Fermi polaron revisited: polaron-molecule transition and coexistence

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We revisit the polaron-molecule transition in three-dimensional (3D) fermion systems using the well-established variational approach. It is found that the molecule is in fact an asymptotic limit of a finite-momentum polaron in the strong coupling regime, which can be continuously connected to the weak coupling polaronic state in the same momentum sector. The polaron-molecule transition can therefore be reinterpreted as a first-order transition between Fermi polarons with different momenta. Within certain interaction window near their transition, both states appear as local minima in the dispersion curve, indicating they can coexist in a realistic system. We have further confirmed the polaron-molecule coexistence in the presence of a finite impurity concentration and at low temperature, which directly leads to a smooth polaron-molecule transition as observed in recent experiments of 3D ultracold Fermi gases. Our results have provided an unambiguous physical picture for the competition and conversion between polaron and molecule, and also shed light on Fermi polaron properties in low dimensions.

\textbf{Introduction}. Fermi polaron is a quasi-particle describing an impurity dressed by surrounding fermions. In recent years it has attracted great attention and also been successfully realized in the field of ultracold gases\cite{1–8}, thanks to the high controllability of spin numbers and interaction strength. Nearby a Feshbach resonance, the Fermi polaron exhibits an attractive lower branch \cite{9–20} and a repulsive upper branch \cite{21–25}. These two branches are crucially important for understanding, respectively, the stability of fermion superfluidity and itinerant ferromagnetism in the high polarization limit of fermion system.

Despite the extensive investigations on Fermi polarons, there still exist unsettled issues that need to be addressed. In particular, one key question is whether there is a polaron-molecule transition in the attractive Fermi polaron. Many theories have predicted a first-order transition between a polaronic state (impurity dressed by many fermions surrounded) and a molecular state (impurity bound with one fermion on top of Fermi sea) as the attraction increases in both three-dimension(3D)\cite{13–18} and two-dimension(2D)\cite{19,20}, while a distinctive claim of a smooth polaron-molecule crossover was also proposed based on wave-function argument\cite{26}. In the experimental side, previous studies in 3D\cite{1} and 2D\cite{5} have reported the polaron-molecule transition with a continuous zero-crossing of quasi-particle residue $Z$, instead of a sudden jump of $Z$ associated with a first-order transition. Furthermore, a very recent experiment of a 3D Fermi gas\cite{8} has observed a smooth evolution of various physical quantities from weak to strong coupling regime, and also pointed to a coexistence between polaron and molecules nearby their transition. These features cannot be fully explained by the trap inhomogeneity, thus requiring further exploration of the physics behind.

To address above issues, in this work we revisit the polaron problem in 3D fermion systems using the well-established variational approach\cite{9,11,12,14,15,18–21,24}. The main contributions are in three fold:

(1) The molecule is found to be an asymptotic limit of polaron state in the strong coupling regime with finite momentum $Q = k_F$ ($k_F$ is the Fermi momentum of majority fermions). By switching the interaction strength, the molecule can be continuously connected to the weak coupling polaronic state ($Q = k_F$ sector) with large quasi-particle residue. Therefore, the literally called polaron-molecule transition can be reinterpreted as a first-order transition between Fermi polarons with different momenta $Q = 0$ and $Q = k_F$. This observation naturally resolves the theoretical debate in literature on the existence of polaron-molecule transition.

(2) Within certain interaction window near their transition, the two $Q$-states are found to appear simultaneously as local minima in the dispersion curve. This provides the underlying mechanism for polaron-molecule coexistence in realistic systems.

(3) Taking the realistic condition in experiment with a finite impurity concentration and at low temperature, we have confirmed the polaron-molecule coexistence and reproduced a smooth evolution of all physical quantities as measured in Ref.\cite{8}. This provides an intrinsic reason for the smooth polaron-molecule transition as observed in 3D Fermi gases\cite{1,8}, and also sheds light on similar phenomenon in 2D system\cite{5}.

