectrum E_ν when the impurity is in the noninteracting state (black arrow up) at zero temperature. When the impurity is in the interacting polaron state (black arrow down), the spectrum $\tilde{E}_\nu$ are shown in (b) at zero and (c) finite temperature.

Hamiltonian in the absence (presence) of the impurity scattering and $\hat{\rho}_0$ is the initial state of the Fermi system (hereafter, we use the units of $\hbar \equiv 1$). Complementarily, the frequency-resolved spectral function $A(\omega) = \mathrm{Re} \int_0^\infty e^{i\omega t} S(t) dt / \pi$, which determines the radio-frequency (rf) spectroscopy, can be obtained by a Fourier transformation [9,65]. Since the complexity of the many-body Hamiltonians increases exponentially with the numbers of particles N in the system, an exact calculation of $S(t)$ is usually inaccessible. However, in the case that $\mathcal{H}_i$ and $\mathcal{H}_f$ are both fermionic, bilinear many-body operators, the overlap function can reduce to a determinant in single-particle Hilbert space that grows only linearly to N [53–56]:

$$S(t) = e^{-i\omega_0 t} \det[1 - \hat{n} + e^{i\hat{h}_i t} e^{-i\hat{h}_f t} \hat{n}], \quad (1)$$

where $\hat{n}$ is the occupation number operator, and $\hat{h}_i$ ($\hat{h}_f$) are the single-particle representatives of $\mathcal{H}_i$ ($\mathcal{H}_f$) up to some constant terms that ω_0 compensates. For example, $\mathcal{H}_f = K_0 + \omega_0 + \int d\mathbf{r} \hat{\phi}^\dagger(\mathbf{r}) h_f(\mathbf{r}) \hat{\phi}(\mathbf{r})$, where K_0 is an unimportant constant and

$$h_f(\mathbf{r}) = \begin{pmatrix} -\frac{\nabla^2}{2m} + V_\uparrow(\mathbf{r}) - \mu & \Delta \\ \Delta & \frac{\nabla^2}{2m} - V_\downarrow(\mathbf{r}) + \mu \end{pmatrix}, \quad (2)$$

with $V_\sigma(\mathbf{r})$ being the potential between impurity and σ-component fermion. Note that, here we already extend the FDA to the case of a BCS Fermi superfluid, which is characterized by the pairing gap Δ and chemical potential μ to be determined by a given scattering length a between unlike fermions, temperature T and Fermi momentum $k_F = (3\pi^2 N/\mathcal{V})^{1/3}$, where $\mathcal{V}$ is the system volume. It is convenient to use the Nambu spinor operators as $\hat{\phi}^\dagger(\mathbf{r}) = [c_\uparrow^\dagger(\mathbf{r}), c_\downarrow(\mathbf{r})]$, where $c_\sigma^\dagger(\mathbf{r})$ [$c_\sigma(\mathbf{r})$] being the creation (annihilation) operator for a σ-component fermion at position $\mathbf{r}$. We also have $\omega_0 = \mathrm{Tr}V_\downarrow$, which corresponds to the phase factor in Eq. (1) with $V_\downarrow$ being the matrix format of $V_\downarrow(\mathbf{r})$ in a complete orthogonal set of basis. Finally, $h_i(\mathbf{r})$ can be obtained by setting $V_\sigma(\mathbf{r})$ equals zero in Eq. (2). In what follows, we briefly describe the computation procedure and present our main physical results, but relegate numerical details and additional discussions to a companion paper [66].

