Polarons in Ultracold Fermi Superfluids

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We study a new type of Fermi polaron induced by an impurity interacting with an ultracold Fermi superfluid. Due to the three-component nature of the system, we can make the polaron become trimer-like with a non-universal energy spectrum. We identify multiple avoided crossings between impurity- and trimer-like solutions in both the attractive and the repulsive polaron spectra. In particular, the widths of avoided crossings gradually increase as the Fermi superfluid undergoes a crossover from the BCS side towards the BEC side, which suggests instabilities towards three-body losses. Such losses can be reduced for interaction potentials with small effective ranges. We also demonstrate, using the second-order perturbation theory, that the mean-field evaluation of the fermion-impurity interaction energy is inadequate even for small fermion-impurity scattering lengths, due to the essential effects of Fermi superfluid and short-range physics in such a system. Our results are practically useful for cold atom experiments on mixtures.

Quasiparticles serve as the cornerstone of complex collective phenomena in interacting many-body systems. As an example, the polaron, an impurity dressed by particle-hole excitations from the environment, is a typical quasiparticle that has stimulated much interest in the study of solid-state and cold-atom systems with highly polarized components. In cold atoms, polarons have been successfully explored in both the attractive and the repulsive branches of impurities interacting with a Fermi sea of identical fermions \cite{14}. These studies are crucial for understanding the nature of normal states either against pairing physics in the case of strong attraction \cite{5,10}, or in the context of itinerant ferromagnetism with strong repulsion \cite{11,12}. However, much less is known about the fate of impurities immersed in a Fermi superfluid, where the impurity can be dressed by pairs of particles in the superfluid \cite{13}. Given the growing number of experiments on atomic mixtures, it becomes pressing to understand the fundamental physics of the underlying quasiparticles, such as polarons, in these systems.

Particularly, in the recent ENS experiment, a mixture of Bose and Fermi superfluids has been realized \cite{15}. The two superfluids not only coexist, but also interact with each other, constituting the most charming character of this system. How to characterize the interaction energy between these two superfluids, however, is still an open question. Exact three-body calculations show that, in the BEC limit of fermions, the interaction between a bosonic atom and a molecule of two fermions cannot be faithfully described by the mean-field theory, even when the boson-fermion scattering length is small \cite{16,17}. It then becomes essential to investigate the validity of the mean-field theory on the many-body level throughout the whole BCS-BEC crossover regime of fermions, and identify the underlying mechanism wherever it fails to apply. Here, we approach this goal via the study of polarons.

We use the variational approach to investigate the polaron physics when an impurity is immersed in a Fermi superfluid with tunable interactions. With a pairing superfluid as the background, the polaron wave function naturally acquires trimer-like terms which originate from the impurity-induced pair-breaking processes in the superfluid bath. As a result, the polaron spectrum is composed of both impurity- and trimer-dominated solutions. Due to the couplings inbetween, many avoided level crossings occur, whose widths depend sensitively on both the interaction strength and the effective range of the system. In particular, as fermions are tuned from the BCS to the BEC side, the widths of the avoided crossings gradually increase, which suggests instabilities towards three-body losses. On the contrary, the widths become narrower at smaller effective ranges, which can help stabilizing the system. For small fermion-impurity scattering lengths, the second-order perturbation theory captures the essential effects of Fermi superfluid and short-range physics in the system, and consequently shows the insufficiency of mean-field descriptions. These results rectify our understanding of interaction effects in multicomponent mixtures on the mean-field level, and provide guidance for maintaining stability from three-body losses in cold atom experiments on mixtures.