\textbf{Model}. We consider the following Hamiltonian for the 3D Fermi gases with contact interaction:

\begin{equation}
H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{Q,\mathbf{k},\mathbf{k}'} U_{Q,\mathbf{k},\mathbf{k}'} c_{\mathbf{Q}-\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\downarrow} c_{\mathbf{k}'\downarrow}^{\dagger} c_{\mathbf{Q}-\mathbf{k}'\uparrow} \tag{1}
\end{equation}

Here $c_{\mathbf{k}\sigma}^{\dagger}$ is the creation operator of spin-$\sigma$($\uparrow, \downarrow$) fermion with momentum $\mathbf{k}$ and energy $\epsilon_{\mathbf{k}} = \mathbf{k}^2/(2m)$; $U$ is the bare interaction that can be connected to the s-wave scat-
tering length $a_s$ via $1/U = m/(4\pi a_s) - 1/V \sum_k m/k^2$. For brevity we will take $\hbar = 1$ throughout the paper.

From now on, we choose spin-up as majority fermions and spin-down as minority impurities. For a single ↓-impurity immersed in the Fermi sea of ↑-atoms with number $N$, based on the variational approach\cite{9, 11, 12, 14, 15, 18–21, 24} we write down a general ansatz for the polaron state with total momentum $Q$:

$$|P(Q)\rangle = \left(\phi_0 c_{Q,\uparrow} + \sum_{k,q} \phi_{k,q} c_{Q+q-k,\uparrow} c_{k,\downarrow} + \ldots\right) |FS\rangle_N;$$

and the molecule state:

$$|M(0)\rangle = \left(\sum_{k} \psi_k c_{-k,\downarrow} c_{k,\uparrow} + \ldots\right) |FS\rangle_{N-1}. (3)$$

Here $\sum'$ refers to summation under $|k| > k_F$ and $|q| \leq k_F$ ($k_F$ the Fermi momentum of spin-up, which sets the Fermi energy $E_F = k_F^2/(2m)$); “…” refers to terms with higher-order particle-hole excitations, which are neglected in this work in view of their destructive interference for the attractive branch\cite{13–18}. The impact of these higher-order excitations will be discussed later.

The two ansatz above give rise to very different pictures for the impurity state: (2) describes a fermionic quasi-particle where the impurity is dressed by majority fermions with particle-hole excitations, while (3) represents a bosonic molecule where the impurity is bound with a single fermion on top of the Fermi sea. Given such distinct features and an energy crossing of according states, many theories have predicted a first-order transition for this single-impurity problem. Due to the rotational invariance of $Q$ in $|P(Q)\rangle$, we choose a specific case with $Q = Q e_z$.

By directly comparing (2) and (3), one can see that if set $Q = k_F$, $\phi_0 = 0$ and $\phi_{k,q} = \delta_{q=-Q}\phi_k$, then (2) exactly reduces to (3). In other words, the molecule state corresponds to only considering a particular type of particle-hole excitation in the polaron state $P(Q)$ with $Q \equiv |Q| = k_F$, which will be denoted as $|P(k_F)\rangle$ for short. For this particular excitation, the hole sits right at Fermi surface and points opposite to $Q$. However, this type of excitation is not self-closed even in the lowest particle-hole excitation subspace. As shown in Fig.1, it can scatter back to the bare impurity at $Q$ together with an unperturbed Fermi sea, and then couple to other particle-hole excitations with holes covering all other momenta inside the Fermi sea\cite{27}. These couplings will generate a lower variational energy, and thus $|P(k_F)\rangle$ is always energetically more favorable than $|M(0)\rangle$. Nevertheless, we will show that the significance to introduce $|M(0)\rangle$ lies in that it is the asymptotic limit of $|P(k_F)\rangle$ in the strong coupling regime.

To demonstrate this, we study the quasi-particle residue of $|P(k_F)\rangle$, $Z(k_F)$, which follows

$$Z(k_F)^{-1} = 1 + \sum_{k,q} |\phi_{k,q}|^2/|\phi_0|^2 = 1 + \int_0^1 (q/k_F) \int_{-1}^1 (d(q/k_F)f(q/k_F, \cos \theta_q). (4)$$

As shown in Fig.2(a), $Z(k_F)$ continuously decreases from unity to nearly zero as the interaction strength increases from weak coupling to $1/(k_F a_s) \sim 0.8$. This behavior can be traced back to the rapid increase of molecular weight compared to the bare one in $|P(k_F)\rangle$, as given by $f(1, -1)$ in Eq.4 and shown in the inset of Fig.2(a)). These fea-
tures indicates a smooth crossover between a polaronic state in $Q = k_F$ sector to a molecular state as the interaction strength increases. The polaron to molecule crossover is further confirmed by examining the energies of $|P(k_F)|$ and $|M(0)|$, denoted respectively as $E(k_F)$ and $E_M$, in Fig.2(b). Despite a clear deviation at the weak and intermediate couplings, the two energies get closer when the interaction is tuned across resonance, and finally merge together for $1/(k_F a_s) \gtrsim 0.8$. In this strong coupling regime, the molecule $|M(0)|$ can be justified as a good approximation of the full $|P(k_F)|$.

