Rapid Communications

Fermi polaron revisited: Polaron-molecule transition and coexistence

Xiaoling Cui*

Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China and Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China

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We revisit the polaron-molecule transition in three-dimensional (3D) fermion systems using the well-established variational approach. The molecule is found to be intrinsically unstable against lowest-order particle-hole excitations, and it can only approximate the ground state of impurity systems with a finite total momentum in the strong-coupling regime. The polaron-molecule transition can therefore be reinterpreted as a first-order transition between single impurity systems with different total momenta. Within a 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 a polaron and molecule, and also shed light on Fermi polaron properties in low dimensions.

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Introduction. A Fermi polaron is a quasiparticle describing an impurity dressed by surrounding fermions. In recent years it has attracted a great deal of attention and also has been successfully realized in the field of ultracold gases [1–8], owing to the high controllability of spin numbers and the interaction strength. Nearby a Feshbach resonance, the Fermi polaron exhibits an attractive lower branch [9–20] and a repulsive upper branch [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 systems.

For an attractive Fermi polaron, it is commonly believed that there is a first-order transition between a polaronic state (an impurity dressed with fermions surrounding it) and a molecular state (an impurity bound with one fermion on top of a Fermi sea) when the attraction increases, as theoretically studied in both three dimensions (3D) [13–18] and two dimensions (2D) [19,20]. Many theories are based on the energy comparison from two distinct variational *Ansätze* for a polaron and molecule with truncated particle-hole excitations [14,15,18–20], while an alternative claim of a smooth polaron-molecule crossover was also proposed by arguing that the two *Ansätze* are mutually contained when including more particle-hole excitations [26]. Thus it is important to identify the nature of the polaron-molecule transition, if it exists, based on a unified treatment for polaronic and molecular states [27]. Moreover, on the experimental side, previous studies in 3D [1] and 2D [5] have reported a polaron-molecule transition with a continuous zero crossing of quasiparticle 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 [8] has observed a smooth evolution of various physical quantities from the weak- to strong-coupling regime, and also pointed to a coexistence between the polaron and molecule nearby their transition. As these observations cannot be fully explained by the trap inhomogeneity [8], the underlying mechanism for the polaron-molecule coexistence is still an open question.

To address the above issues, in this Rapid Communication we revisit the 3D Fermi polaron problem using the well-established variational approach [9,11,12,14,15,18–21,24]. The main contributions are threefold:

(1) The molecule is found to be intrinsically unstable against lowest-order particle-hole excitations. However, it can serve as a good approximation to describe the impurity system at finite momentum $Q = k_F$ in the strong-coupling regime (k_F is the Fermi momentum of majority fermions). It follows that the literally called polaron-molecule transition can be reinterpreted as a first-order transition between single impurity systems with different total momenta $Q = 0$ and $Q = k_F$ (see the illustration in Fig. 1). Since different-Q states cannot be smoothly connected by particle-hole excitations, the theoretical debate in Ref. [26] is naturally resolved.

(2) Within a 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 the 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. [8]. This provides an intrinsic reason for the smooth polaron-molecule transition as observed in 3D Fermi gases [1,8], and also sheds light on a similar phenomenon in 2D systems [5].

*xlcui@iphy.ac.cn

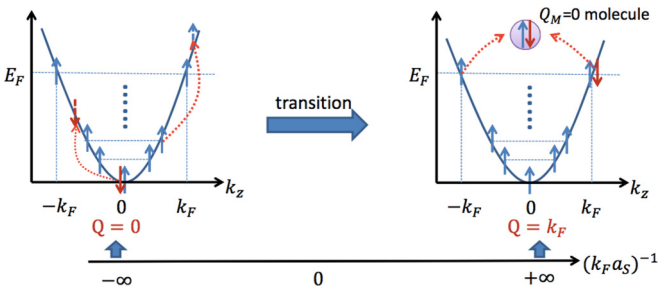

FIG. 1. Illustration of a polaron-molecule transition for a single impurity (spin-↓) imbedded in a spin-↑ Fermi sea (with Fermi energy E_F and Fermi momentum k_F). In the regime $(k_F a_s)^{-1} \to -\infty$, the ground state is a zero-momentum polaron dressed by particle-hole excitations. In the regime $(k_F a_s)^{-1} \to +\infty$, the ground state switches to total momentum $Q = k_F$, such that the impurity can pair with a spin-↑ originally at the Fermi surface to form a deeply bound molecule with zero center-of-mass momentum. Due to the rotational invariance of $\mathbf{Q}$, here we take it along the z axis and only plot out the k-space excitations with $k_x = k_y = 0$.