Polaron ansatz. We start from the Hamiltonian of our system $\mathcal{H} = H - \mu N_F$ ($N_F$ is the total number of fermions):\text{
\begin{equation}
\mathcal{H} = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \frac{g_{\text{f}}}{\sqrt{V}} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{q-k}\sigma}^\dagger a_{\mathbf{q-k'}\sigma} a_{\mathbf{k'}\sigma} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + \frac{g_{\text{f}}}{\sqrt{V}} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{q-k-k'}\sigma} a_{\mathbf{q-k}\sigma}^\dagger a_{\mathbf{q-k'}\sigma}^\dagger,
\end{equation}
where $a_{k\sigma}$ and $b_k$ are respectively the annihilation operators for the superfluid fermions and the impurity atom with the dispersion $\epsilon_k = k^2/(2m)$ ($h$ is taken to be unity); $\mu$ is the chemical potential of the two-species ($\sigma = \uparrow, \downarrow$) spin-balanced Fermi gas. $g_\text{ff}$ ($g_\text{fi}$) is the bare fermion-fermion (fermion-impurity) interaction, which is related to the scattering length $a_\text{ff}$ ($a_\text{fi}$) via the standard renormalization relation $1/g_\beta = m/(4\pi a_\beta) - 1/V \sum_k 1/(2\epsilon_k)$, where $V$ is the quantization volume and $\beta = \text{ff, fi}$. For simplicity, we only consider the case where the impurity has the same mass as that of a fermion, and interact equally with two fermion species. Our results can be straightforwardly generalized to cases with unequal masses or imbalanced interactions.

The Fermi superfluid at zero temperature can be described by the standard BCS wave function:

$$|\text{BCS}\rangle = \prod_k (u_k + v_k a_k^\dagger a_{-k}^\dagger)|\text{vac}\rangle \sim \prod_k \alpha_{-k\uparrow}\alpha_{k\uparrow}|\text{vac}\rangle.$$  \hfill (2)

Here, $\alpha_{k\sigma} = u_k a_{k\sigma} + \eta_\sigma v_k a_{-k\sigma}$ is the annihilation operator for the Bogoliubov quasiparticles, where $\eta_\uparrow = -\eta_\downarrow = 1$, $u_k = (\sqrt{E_k + \epsilon_k - \mu})/(2E_k)$, and $v_k = \sqrt{1 - u_k^2}$; the corresponding quasiparticle energy $E_k = \sqrt{(\epsilon_k - \mu)^2 + \Delta^2}$ with $\Delta$ the pairing order parameter.

To depict the impurity-induced polaron excitations in a Fermi superfluid, we adopt the following ansatz:

$$|P\rangle_Q = \left(\psi_{Q}^b b_k^\dagger + \sum_{kk'} \psi_{kk'} b_k^\dagger|Q-k\rangle \alpha_{k\uparrow}^\dagger a_{-k\uparrow}^\dagger\right)|\text{BCS}\rangle,$$  \hfill (3)

where $Q$ indicates the center-of-mass momentum of the polaron. The second term in the bracket, which effectively describes impurity-induced pair breaking in the superfluid and is therefore trimer-like, includes contributions from excitations like $a_{k\uparrow}^\dagger a_{-k\uparrow}^\dagger$, $a_{k\downarrow}^\dagger a_{-k\downarrow}^\dagger$, $a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger$ or $a_{-k\uparrow}^\dagger a_{k\downarrow}^\dagger$. The existence of trimer-like terms in polaron wave functions is unique for a pairing-superfluid background, which significantly affects the polaron spectra as shown below. Note that here we only keep excitations to the lowest order, as they have been shown to be adequate to provide quantitatively accurate results in polarized Fermi systems when compared with results from quantum Monte Carlo studies [6,10].

