Crystalline correlations emergent from a smooth crossover of mass-imbalanced Fermi polaron

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Identifying few-body correlations is an efficient tool to solve complex many-body problems. The polarons, interpolating between few- and many-body systems, serve as an ideal platform to achieve the goal. In this work, we reveal various crystalline few-body correlations emergent from a smooth crossover of mass-imbalanced Fermi polarons in two dimension. Here a unified variational approach up to three particle-hole excitations allows us to extract the dominant $n$-body correlations for $n$ ranging from 2 (dimer), 3 (trimer) to 4 (tetramer). It is found that when the fermion-impurity mass ratio is beyond certain critical value, the Fermi polaron will undergo a smooth polaron-trimer or polaron-trimer-tetramer crossover as increasing the fermion-impurity attraction, in contrast to the polaron-molecule transition for the equal mass case. During the crossover, the 3- and 4-body correlations gradually emerge and become dominant, which can manifest themselves in the momentum-space crystallization, i.e., the particle-hole excitations of majority fermions tend to distribute with equal interval near the Fermi surface forming a stable diagonal or triangular structure. Such emergent crystallization can be detected through the density-density correlation of majority fermions. Our results shed light on the intriguing quantum phases in the mass-imbalanced Fermi-Fermi mixtures beyond the pairing superfluid paradigm.

INTRODUCTION

Many-body problems are usually complex, and an efficient tool to tackle them is through identifying few-body correlations. A famous example is the Cooper instability, which tells the molecule formation on top of a spin-1/2 Fermi sea, providing the foundation for the theory of Cooper pair superfluidity[1]. However, the hardest part of the approach is to foresee the dominant correlation from a complicated many-body environment. In this regard, the $1+N$ polaron system, which consists an impurity immersed in a sea of majority atoms, serves as an ideal platform for this study as it just interpolates between the few- and many-body systems and constitutes the simplest model for the few-to-many crossover[2, 3].

The concept of polaron, as raised by Landau nearly a century ago for an electron moving in solid[4], has been successfully applied to various physical systems. In recent years, the polaron study has gained rapid development in ultracold atoms thanks to the high controllability over spin species, number, and interaction therein. For instance, by choosing majority atoms with different statistics, the cold atoms experiments have successfully realized the Fermi polaron[5–13], Bose polaron[14–17] and even both of them in a single system[18]. Similar polaron spectra have also been observed in semiconductor microcavities[19, 20]. Among all circumstances, the few-body correlation in an attractive Fermi polaron is of particular interest. It has been shown that the 3D and 2D Fermi polarons with equal mass can undergo a first-order transition from polaronic to molecular phase as increasing the impurity-fermion attraction[21–29], a consequence of enhanced two-body correlation therein. Using a unified treatment of polaron and molecule, such transition can be interpreted as the energy competition between different momentum states[30, 31], where the molecule serves as a good approximation for the finite-momentum state in strong coupling limit (see also [32]) and possesses a huge hidden degeneracy. The inclusion of finite-momentum states[30, 31, 33] is crucial for explaining the smooth polaron-molecule evolution in realistic experiment with a finite impurity density and at finite temperature[5, 8, 12]. Besides, the polaron-molecule transition has profound implications to the property of highly-polarized spin-1/2 fermions, where a phase separation between normal and superfluid states can occur[34] as observed in cold atoms experiments[35, 36].

The recent realization of mass-imbalanced Fermi-Fermi mixtures in cold atoms, such as $^{40}$K-$^{6}$Li[37–39], $^{161}$Dy-$^{40}$K[40, 41], $^{53}$Cr-$^{6}$Li[42], offers an unprecedented opportunity for uncovering intriguingly new correlation effect in Fermi polarons. Here an important hint is from the few-body physics, where the mass-imbalance has been found to greatly facilitate the formation of cluster bound states. For instance, a light atom can bind with two heavy fermions to form an Efimov trimer[43] or a universal trimer[44, 45], and bind with three or four fermions to form a tetramer[46–49] or pentamer[49, 50], as long as the heavy-light mass ratio is beyond certain critical value. An important follow-up question is how would their associated few-body correlations affect the many-body physics, such as, in 1 + $N$ Fermi polarons. In literature, there have been a number of studies on the competition and conversion between polaron and trimer...
in Fermi polarons [51–57]. However, a clear understanding on the relation between polaron, trimer and other highly correlated states is still missing, due to the lack of a unified perspective on them. It is still open questions how the different few-body correlations evolve and manifest themselves in polaron systems. The problem is quite challenging as it requires a theoretical approach to incorporate all essential correlations in a single framework.