Model. We consider the following Hamiltonian for the 3D Fermi gases with a contact interaction,

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{Q},\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{Q}-\mathbf{k},\uparrow} c^\dagger_{\mathbf{k},\downarrow} c_{\mathbf{k}',\downarrow} c_{\mathbf{Q}-\mathbf{k}',\uparrow}. \quad (1)$$

Here, $c^\dagger_{\mathbf{k},\sigma}$ is the creation operator of the 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 scattering length a_s via $1/U = m/(4\pi a_s) - 1/V \sum_{\mathbf{k}} m/\mathbf{k}^2$. For brevity we will take $\hbar = 1$ throughout this Rapid Communication.

For a single ↓ impurity immersed in the Fermi sea of ↑ atoms with number N [giving the Fermi momentum k_F and Fermi energy $E_F = k_F^2/(2m)$], based on the variational approach [9,11,12,14,15,18–21,24] we can write down a general *Ansatz* for the system with total momentum $\mathbf{Q}$,

$$|P(\mathbf{Q})\rangle = \left(\phi_0 c^\dagger_{\mathbf{Q},\downarrow} + \sum_{\mathbf{k},\mathbf{q}}{}' \phi_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{Q}+\mathbf{q}-\mathbf{k},\downarrow} c^\dagger_{\mathbf{k},\uparrow} c_{\mathbf{q},\uparrow} + \cdots\right)|\mathrm{FS}\rangle_N, \quad (2)$$

and the molecule ansatz is

$$|M(0)\rangle = \left(\sum_{\mathbf{k}}{}' \psi_{\mathbf{k}} c^\dagger_{-\mathbf{k},\downarrow} c^\dagger_{\mathbf{k},\uparrow} + \cdots\right)|\mathrm{FS}\rangle_{N-1}. \quad (3)$$

Here, $\sum'$ refers to summation under $|\mathbf{k}| > k_F$ and $|\mathbf{q}| \leqslant k_F$; "…" refers to terms with higher-order particle-hole excitations, which are neglected in this work given their destructive interference for the attractive branch [12].

The two *Ansätze* above give rise to very different pictures: (2) describes a fermionic quasiparticle 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 as the attraction is increased, many theories have predicted a first-order transition from $|P(0)\rangle$ to $|M(0)\rangle$ [13–18], called the *polaron-molecule transition*. On the other hand, an alternative