**Polaron spectrum and residue.** The polaron energy $E_p$ and the coefficients in ansatz (3) can be obtained by enforcing the Schrödinger’s equation:

$$\mathcal{K}|P\rangle_Q = (E_p + E_{\text{BCS}})|P\rangle_Q,$$  \hfill (4)

where $E_{\text{BCS}}$ is the energy of superfluid fermions based on Eq. (2). Introducing three auxiliary variables: $A_k = g_\text{fi}(v_k\psi_Q + \sum_{k'} v_{k'}\psi_{kk'})$, $B_k = g_\text{fi}(v_k\psi_Q + \sum_{k'} u_{k'}\psi_{kk'})$ and $C_k = g_\text{fi} \sum_{k'} \psi_{k-k'} u_{k'}\psi_{k'}$, while noting $A_k = B_k$ due to the spin-independent fermion-impurity interaction, we arrive at two sets of equations [20]:

$$\begin{align*}
\left(\frac{V}{g_\text{fi}} - \sum_{k'} \frac{u_{k'}^2}{A_{kk'}}\right) A_k &= \sum_{k'} \frac{2v_{k'}v_k A_{k'}}{E_p - \epsilon_Q - \frac{u_k u_{k'} A_{k'}}{A_{kk'}} + \frac{u_k u_{k'}^2 C_{k+k'}}{A_{kk'}}}; \\
\left(\frac{V}{g_\text{fi}} - \sum_{k'} \frac{u_{k'}^2 u_{k-k'}}{A_{kk'}-k-k'}\right) C_k &= \sum_{k'} \frac{2u_{k'}^2 u_k A_{k'}}{A_{kk'}-k-k'}.
\end{align*}$$  \hfill (5, 6)

with $A_{k,k'} = E_p - \epsilon_Q - k - k' - E_k - E_{k'}$. $E_p$ and variables $A_k, C_k$ can then be numerically solved by imposing a certain momentum cutoff $k_c$. Physically, $k_c$ corresponds to setting a finite effective range $r_0 \sim 1/k_c$ in the two-body collision. The coefficients in ansatz (3) can be easily deduced from the Schrödinger’s equation (4), which gives the polaron residue [18]:

$$Z = \frac{\psi_{Q}^2}{\psi_{Q}^2 + \sum_{kk'} \psi_{kk'}^2}.$$  \hfill (7)

Apparently, the polaron residue $Z \sim 1$ ($Z \sim 0$) when the system is impurity (trimer) dominated. In the rest of the work, we will focus on polarons in the $Q = 0$ sector.

By explicitly solving Eqs. (5,6), we get the typical polaron spectrum for a unitary Fermi superfluid (see Fig. 1(a)). The spectrum exhibits many avoided level crossings between impurity- and trimer-dominated solutions, which are also apparent in the residue plots in Fig. 1(b1, b2). Particularly, a wide avoided crossing exists between the two lowest branches at $(k_F a_\text{fi})^{-1} \sim 3$, where $k_F$ is the Fermi momentum of a non-interacting Fermi gas with the same number density as the Fermi superfluid. When $a_\text{fi}^{-1}$ is tuned through the avoided crossing, the wave function continuously evolves from impurity dominated ($Z \sim 1$) to trimer dominated ($Z \sim 0$) in the lowest branch [19]. Similar atom-trimer crossover has been reported for the ground state of a two-channel model in Ref. [14], where equal fermion-fermion and fermion-impurity interactions are considered. A polaron to molecule transition [9,10,14] can also occur within the second lowest branch of our system, when the fermion-impurity interaction is tuned towards the BEC limit [20].

Compared to the two lowest branches, the higher branches at positive $a_\text{fi}$ in Fig. 1(a) show more interesting properties, as multiple avoided crossings occur with widths tunable by $a_\text{fi}$. At small $a_\text{fi}$, the avoided crossings are very narrow, which allows us to identify a repulsive atomic branch by following the trajectory of the impurity-dominated solutions ($Z \sim 1$) while $a_\text{fi}$ varies. The energy of the repulsive branch increases with $a_\text{fi}$, while the width of avoided crossings becomes broader due to the enhanced coupling between the impurity and the trimer terms in Eq. (3). This repulsive branch eventually runs into a dense spectrum of trimer-dominated solutions.
Perturbative Corrections. To gain further insights into the polaron state, we apply the second-order perturbation theory at small \(|a_\parallel|\) \[20\]. Intuitively, up to \(a_\parallel^2\), the perturbative energy caused by the fermion-impurity scattering can be written as:

\[
E_{PT} = \frac{4\pi a_\parallel \rho}{m} + 2\left(\frac{4\pi a_\parallel}{mV}\right)^2 \sum_{kq} \left[ v_q^2 \left( \frac{1}{2\epsilon_k} - \frac{u_k^2}{\epsilon_{-q-k} + E_q + E_k} \right) - \frac{u_k v_k u_q v_q}{\epsilon_{-q-k} + E_q + E_k} \right] \tag{8}
\]

Here, the first term is the mean-field contribution, with \(\rho\) the total density of fermions; while the second term accounts for the intermediate scatterings processes shown in Fig. 2(a). Eq. (8) can be continuously reduced to the case of non-interacting fermions \[10\] with decreasing fermion-fermion interaction. However, for a unitary Fermi superfluid, \(E_{PT}\) is well above the polaron energy \(E_\rho\) even at relatively small \(|a_\parallel|\) (see Fig. 1(a)). This can be attributed to the effects of intermediate fermion-fermion scatterings, as shown diagrammatically in Fig. 2(b). The sum of all relevant diagrams gives an additional energy correction up to the order of \(a_\parallel^3\):

\[
E_{PT}' = 2\left(\frac{4\pi a_\parallel}{mV}\right)^2 \sum_{k,q,k'} \frac{(u_k v_q + u_q v_k) T_{k,q,k',k+q-k'}(u_{k'} v_{k+q-k'} + v_{k'} u_{k+q-k'})}{(\epsilon_{-q-k} + E_k + E_q)(\epsilon_{-q-k} + E_{k'} + E_{k+q-k'})} \tag{9}
\]

As shown in Fig. 1(a), the inclusion of \(E_{PT}'\) considerably lowers the perturbative energy based on Eq. (8). The remaining discrepancy is attributed to higher-order scattering processes beyond the diagrams in Fig. 2.

The second-order perturbation results reveal several remarkable properties of polarons in the presence of pairing superfluid. First, through the inclusion of \(E_{PT}'\) (Eq. (9)) and \(u_k, v_k, E_k\) (Eqs. (8)(9)), the second-order terms rely crucially on the interaction between fermions. Thus, sweeping the Fermi superfluid across the resonance is ex-
Although the Pauli principle. Accordingly, more impurity-induced excitations emerge in the Fermi superfluid, which effectively enhances the impurity-trimer coupling in Eq. (3).

In addition, from Fig. 3(b,d) one can see increasing deviations from the perturbative results when the fermions are tuned from the BCS to the BEC side. This suggests that a strong Fermi superfluid can dramatically affect the polaron spectra through higher-order scattering processes, which are beyond the ones shown in Fig. 2.

Effect of effective range. As the effective range ($r_0$) corresponds to the inverse of the cutoff momentum ($k_c$) in our formalism, its effect can be studied by changing $k_c$ in numerical simulations of Eqs. (5,6). In Fig. 4 we show the polaron spectra for two different $k_c$, where Fig. 4(a) and (b) are respectively for the lower and the higher branches. A common feature is that for larger $k_c$, or smaller $r_0$, the avoided crossings move towards weaker fermion-impurity interactions, i.e., towards smaller $|a_{fi}|$. Accordingly, the coupling between impurity- and trimer-dominated solutions also becomes smaller, which naturally leads to narrower avoided crossings. In practice, these results suggest that a system with a smaller $r_0$ can be more stable, as a narrower crossing with trimer-dominated solutions makes the decay into deep trimers less likely.