We consider a finite system confined in a sphere of radius R and take the system size towards infinity, while keeping the density constant, until numerical results are converged [9]. We focus on the s-wave channel and use finite-range potentials $V_\sigma(r)$ whose corresponding energy-dependent scattering length $a_\sigma(E_F) = -\tan \eta_\sigma(k_F)/k_F$, where $\eta_\sigma(k_F)$ is the s-wave scattering length between the impurity and σ-component fermions at the Fermi energy $E_F = k_F^2/(2m)$. We find that numerical results

are not sensitive to other short-range details of the potential. Therefore, for simplicity we denote $a_\sigma \equiv a_\sigma(E_F)$ hereafter [67]. Finally, for a given set of parameters $\{k_F, a, a_\uparrow, a_\downarrow, T\}$, we can calculate Eq. (1) by finding the eigenpairs $E_\nu, \phi_\nu \equiv [\phi_{\nu,\uparrow}(r), \phi_{\nu,\downarrow}(r)]$ for $h_i(r)$ and $\tilde{E}_\nu, \tilde{\phi}_\nu$ for $h_f(r)$. In this presentation, the occupation operator $\hat{n}$ is given by a diagonal matrix with elements $n_{\nu\nu} = [e^{-E_\nu/(k_B T)} + 1]^{-1}$, where k_B is the Boltzmann constant. Figure 1(a) gives a sketch of the occupation and structure of single-particle spectrum E_ν without impurity at $T = 0$, which includes a completely filled Fermi sea (filled circles in the lower branch) and an empty one (empty circles on the top) separated by 2Δ. The presence of impurity scattering leads to a shift of the single-particle levels $E_\nu \to \tilde{E}_\nu$ as shown in Fig. 1(b), where the small blue dots shows E_ν for comparison. In the case of a magnetic impurity scattering $(a_\uparrow \neq a_\downarrow)$, there also exists a subgap YSR bound state with energy E_{YSR} [60–63].

Ramsey response.—As reported in Fig. 2, our numerical examples here focus on the BCS side of the crossover $k_F a = -2 < 0$, where $\mu \approx 0.85 E_F$ and $\Delta \approx 0.40 E_F$ at zero temperature. While our method applies to the whole crossover regime, mean-field description becomes only qualitatively reliable on the BEC side. In addition, BCS treatment also cannot describe the gapless collective bosonic excitations, which might become more important and induce OC on the deep BEC side. We also focus on the simplest case, where the impurity only interacts with the spin-up component fermion, i.e., $V_\downarrow(r) = 0$. For comparison, we show also the results for $k_F a = 0$ (with $\mu = E_F$ and $\Delta = 0$), where the $\uparrow$ component of medium reduces to a
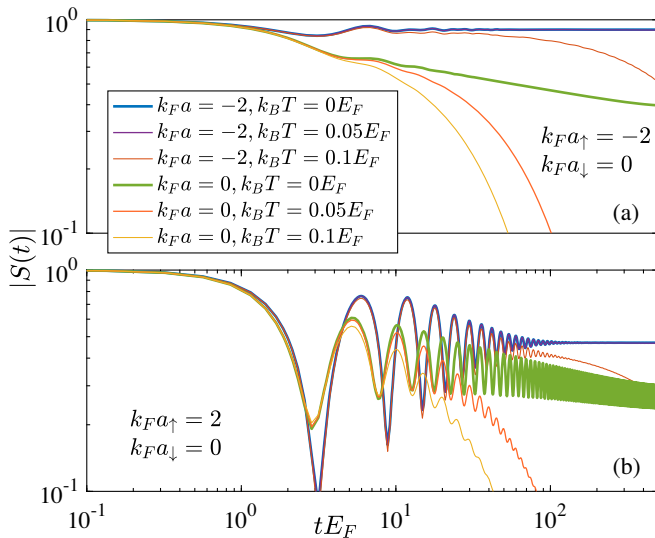

FIG. 2. Ramsey response $|S(t)|$ for a magnetic impurity scattering with (a) attractive scattering lengths $a_\uparrow < 0$ and (b) repulsive scattering lengths $a_\uparrow > 0$ are shown for different values of the scattering length a between the two-component fermions and different temperature T; see legend.

noninteracting Fermi gas that couples with the impurity, and the $\downarrow$ component being simply a spectator. These results agree with previous studies for both zero and finite temperature [9].