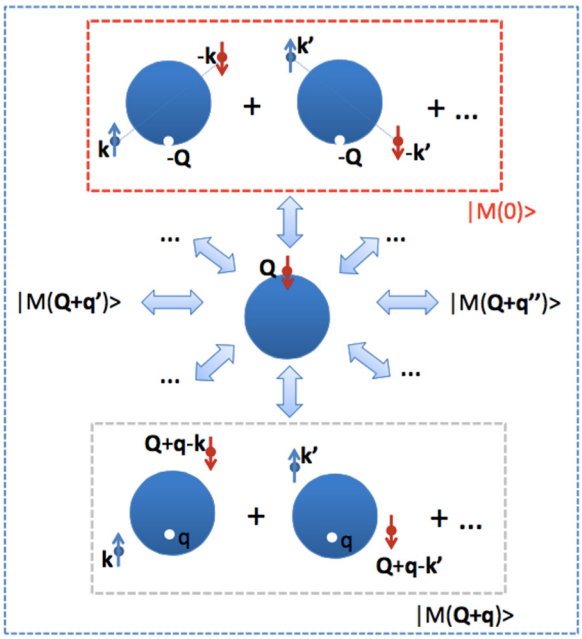

FIG. 2. Schematics for the instability of the molecule state $|M(0)\rangle$ (upper red rectangle), which is constructed by a singlet pair $(\uparrow,\downarrow)$ outside the Fermi sea with a zero center-of-mass momentum and a hole at $-\mathbf{Q} = -k_F \mathbf{e}_z$. $|M(0)\rangle$ can become unstable through coupling to the unperturbed bare state (central picture), and then from this state to other particle-hole excitations with the hole at other momenta [see, for instance, $|M(\mathbf{Q}+\mathbf{q})\rangle$ in the lower gray rectangle]. All these configurations compose a $|P(\mathbf{Q})\rangle$ state.

claim of a smooth crossover, instead of a sharp transition, was proposed based on the argument that $|M\rangle$ is a special case of the $|P\rangle$ family and vice versa if including arbitrarily many particle-hole excitations [26]. In this sense, it is highly demanded that we reexamine the relation between the two *Ansätze*. Due to the rotational invariance of $\mathbf{Q}$, from now on we choose a specific case with $\mathbf{Q} = Q\mathbf{e}_z$.

Molecule versus finite-Q polaron. By directly comparing (2) and (3), one can see that if we set $Q = k_F$, $\phi_0 = 0$, and $\phi_{\mathbf{k},\mathbf{q}} = \delta_{\mathbf{q},-\mathbf{Q}} \psi_{\mathbf{k}}$, then (2) exactly reduces to (3). In other words, $|M(0)\rangle$ corresponds to only considering a particular type of particle-hole excitation in $|P(\mathbf{Q})\rangle$ with $|\mathbf{Q}| \equiv Q = k_F$, which will be denoted as $|P(k_F)\rangle$ for short. In such a particular excitation, the hole sits right at the Fermi surface and points opposite to $\mathbf{Q}$. However, this type of excitation is not self-closed even in the lowest-order excitation subspace. As shown in Fig. 2, it can scatter back to the bare impurity at $\mathbf{Q}$ together with an unperturbed Fermi sea, and then couple to other excitations with holes covering all other momenta inside the Fermi sea [28]. Here, we denote $|M(\mathbf{Q}+\mathbf{q})\rangle$ as a set of excitation states with total momentum $\mathbf{Q}$ and the hole sitting at $\mathbf{q}$. $|P(k_F)\rangle$ is thus a superposition of the bare term and all $|M(\mathbf{Q}+\mathbf{q})\rangle$ states, and it is self-closed up to the lowest particle-hole excitation. As the coupling between the bare term and different $|M(\mathbf{Q}+\mathbf{q})\rangle$ will generate a lower variational energy, $|P(k_F)\rangle$ is always energetically more favorable than $|M(0)\rangle$. Therefore, the necessity to introduce such a $|M(0)\rangle$ state seems quite questionable.

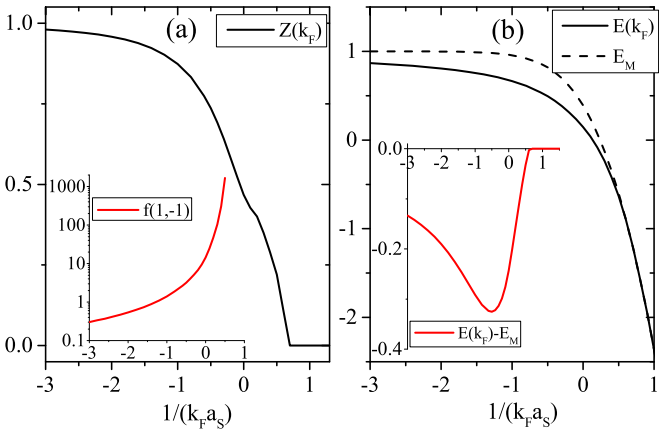

FIG. 3. (a) Residue of $|P(k_F)\rangle$ as a function of $1/(k_F a_s)$. The inset of (a) shows the weight between the molecular component and bare one (see text). (b) Energies of $|P(k_F)\rangle$ $[E(k_F)]$ and $|M(0)\rangle$ (E_M) as functions of $1/(k_F a_s)$. The inset shows their difference. The unit of energy is E_F.