Conclusion and final remark. We have studied the polaron excitations when an impurity is interacting with a Fermi superfluid. In particular, we show the importance of higher-order scattering processes caused by the superfluid fermions in evaluating the polaron energy. Consequently, the mean-field description of polars becomes inadequate even for small fermion-impurity scattering lengths, especially when the fermions are tuned across resonance to the BEC side. These results suggest that in a mixture system with multiple interaction channels, the interplay between these channels can produce intriguing interaction effects. This poses new challenges on the theoretical treatment of these systems beyond the mean-field or perturbative approaches. Moreover, our work shows that the impurity-trimer coupling can be greatly enhanced by increasing the fermion-fermion and fermion-impurity interaction strengths or by decreasing the effective range, which all lead to broader avoided level crossings. Our results can therefore serve as a guideline to
reduce three-body losses and maintain the stability of mixture systems in cold-atom experiments.

Finally, we note that our polaron ansatz does not apply in the deep BEC regime of fermions, where the dominant excitations should be Bogoliubov phonons above a molecular BEC. This regime can be effectively modeled by a polaron on top of a BEC [21, 22], with impurity-boson and boson-boson scattering lengths given by three-body [16, 17] and four-body [29] solutions, respectively.

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[18] The residue here refers to the weight of bare impurity term in the background of the ground state Fermi superfluid. Thus, it does not include the excitation term with \( k + k' = 0 \), though the impurity still stays at initial momentum \( Q \).
[19] Close to \((k_F a_0)^{-1} \sim -4\), an avoided crossing exists between the second lowest and the third lowest branch. This is why the residue \( Z \) in the second lowest branch does not immediately go to small value (\( \sim 0 \)) beyond the avoided crossing with the lowest branch (see Fig. [b1]).
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Supplemental Materials

In this Supplemental Materials, we provide more details on the derivations of closed equations, the perturbative corrections, and the polaron to molecule transition.

Derivation of the Polaron Equations

We adopt the polaron ansatz:

$$ |P⟩_Q = ψ_Q b_0^† |BCS⟩ + \sum_{kk'} ψ_{kk'} b_{k'-k}^† a_{kk'}^† |BCS⟩, \quad (S1) $$

where the annihilation operator for the Bogoliubov quasiparticles $a_{kk'}$ is defined via:

$$ a_{kk'}^+ = u_k a_{kk'} + v_k a_{-k,k'}, \quad (S2) $$

and we have assumed the coefficients $u_k, v_k$ to be real. According to standard BCS theory, we have

$$ ⟨BCS⟩ \sim \prod_k (u_k + v_k c_k^† c_{-k}) |vac⟩ \sim \prod_k ψ_{kk'}^†, \quad (S3) $$

with $E_{BCS} = \sum_k (ε_k - μ) + \sum_k Δ^2/(2E_k)$, and $E_k = \sqrt{(ε_k - μ)^2 + Δ^2}$. For the excited state $|e_k⟩ = a_{kk'}^† |BCS⟩$, the energy is given by $⟨e_k |K| e_k⟩ = E_{BCS} + E_k$, where $K = H - μN$ is given in the main text.

Given the trial wave function and the Hamiltonian, we can get the ground state solution by minimizing $E_p = ⟨P|K|P⟩ - E_{BCS}$. Note that it is convenient to express the fermion-fermion interaction term in $K$ in terms of the scattering between different quasiparticle states: $k, q - k → k', q - k'$. Since in the large-$k$ limit, $u_k \to 1, v_k \to 0$, only one term has finite contribution to the energy:

$$ g_{ff} = \frac{1}{V} \sum_{q,k,k'} u_q u_{q-k} v_{q-k'} u_{k'} a_{kk'}^† a_{q-k,1} a_{q-k',1} a_{k,1}^†. \quad (S4) $$