At $k_F a = 0$ and $T = 0$, the asymptotic behavior of $|S(t)|$ at large t exhibits a power-law decay $|S(t)| \sim t^{-\alpha}$, reflecting Anderson's OC and x-ray infrared singularity $\epsilon^{\alpha-1}$ at the low-energy scale set by the inverse time $\epsilon \sim \hbar/t$ [3,9,48]. In contrast, in the presence of a pairing gap $\Delta \neq 0$, $|S(t)| \sim t^0$ at $T = 0$, indicating OC is prevented as the low-energy scale is now cut by Δ [68]. At finite temperature, although both with or without the pairing gap, $|S(t)|$ shows an exponential decay at large t, such behavior appears at a much later time for finite Δ. In particular, for nonzero Δ the results at $T = 0$ and $T = 0.05 E_F/k_B$ are almost overlapping at $tE_F \leq 500$, showing that the pairing gap can also protect the response signal against thermal fluctuation if $k_B T \ll \Delta$.

More quantitatively, at nonzero pairing gap we have the following analytic result,

$$S(t \to \infty) \simeq \begin{cases} D_a e^{-iE_a t}, & a_\uparrow < 0, \\ D_a e^{-iE_a t} + D_r e^{-iE_r t}, & a_\uparrow > 0, \end{cases} \quad (3)$$

which fits excellently well to our numerical results, with D_a E_a, D_r, and E_r being fitting parameters. At small Δ, the coefficients $|D_a| \propto (\Delta/E_F)^{\alpha_a}$ and $|D_r| \propto (\Delta/E_F)^{\alpha_r}$, making the asymptotic form that agrees with the modification of the analytic expression of $S(t)$ for a noninteracting Fermi gas medium via replacing the low-energy cutoff $1/t \to \Delta$ [see, i.e., Eqs. (12) and (15) of Ref. [9]]. However, our numerical results indicate the power-law exponents α_r and α_a are close to but not exactly the same as the analytical results given in [9], see Ref. [66] for details. At $T = 0$, E_a is purely real and corresponds to the attractive polaron energy that satisfies $E_a = \sum_\nu n_{\nu\nu}(E_\nu - \tilde{E}_\nu)$, indicating that the attractive polaron can be regarded as the renormalization of the Fermi sea due to the impurity level. The repulsive polaron energy E_r is in general complex, where we denote the real and imaginary part as $\mathrm{Re}E_r$ and $\mathrm{Im}E_r$.

rf spectroscopy.—One of the key observations of this Letter is the saturation of $|S(t)|$ at large time, which implies a finite polaron quasiparticle residue $Z = |D_a| \propto \Delta^{\alpha_a}$. To check this, we calculate the frequency response $A(\omega)$ accurately with a Fourier transformation of $S(t)$. We choose a large cutoff $t^* \sim 500/E_F$, evaluate $S(t)$ numerically for $t < t^*$, and use the fitting formula in Eq. (3) for $t \geq t^*$. As shown in Fig. 3 by thick blue solid curves for zero-temperature results, the attractive polaron is characterized by a δ-function peak at E_a (with a small artificial width for visibility), unambiguously confirming the existence of a well-defined quasiparticle. The attractive polaron peak separates with a molecule-hole continuum by a region of anomalously low spectral weight, namely the "dark continuum." This spectral gap has previously been shown in
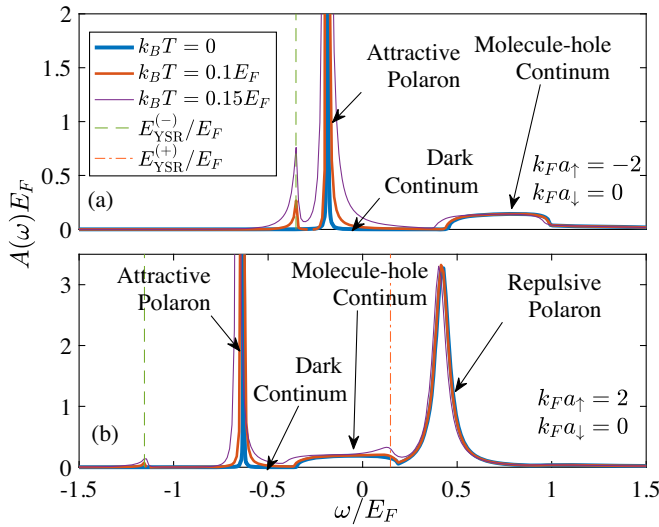
FIG. 3. The spectral function $A(\omega)$ at $k_F a = -2$ for different temperature (see legend) and different scattering length $a_\uparrow < 0$ in (a) and $a_\uparrow > 0$ in (b).