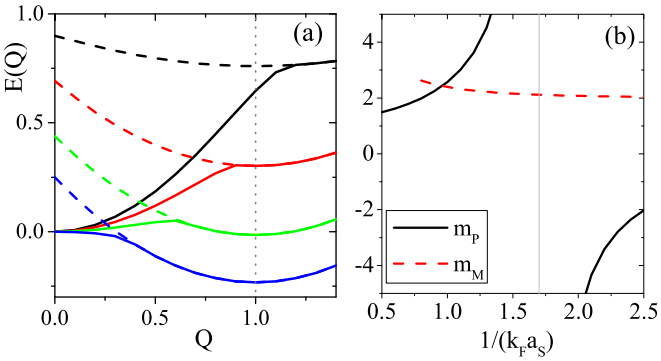

FIG. 4. First-order transition between $|P(0)\rangle$ and $|P(k_F)\rangle$. (a) Solid lines: Energies of $|P(Q)\rangle$ as functions of Q for $1/(k_F a_s) = 0.3$, 0.8, 1.3, and 2 (from top to bottom). Dashed lines show results by only including the $\mathbf{q} = -k_F \mathbf{e}_z$ hole states in $|P(Q)\rangle$. (b) Effective masses near $Q = 0$ and $Q = k_F$, denoted respectively by m_P and m_M, as functions of $1/(k_F a_s)$. The units of momentum and energy are respectively k_F and E_F.

Here, we show that the significance of $|M(0)\rangle$ lies in that it represents the asymptotic limit of $|P(k_F)\rangle$ in the strong-coupling regime. To see this, we study the quasiparticle residue of $|P(k_F)\rangle$, $Z(k_F)$, which follows

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

As shown in Fig. 3(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. 3(a). This indicates a smooth crossover in the $Q = k_F$ sector from a polaronic to a molecular state as the attraction increases. Such a crossover is further confirmed by examining the energies of $|P(k_F)\rangle$ and $|M(0)\rangle$, denoted respectively as $E(k_F)$ and E_M, as shown in Fig. 3(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, $|M(0)\rangle$ can be justified as a good approximation for $|P(k_F)\rangle$.

A physical picture to understand the above results is as follows. As increasing the attraction strength, the particle-hole excitations become more dominated in $|P(k_F)\rangle$, leading to a reduced $Z(k_F)$. Due to the reduced weight of the bare term, the coupling effect between $|M(0)\rangle$ and the other states, as depicted in Fig. 2, becomes less significant. In the strong-coupling regime with $Z(k_F) \sim 0$, the coupling effect is negligible, and $|M(0)\rangle$ is nearly isolated from all other hole excitations [these hole states are all energetically unfavorable as compared to $|M(0)\rangle$]. In this limit, $|M(0)\rangle$ can well approximate $|P(k_F)\rangle$ and E_M becomes identical to $E(k_F)$. We find these results are robust against higher-order particle-hole excitations [29].

We note that the competition between the molecule and finite-Q polaron was also discussed in Refs. [18,30], and their resemblance in the strong-coupling limit was pointed out in multichannel alkali-earth fermions [31]. Nevertheless, in these studies the two states were treated separately from the independent *Ansatz*, and their generic relation (as depicted in Fig. 2) has not been revealed.

Polaron-molecule transition. Having demonstrated the molecule as an asymptotic limit of the finite-Q state, now we are ready to search for a possible transition under $|P(\mathbf{Q})\rangle$ throughout all Q. In Fig. 4(a), we show the dispersion $E(Q)$ for various coupling strengths. One can see that in weak couplings, the only minimum of $E(Q)$ is at $Q = 0$, thus $|P(0)\rangle$ is the unique ground state; while increasing $1/(k_F a_s)$ to $\sim$0.8, another local minimum appears at $Q = k_F$ but with a higher energy than $E(Q = 0)$. 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 $|P(0)\rangle$ and $|P(k_F)\rangle$. At this point, $|M(0)\rangle$ is already a good approximation for $P(k_F)$. Further increasing $1/(k_F a_s)$ to $\sim$1.7, $|P(0)\rangle$ becomes a local maximum in the dispersion, and accordingly its effective mass undergoes a resonance from large positive to large negative [see Fig. 4(b)]. Beyond this point, the only energy minimum occurs at $Q = k_F$, and the ground state is well approximated by $|M(0)\rangle$.