Finally, we have the equations:

$$ (E_p - ε_Q)ψ_Q = g_{ff} \left( 2 \sum_k |v_k|^2 ψ_Q + \sum_{kk'} v_k u_{k'} ψ_{kk'} + \sum_{kk'}^\prime u_k v_{k'} ψ_{kk'} \right) \quad (S5) $$

$$ A_{kk'} ψ_{kk'} = g_{ff} \left( u_k' \sum_{k'''} u_{k'''} a_{kk'''}^† a_{kk'} - v_k \sum_{k''} u_{k''} a_{kk''}^† a_{kk'} + v_k \sum_{k''} u_{k''} a_{kk''}^† a_{kk'} - v_k' \sum_{k''} v_{k''} a_{kk''}^† a_{kk'} + ψ_{kk'}^† \sum_{q,k,k'} u_q u_{q-k} v_{q-k'} u_{k'} a_{kk'}^† + v_{k'} u_{k'} ψ_Q + u_k v_{k'} ψ_Q \right) $$

$$ \quad + g_{ff} \sum_{k''} ψ_{kk'', k+k'-k''} u_{k''} u_{k+k'-k''}. \quad (S6) $$

As $g_β$ ($β = ff, fi$) would become vanishingly small after renormalization, terms including $g_β \sum_k v_k ...$, where $v_k \sim 1/k^4$ at large momentum $k$, should also vanish. We therefore neglect terms including $g_β \sum_k v_k ...$, and define:

$$ A_k = g_{ff} (v_k ψ_Q + \sum_{k'} u_{k'} ψ_{kk'}); \quad (S7) $$

$$ B_k = g_{ff} (v_k ψ_Q + \sum_{k'} u_{k'} ψ_{kk}); \quad (S8) $$

$$ C_k = g_{ff} \sum_{k'} ψ_{k', k-k'} u_{k'} u_{k-k'} \quad (S9) $$

We then have:

$$ (E_p - ε_Q)ψ_Q = \frac{1}{V} \sum_k v_k (A_k + B_k); \quad (S10) $$

$$ A_{kk'} ψ_{kk'} = \frac{1}{V} (u_{k'} A_k + u_k B_k' + u_{k'} u_{k-k'} C_{k+k'}). \quad (S11) $$
where \( A_{kk'} = E_p - E_k - E_{k'} - \epsilon_{k-k'} \). From these two equations, we can get \( \psi_Q \) and \( \psi_{kk'} \) in terms of \( A_k, B_k, C_k \), which, when plugged into Eqs. (S17, S8, S9), yield a set of three closed equations:

\[
\begin{align*}
\left( \frac{V}{g_{fi}} - \sum_{k'} \frac{|u_k|^2}{A_{kk'}} \right) A_k &= \sum_{k'} \left[ \frac{v_k v_{k'} (A_{kk'} + B_{kk'})}{E_p - E_Q} + \frac{u_k u_{k'}}{A_{kk'}} + \frac{u_k |u_k|^2 C_{kk'}}{A_{kk'}} \right]; \\
\left( \frac{V}{g_{fi}} - \sum_{k'} \frac{|u_k|^2}{A_{kk'}} \right) B_k &= \sum_{k'} \left[ \frac{v_k v_{k'} (A_{kk'} + B_{kk'})}{E_p - E_Q} + \frac{u_k u_{k'}}{A_{kk'}} + \frac{u_k |u_k|^2 C_{kk'}}{A_{kk'}} \right]; \\
\left( \frac{V}{g_{fi}} - \sum_{k'} \frac{|u_k|^2 |u_{k-k'}|^2}{A_{kk',k-k'}} \right) C_k &= \sum_{k'} \left[ \frac{|u_{k-k'}|^2 u_k A_{kk'}}{A_{kk',k-k'}} + \frac{|u_{k'}|^2 u_{k-k'} B_{k-k'}}{A_{kk',k-k'}} \right].
\end{align*}
\]  

Physically, as we only consider the case of spin-independent impurity-fermion interactions, we expect \( A_k = B_k \), \( \psi_{kk'} = \psi_{k'k} \). The above three equations can then be reduced to two. We have numerically checked that this is the case.