A physical picture to understand above crossover is as follows. In the weak coupling limit, a free impurity plus an unperturbed Fermi sea (bare term in (2)) dominates the polaron $|P(k_F)|$, while the molecule $|M(0)|$ is extremely unstable due to the coupling to bare term and further to other particle-hole states, as illustrated in Fig.1. Such coupling leads to an obvious deviation between the energies $E(k_F)$ and $E_M$. However, as increasing the attraction, more weight transits from the bare term to particle-hole excitations in $|P(k_F)|$, leading to a reduced $Z(k_F)$; meanwhile, the coupling effect between $|M(0)|$ and the other states becomes less significant due to the reduced weight of bare term. Finally, in the strong coupling regime with $Z(k_F) \sim 0$, the coupling effect is negligible, and $|M(0)|$ becomes nearly independent from the other hole excitations (these hole states are all energetically unfavorable as compared to $|M(0)|$). In this limit, $|M(0)|$ can well approximate $|P(k_F)|$ and $E_M$ becomes identical to $E(k_F)$. We note that the resemblance between molecule and finite-$Q$ polaron in strong coupling limit was pointed out previously in the multi-channel alkali-earth fermions[28], where the two states were treated separately and their generic relation (as depicted in Fig.1) has not been discussed.

**Polaron-molecule transition.** Having demonstrated the molecule as an asymptotic limit of finite-$Q$ polaron, now we are ready to search for possible transition under $|P(Q)|$ ansatz throughout all momenta. In Fig.3(a), we show the dispersion $E(Q)$ for different coupling strengths. One can see that for weak couplings, the only minimum of $E(Q)$ is at $Q = 0$, thus the zero-momentum polaron is the unique ground state; while increasing $1/(k_F a_s)$ beyond $\sim 0.8$, another local minimum appears at $Q = k_F$, though still with a higher energy than $Q = 0$ state. At $1/(k_F a_s) \sim 1.27$, the two minima have the same energy, setting the location of the first-order transition between $|P(0)|$ and $P(k_F)$. At this point, $|M(0)|$ is already a good approximation for $P(k_F)$. Further increasing $1/(k_F a_s)$ beyond $1.7$, $Q = 0$ state becomes a local maximum rather than a minimum in the dispersion curve, and correspondingly, the effective mass of $|P(0)|$ goes through a resonance from large positive to large negative (see Fig.3(b)). For even stronger interactions, the only energy minimum occurs at $Q = k_F$, and the ground state is well approximated by the molecule $|M(0)|$.

Fig.3 delivers two important points. First, the literally called polaron-molecule transition for the single impurity system does exist. Nevertheless, the transition by its nature is between impurity systems with different momenta($Q = 0$ and $Q = k_F$), rather than between different forms of preset ansatz. This naturally resolves the theoretical debate on the existence of such transition based on wave-function argument[26]. Second, within an interaction window near their transition, the two-$Q$
states are both locally stable against any momentum fluctuation. This provides the underlying mechanism for their possible coexistence in realistic systems, as will be discussed below.

**Polaron-molecule coexistence and smooth transition in realistic systems.** Considering the realistic condition in experiments, we take a small impurity concentration \( n_\perp = 0.05 n_t \) and a low temperature \( T = 0.02 E_F \). The finite impurity density and finite temperature effects to the spectroscopy of Fermi polarons were studied previously in [29–32]. Here, to highlight the essential physics of polaron-molecule coexistence, we will neglect the distortion of spin-\( \uparrow \) Fermi sea (due to thermal effect) and the mediated interactions between the same spins. We just focus on two possible configurations for the dressed impurities: one is nearby zero-momentum polaron with dispersion \( \epsilon_Q^P = E_P + Q^2/(2m_P) \) \( (E_P = E(0)) \), which obeys fermionic statistics; the other is nearly \( Q = k_F \) with dispersion \( \epsilon_Q^M = E_M + (|Q| - k_F)^2/(2m_M) \), which obeys bosonic statistics and holds for \( 1/(k_F a_s) \geq 0.8 \) when the molecule solution is approached. Here \( m_P \) and \( m_M \) are respectively the effective masses of polaron and molecule, as shown in Fig.3(c). These two configurations can stay in equilibrium with each other under the same chemical potential \( \mu \) for spin-\( \perp \), which leads to the number equation \( N_\perp = N_P + N_M \) with:

\[
N_P = \sum_Q f_+(\epsilon_Q^P - \mu); \quad N_M = \sum_Q f_-(\epsilon_Q^M - \mu); \quad \tag{5}
\]

here \( f_\pm(\epsilon) = (e^{\epsilon/T} \pm 1)^{-1} \). The total energy is

\[
E = \sum_Q \left( \epsilon_Q^P f_+(\epsilon_Q^P - \mu) + \epsilon_Q^M f_-(\epsilon_Q^M - \mu) \right). \quad \tag{6}
\]

In the coexistence region \( 1/(k_F a_s) \in (0.8,1.7) \) where both polaron and molecule are locally stable, one can obtain \( \mu \) from (5) and further \( E \) from (6), by employing the data of \( E_P, E_M, m_P, m_M \) as presented in Fig.3. Near the boundaries of coexistence region, Eq.(5) automatically guarantees a negligible occupation either on polaron \( (N_P \sim 0) \) or on molecule \( (N_M \sim 0) \), due to their visible energy difference \( |E_P - E_M| \). Therefore (5,6) can be continuously connected to non-coexistence region, where the system is solely composed by polarons or molecules.

In Fig.4(a-d), we show the polaron weight \( w_P \equiv N_P/N_\perp \), residue \( Z = Z_P N_P/N \) \( (Z_P = Z(0)) \), energy \( E \), and contact \( C = (4\pi n_\perp) dE/d(1/a_s) \). We can see that all these values evolve continuously from the weak to strong coupling regime, consistent with the experimental observations[8]. In the weak (strong) coupling regime, both \( E \) and \( C \) can be well fit by the polaron (molecule) results (see dashed lines in Fig.4). All these features demonstrate a smooth polaron to molecule transition in realistic Fermi polaron systems. In particular, we note that the polaron weight shows an obvious decrease from unity to zero within \( 1/(k_F a_s) \in [0.9,1.3] \), as marked by shaded area in Fig.4, which sets the region for visible polaron-molecule coexistence. Such coexistence washes out all the discontinuities at the first-order polaron-molecule transition, and turns it to be a smooth one in realistic system. We also note that the visible coexistence terminates at \( 1/(k_F a_s) \sim 1.3 \), very close to the transition point \( \sim 1.27 \). This can be attributed to the bosonic enhancement, where particles tend to condense as molecular bosons once across the transition. This also implies that the experimentally measured zero-crossing points of the residue \( (Z \sim 0)[1,8] \) are indeed very close to the location of polaron-molecule transition.

**Discussion and outlook.** Our results can be further improved by including the second-order particle-hole excitations in variational ansatz, which has been shown to be as accurate as Monte Carlo method[13, 14]. Its inclusion will not change qualitatively the essential physics revealed in this work, but is expected to shift the location of polaron-molecule transition[14], and thus their coexistence region, to weaker couplings. This would generate a quantitatively better fit to experimental observations in Ref.[8]. On the other hand, it should be noted that the trap inhomogeneity in existing experiments[1, 8] can also contribute to the polaron-molecule coexistence and smooth the transition, as the two phases can appear in
different locations inside the trap even without the mechanism shown in this work. Therefore, a more transparent testbed for our theory is a homogeneous Fermi gas, which has become accessible in cold atoms laboratories[33, 34].

Finally, our analyses on the instability of molecule state, the competition between different-\(Q\) sectors, and the smooth polaron-molecule transition in realistic system can in principle be applied to Fermi polarons in low dimensions. In the 2D case, the experiment has reported a continuous zero crossing of quasi-particle residue[5], while for the theory of single impurity system, it is still an open question regarding the existence of a polaron-molecule transition given different conclusions from variational approaches[19, 20, 35, 36] and from Monte Carlo methods[37–39]. In the 1D case, the situation is even more intriguing due to the strong fluctuations therein. For instance, in 1D different hole states can directly couple with each other in all coupling regime[40], instead of being isolated as shown in Fig.1. Exact solutions of single impurity problem in 1D have shown a smooth crossover, instead of a sharp transition, from polaron to molecule, and the effective mass never displays a resonance[41, 42]. A detailed investigation of the polaron and molecule physics with respect to a dimension reduction is required and will be put to future studies.

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