Figure 4 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 *Ansätze*. Since the transition is between different-Q states, it cannot be accomplished by reshuffling the Fermi sea via the interaction-induced particle-hole excitations, which conserve the total momentum. This naturally resolves the theoretical debate on the existence of such a transition as in Ref. [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 coexistence in realistic systems, as discussed below.

Polaron-molecule coexistence and smooth transition in realistic systems. We consider a small impurity concentration $n_\downarrow = 0.05n_\uparrow$ and a low temperature $T = 0.02E_F$ to mimic the realistic condition in experiment. The effects of finite $n_\downarrow$ and finite T to the spectroscopy of Fermi polarons were studied in Refs. [32–35]. Here, to highlight the essential physics of polaron-molecule coexistence, we just focus on two possible configurations for the dressed impurities: One is nearby a zero-momentum polaron with dispersion $\epsilon^P_{\mathbf{Q}} = E_P + \mathbf{Q}^2/(2m_P)$ [$E_P = E(0)$], which obeys fermionic statistics; the other is nearby $Q = k_F$ with dispersion $\epsilon^M_{\mathbf{Q}} = E_M + (|\mathbf{Q}| - k_F)^2/(2m_M)$, which obeys bosonic statistics and holds for $1/(k_F a_s) \gtrsim 0.8$ when the molecule solution is approached. Here, m_P and m_M are respectively the effective masses of the polaron and molecule, as shown in Fig. 4(c). These two configurations can stay in equilibrium with each other under the same impurity chemical potential μ, which leads to the number equation $N_\downarrow = N_P + N_M$ with

$$N_P = \sum_{\mathbf{Q}} f_+\big(\epsilon^P_{\mathbf{Q}} - \mu\big), \quad N_M = \sum_{\mathbf{Q}} f_-\big(\epsilon^M_{\mathbf{Q}} - \mu\big); \quad (5)$$

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

$$E = \sum_{\mathbf{Q}} \big[\epsilon^P_{\mathbf{Q}} f_+(\epsilon^P_{\mathbf{Q}} - \mu) + \epsilon^M_{\mathbf{Q}} f_-(\epsilon^M_{\mathbf{Q}} - \mu)\big]. \quad (6)$$

In the coexistence region $1/(k_F a_s) \in (0.8, 1.7)$ where both the polaron and molecule are locally stable, one can obtain μ from (5) and further E from (6), by employing the data of E_P, E_M, m_P, m_M as presented in Fig. 4. Near the boundaries of the coexistence region, Eq. (5) automatically guarantees a negligible occupation either on the polaron ($N_P \sim 0$) or on the molecule ($N_M \sim 0$), due to their visible energy difference $|E_P - E_M|$. Therefore (5) and (6) can be continuously connected to a noncoexistence region, where the system is solely composed by polarons or molecules.

In Figs. 5(a)–5(d), we show the polaron weight $w_P \equiv N_P/N_\downarrow$, residue $Z = Z_P w_P$ [$Z_P = Z(0)$], energy E, and contact $C = (4\pi m) dE/d(1/a_s)$. We can see that all quantities evolve continuously from the weak- to strong-coupling regime, consistent with experimental observations [8]. In the weak- (strong-) coupling regime, both E and C are well explained by the polaron (molecule) results (see the dashed lines). All these features demonstrate a smooth polaron to molecule transition in realistic impurity systems. In particular, we note that Z_P shows an obvious reduction from unity to zero within $1/(k_F a_s) \in [0.9, 1.3]$, as marked by the shaded area in Fig. 5, which sets the region for a visible polaron-molecule coexistence. Such a coexistence washes out all the discontinuities at the first-order transition, and turns it into a smooth one in a 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. It can be attributed to the bosonic enhancement, where particles tend to condense as molecular bosons once across the transition. This implies the experimentally measured zero-crossing locations of Z [1,8] are indeed close to the transition point.