**Perturbative approach**

For weak fermion-impurity interactions (small \( |a_{fi}| \)), it is tempting to analytically expand the polaron energy \( E_p \) based on the 2nd-order perturbation theory. Neglecting scattering between the Bogoliubov quasiparticles, we have

\[
E_{PT} = E_{PT}^{(1)} + E_{PT}^{(2)} = 2 \frac{g_{fi}^2}{V} \sum_k u_k^2 \left[ q < k_F \right] - \frac{4 \pi a_{fi}^2}{m V} \frac{1}{(2 \epsilon_k)^2} \sum_{q < k_F} \frac{1}{2 \epsilon_k} + \ldots
\]

Using RG equation \( 1/g_\beta = m/(4 \pi a_\beta) - 1/V \sum_k 1/(2 \epsilon_k) \), we can expand

\[
g_\beta = \frac{4 \pi a_\beta}{m} + \left( \frac{4 \pi a_\beta}{m} \right)^2 \frac{1}{V} \sum_k \frac{1}{2 \epsilon_k} + \ldots
\]

Plugging the expression above into Eq. (S15), we get the expression of \( E_{PT} \) as Eq. (8) in the main text.

Eq. (8) in the main text can be smoothly reduced to the non-interacting Fermi-Sea case. In this case, \( v_k = 1 \) if \( k < k_F \) and \( v_k = 0 \) otherwise; \( u_k = 1 \) if \( k > k_F \) and \( u_k = 0 \) otherwise; \( E_k = |\epsilon_k - E_F| \). Then we have

\[
E_{PT} = \frac{8 \pi a_{fi}}{m V} \sum_{k < k_F} 1 + 2 \frac{4 \pi}{m V} a_{fi}^2 \sum_{q < k_F} \left( \sum_{k} \frac{1}{2 \epsilon_k} - \sum_{k > k_F} \frac{1}{2 \epsilon_k} \right).
\]

The result was shown previously in Ref. 11 in the main text.

However, as we have analyzed in the main text, the effects of high-order scattering between the quasiparticles cannot be neglected. To see this, we perform the diagram summation illustrated in Fig. 2(b) of the main text to include the effects of the fermion-fermion interactions into the second-order perturbation, and get the expression of Eq. (9) in the main text.

It is worthwhile to study how the second-order terms in Eqs. (8,9) of the main text depend on the momentum cutoff \( k_c \). As illustrated in Fig. 3, both second-order terms in Eqs. (8,9) scale logarithmically with \( k_c \). This log-scaling indicates that the polaron energy is generically non-universal. Moreover, it tells us that the mean-field evaluation is far from sufficient to predict the full polaron energy, where the higher-order terms (in \( |a_{fi}|^n \), \( n \geq 2 \)) also play essential roles due to the ultraviolet divergence of the summed contributions.

The polaron residue \( Z \) can also be estimated based on first-order (in \( |a_{fi}| \)) wave functions derived from the perturbation theory

\[
\psi_Q \approx 1
\]

\[
\psi_{kk'} \approx \frac{4 \pi a_{fi}}{m V} \left( \frac{u_{kk'} v_k + u_{kk} v_{k'}}{\xi_{kk'}} + \frac{u_k u_{k'} \sum_{k''} u_{k-k''} u_{k''} (v_{k-k''} v_{k''} + v_{k-k'} v_{k'-k''} u_{k''})}{\xi_{kk''}} \right) \frac{V}{4 \pi a_{fi}} - \sum_k \frac{1}{2 \epsilon_k} - \sum_{k'} \frac{u_k u_{k'} |u_{k-k'}|^2}{\xi_{kk',k-k'}}
\]

with \( \xi_{kk'} = - (\epsilon_{k-k'} + E_k + E_{k'}) \). One may then plug these expressions of \( Z \) in the main text to calculate the polaron residue based on perturbed wave functions, as shown in Fig. 1(b1,b2) of the main text.
Impurity-induced two-body states