other polaron systems with approximate calculations, where the anomalously low spectral weight might be an artifact of the adopted approximations. Only recently, a diagrammatic Monte Carlo study indicates that this dark continuum might be indeed physical [35]. Here, the heavy polaron spectral function is calculated via FDA, and hence can be regarded as an exact proof of the dark continuum. For $a > 0$, a Lorentzian line shape with a peak at $\mathrm{Re}(E_r)$ corresponds to the repulsive polaron. The finite width determined by $\mathrm{Im}(E_r)$ implies that the repulsive polaron has a finite lifetime.

In Fig. 3, finite-temperature results are indicated by the red thin (purple thinner) curves for $k_B T = 0.1 E_F (0.15 E_F)$. Other than the expected thermal broadening, some additional surprising features show up. An enhancement of

spectral weight appears sharply at the energy $E_{\mathrm{YSR}}^{(-)} = E_a - (\Delta - E_{\mathrm{YSR}})$ below the attractive polaron. This spectral feature corresponds to the decay process highlighted by the purple arrow in Fig. 1(c), where an additional particle initially excited to the upper Fermi sea by thermal fluctuation is driven to the YSR state. For the case of $k_F a_\uparrow > 0$, a feature associated with the repulsive polaron appears at $E_{\mathrm{YSR}}^{(+)} = \mathrm{Re}(E_r) - (E_{\mathrm{YSR}} + \Delta)$, as indicated by the green arrow in Fig. 1(c): an additional particle decays from the YSR state to the lower Fermi sea. These features can be better observed in the whole spectrum of $a_\uparrow$ across a resonance, as shown in Fig. 4 for different temperatures. The YSR features are negligible at $k_B T = 0.05 E_F$, and the spectrum in Fig. 4(a) is almost the same as zero-temperature results. This shows the protection against finite temperature provided by the pairing gap. The YSR features become apparent in Fig. 4(b) at $k_B T = 0.15 E_F$ and shows broadening at $k_B T = 0.2 E_F$. We emphasize that this range of temperature is accessible for current experiments. The polaron spectrum can be applied to measure the superfluid gap Δ and E_{YSR}. In particular, we notice, on the positive side $a_\uparrow > 0$, if E_a, $\mathrm{Re}(E_r)$, $E_{\mathrm{YSR}}^{(-)}$, and $E_{\mathrm{YSR}}^{(+)}$ can all be measured accurately, we have $2\Delta = E_a + \mathrm{Re}(E_r) - E_{\mathrm{YSR}}^{(-)} - E_{\mathrm{YSR}}^{(+)}$ that does not depend on E_{YSR}. Since this formula only relies on the existence of the gap and a midgap state, we anticipate it can be used to measure Δ accurately for a Fermi superfluid that cannot be quantitatively described by the BCS theory.