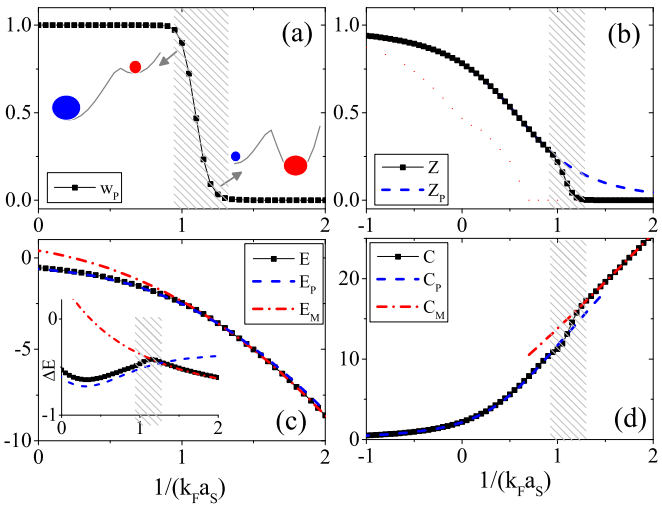

FIG. 5. Smooth polaron-molecule transition with a finite impurity density $n_\downarrow = 0.05n_\uparrow$ and at temperature $T = 0.02E_F$. (a)–(d) respectively show the polaron weight w_P, residue Z, energy E scaled by $N_\downarrow E_F$, and contact C scaled by $(2N_\downarrow k_F)$. For comparison, the blue dashed (red dashed-dotted) lines show results based on the polaron (molecule) *Ansatz*. The shaded areas mark the region of visible polaron-molecule coexistence. The inset of (a) shows two typical situations when the polaron (left blue) or molecule (right red) dominates in the impurity occupation, depending on their energy comparison. The inset of (c) shows the energy per impurity shifted by two-body binding energy $E_{2b} = -1/(ma_s^2)$, for a better view of the smooth transition.

Discussion and outlook. Our results can be further improved by including the second-order particle-hole excitation in a variational *Ansatz*, which has been studied in the $Q = 0$ sector and shown to be as accurate as the Monte Carlo method [12,13,15]. Our preliminary study on finite-Q sectors confirms that their inclusion does not change qualitatively the essential physics revealed in this work, except for shifting the polaron-molecule transition point and the coexistence region to weaker couplings [29]. Moreover, it is noted that the trap inhomogeneity in existing experiments [1,8] can also contribute to smoothening the transition, as polarons and molecules can appear in different locations inside the trap even without the mechanism discussed in this work. Therefore, a more transparent test bed for our theory is a homogeneous Fermi gas, which has become accessible in cold-atom laboratories [36,37].

Finally, our analyses on the molecule instability, the competition between different Q's, and the smoothening mechanism can in principle be applied to Fermi polarons in low dimensions. In 2D, the existence of a polaron-molecule transition for a single impurity system is still an open question given different conclusions from variational methods [19,20,38,39] and quantum Monte Carlo [40–42]. In 1D, the situation is even more intriguing due to contributions from hole scattering [43]. Exact solutions have shown a smooth crossover instead of a sharp transition, and the effective mass never displays a resonance [44,45]. In this context, the physics

of competition and/or conversion between a polaron and molecule in reduced dimensions still requires a careful study in the future.

Note added. Recently, the updated experiment by Ness *et al.* [8] has newly adopted a theory similar to ours to explain the observed smooth polaron-molecule transition. The idea of a polaron-molecule coexistence and equilibrium in the presence of a finite impurity density and at a finite temperature is consistent with ours. However, in Ref. [8], the polaron and molecule dispersions are both centered at zero momentum while here their centers are shown to be differed by k_F.

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