The general variational wave function for a two-body state involving the impurity atom can be written as:

$$|M\rangle_Q = \sum_k \left( \varphi_{k\uparrow}^\dagger b_{Q-k\uparrow} + \varphi_{k\downarrow} b_{Q-k\downarrow} \right) |BCS\rangle.$$  \hfill (S20)

In the case of a spin-independent fermion-impurity interaction, the bound state wave functions $\varphi_{k\uparrow}$ and $\varphi_{k\downarrow}$ are decoupled. There is then simply a two-fold degeneracy in the two-body sector. We therefore write the ansatz as:

$$|M\rangle_Q = \sum_k \varphi_{k\uparrow}^\dagger b_{Q-k\uparrow} |BCS\rangle.$$  \hfill (S21)

From the Schrödinger’s equation, the wave functions $\varphi_{k\uparrow}$ should satisfy

$$E \varphi_{k\uparrow} = \epsilon_{Q-k-k\uparrow} + E_k \varphi_{k\uparrow} + \frac{g_{fi}}{V} \left( u_k \sum_{k'} u_{k'} \varphi_{k'\uparrow} - v_k \sum_{k'} v_{k'} \varphi_{k'\downarrow} + 2 \sum_{k'} |v_{k'}|^2 \varphi_{k'} \right),$$  \hfill (S22)

where the last term is the Hartree term. As the Hartree terms here only serve to shift the molecular energy by a vanishingly small amount after renormalization, they are not important for the two-body bound states. Similarly, we may drop the term $g_{fi} v_k \sum_{k'} v_{k'} \varphi_{k'\downarrow}$. This leads to the equation in the two-body bound state sector:

$$\frac{V}{g_{fi}} = \sum_k \frac{|u_k|^2}{E_m - \epsilon_{Q-k} - E_k}.$$  \hfill (S23)

With the zero energy reference chosen to be the BCS ground state energy, the two-body bound state threshold $E_{th}$ in this sector is the quasi-particle excitation gap: $E_{th} = \Delta$ when $\mu > 0$ and $E_{th} = \sqrt{\Delta^2 + \mu^2}$ when $\mu < 0$. In Fig. S2(a), we show the lowest two branches of the polaron energy and the molecular energy relative to the threshold. While there are no polaron to molecule transitions in the lowest branch, which undergoes an impurity-trimer crossover before crossing with the molecular branch, there are two polaron to molecule transitions in the second-lowest branch. With increasing $k_c$, the two transition points will move towards the BCS and the BEC limit, respectively.

Similar picture for the polaron to molecule transition holds when we consider the special case where $g_{fi} = g_{fi}$, i.e., the fermion-fermion interaction and the fermion-impurity interaction are equal. As shown in Fig. S2(b), with an appropriately chosen cutoff momentum, the avoided crossing between the lowest two branches in the polaron spectrum is very narrow. If one starts from the ground state in the BCS limit and tune the interaction strength $a_s = a_{ff} = a_{fi}$ fast enough, the system would not end up in the trimer-like branch beyond the avoided crossing. In this case, there will be a polaron to molecule transition on the BEC side of the resonance, at which point the ground state of the system undergoes a first-order transition from the non-universal polaron-like state into a universal molecular state.
FIG. S2: (Color Online) (a) Polaron to molecule transition in the $Q = 0$ sector. The solid and the dashed lines correspond to the lowest two branches of the polaron energy, while the dash-dotted curve is the molecular energy relative to the molecular threshold. The fermion-fermion interaction is at resonance ($a_{ff} = \infty$). Cutoff momentum is chosen to be $k_c = 10k_F$, and the unit of energy is $E_F$. (b) Polaron to molecule transition for the case of $a_s = a_{ff} = a_{fi}$, with $k_c = 15k_F$. 