Finally, we discuss briefly our observations for the case of a nonmagnetic impurity scattering with $a_\uparrow = a_\downarrow$, where the YSR features are absent as expected. Interestingly, we also discover that the repulsive polaron exhibits itself as a δ-function peak in the spectral function at zero temperature. We believe the underlying physics might be due to the gapless density fluctuations in the Fermi superfluid
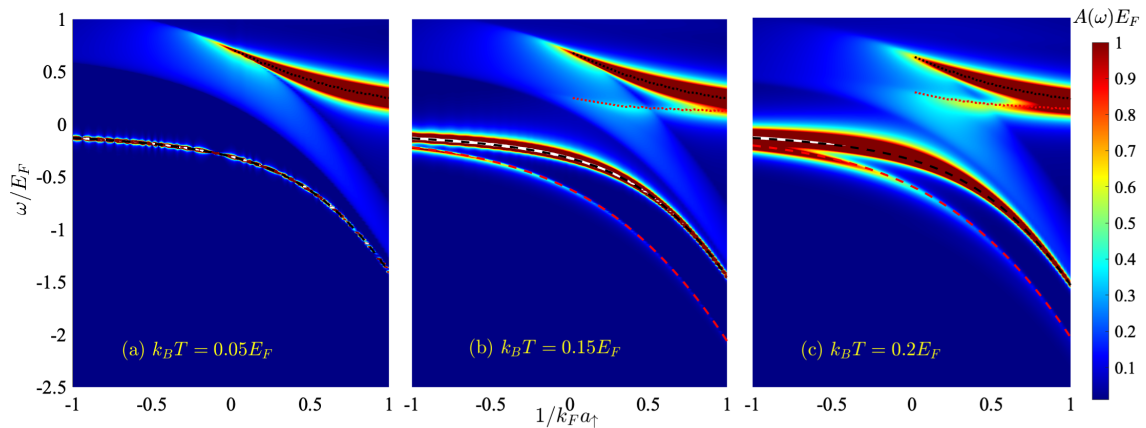

FIG. 4. The spectral function $A(\omega)$ at $k_F a = -2$ as a function of $a_\uparrow$ for different temperature: $k_B T = 0.05, 0.15, 0.2 E_F$ for (a), (b), and (c), respectively. The black dashed (dotted) curves show the attractive (repulsive) polaron energy and the red dashed (dotted) curves show $E_{\mathrm{YSR}}^{(+)}$ ($E_{\mathrm{YSR}}^{(-)}$) at finite temperature.

excited by the perfect balance of the two scattering lengths. As a result, the impurity couples to phonon excitations of the superfluid and forms a long-lived repulsive polaron. For more details, we refer to the companion paper [66].

Experimental realization.—Our predictions can be readily confirmed by immersing heavy ^{133}Cs impurities in a BCS Fermi superfluid of ^{6}Li atoms routinely observed near a broad Feshbach resonance $B_0 \simeq 832$ G. The two interspecies broad resonances located nearby at 843 and 889 G [69] allow us to independently control the ^{133}Cs-^{6}Li scattering lengths $a_{\uparrow,\downarrow}$. Both magnetic and nonmagnetic impurity scatterings can therefore be realized by tuning the magnetic field [66]. The finite mass effect should be negligible due to the large mass ratio [66]. Otherwise, one can also further suppress the finite mass effect by applying a deep optical lattice to localize the impurity [3,9].

Conclusions.—We have calculated the response functions of driving a heavy impurity in a BCS superfluid from noninteracting to interacting hyperfine states. Because of the existence of a pairing gap in the superfluid, the OC is prevented and genuine polaron quasiparticles exit. The underlying physical reason is apparent: exciting particle-hole pairs in this system requires an energy cost for Cooper-pair breaking, and hence multiple particle-hole excitations are energetic unfavored. We emphasize that our FDA can support this conclusion since it is essentially exact, unlike some approximations such as extended Chevy's ansatz [22,26] or T-matrix method [2,36] that allow only a few particle-hole excitations. In this respect, our calculation can be regarded as an exact theoretical model of polarons. Many features of the spectrum structure, such as the existence of a δ-function peak for the attractive polaron and a dark continuum, are rigorously confirmed to be universal. The pairing gap also protects the polaron against thermal fluctuation, preserving clear polaron features in response functions at a finite temperature $k_B T \sim \Delta$. Furthermore, we discover that the polaron spectrum can be applied to measure the background superfluid excitation spectrum, such as the pairing gap Δ. Interestingly, in the case of a magnetic impurity, the polaron spectrum at finite but low temperature has sharp features that can be used to measure the subgap YSR bound state. For nonmagnetic impurity, we predict the existence of a long-lived repulsive polaron.

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