In this work, we address the mass-imbalanced Fermi polaron problem in 2D using a unified variational approach consisting up to three particle-hole excitations. The approach represents the state-of-the-art theoretical tool that allows us to systematically examine the \( n \)-body correlations, with \( n \) ranging from 2 (dimer), 3 (trimer) to 4 (tetramer), in a unified framework. We find that in distinct contrast to the first-order transition in equal mass case, no sharp transition occurs in the mass-imbalanced Fermi polaron if the fermion-impurity mass ratio \( \eta \) is larger than \( \eta_r(= 3.34) \), the critical value to support a trimer bound state in the few-body sector. Depending on the actual \( \eta(> \eta_r) \), the system undergoes a continuous evolution from a polaronic state to the dressed trimer or tetramer states (see Fig. 1), where the dominant 3- and 4-body correlations gradually emerges. In this process, the majority fermions develop the momentum-space crystallization, i.e., the dominant particle-hole excitations distribute with equal interval near the Fermi surface that form a stable diagonal or triangular structure, despite the whole system is rotational invariant. Such emergent crystallization directly characterizes the dominant trimer and tetramer correlations, and can be readily detected via the density-density correlation of majority fermions. Our results reveal a remarkable effect of mass imbalance in changing the few-body correlation in Fermi polarons, which shed light on the novel phases and correlations in mass-imbalanced Fermi-Fermi mixtures that are well beyond the pairing superfluid paradigm.

**UNIFIED VARIATIONAL APPROACH**

We start from the Hamiltonian describing a single impurity immersed in a 2D Fermi sea:

\[
H = \sum_k \left( \varepsilon_k a_k^\dagger a_k + \varepsilon_k^f f_k^\dagger f_k \right) + \frac{g}{S} \sum_{Q,k,k'} a_{Q-k,k'}^\dagger f_k^\dagger f_k a_{Q-k'}.
\]

(1)

Here \( a_k^\dagger \) and \( f_k^\dagger \) respectively create an impurity atom and a majority fermion with momentum \( k \) and energy \( \varepsilon_k = k^2/(2m) \); \( g \) is the bare coupling that follows the renormalization equation \( 1/g = -1/S \sum_k 1/(\varepsilon_k^2 + \varepsilon_k^f + E_{2b}) \), where \( S \) is the system area and \( E_{2b} = (2\mu a_{2d}^2)^{-1} \) is the 2-body binding energy in vacuum that relies on the relative mass \( \mu = m/m_f/(m+2m_f) \) and 2D scattering length \( a_{2d} \). We take \( \hbar = 1 \) for brevity. The Fermi polaron properties are determined by two dimensionless parameters, namely, the mass ratio \( \eta = m_f/m_a \) and the interaction strength \( \ln(k_F a_{2d}) \), where \( k_F \) is the Fermi momentum of majority atoms giving the Fermi energy \( E_F = k_F^2/(2m_f) \).

We write down a generalized version of the Fermi polaron ansatz initially proposed in [58]:

\[
P_{2n+1}(Q) = \left( \psi^{(0)}_Q \right)^4 + \frac{1}{(n!)^2} \sum_{l=1}^n \sum_{q_i} \psi^{(l)}_{Q,q_i} \sum_{j=1}^l a_{P}^\dagger \prod_{i=1}^l f_{k_i}^\dagger f_{q_i} \left| FS_N \right>.
\]

(2)

Here \( \left| FS_N \right> \) is the Fermi sea with number \( N \); all \( q(k) \) are below (above) the Fermi surface and \( P = Q + \sum q_i - \sum k_i \). Taking \( \left| FS_N \right> \) as the reference state, \( P_{2n+1}(Q) \) describes the impurity dressed with up to \( n \) particle-hole (p-h) excitations and with total momentum \( Q \). Because of the rotational invariance, hereafter we will use \( Q = |Q| \) as the momentum index for simplicity.

We emphasize that the generalized ansatz (2) systematically incorporates all the essential few-body correlations and thus can serve as a unified approach for the Fermi polaron problem. First, taking \( Q = 0 \), it describes the polaronic ground state for the weak coupling Fermi polarons, as studied previously with up to one [23, 26, 27, 30, 51, 58, 59, 61] and two [22, 31, 52, 60] p-h excitations. Secondly, taking a finite \( Q = k_F \), it well covers the molecule state with zero center-of-

![FIG. 1. (Color Online). Phase diagram of the 2D Fermi polaron problem. The black line refers to the polaron-molecule phase boundary for small \( \eta < \eta_r \): the ground state above the line is a polaron (P) with total momentum \( Q = 0 \) and below the line is a molecule (M) with \( |Q| = k_F \) (or with center-of-mass momentum \( Q_M = 0 \)). The gray area around the line denotes the coexistence region for polaron and molecule. For \( \eta > \eta_r \), no phase transition is found and the ground state is always at \( Q = 0 \); as increasing the attraction strength, the system undergoes a smooth polaron-trimer ('Tr') crossover for \( \eta \in (\eta_r, \eta_c) \) and a polaron-trimer-tetramer ('Te') crossover for \( \eta > \eta_c \). For the \( Q = 0 \) ground state, we provide the RGB color map according to the weights of different particle-hole excitation terms in its full wave-function, i.e., \( w_3, w_2 \) and \( w_1 + w_0 \) represent the mixing ratio of R (red), G (green) and B (blue) colors, respectively. Here \( \eta_r = 3.34 \) and \( \eta_M = 3.38 \).


mass momentum as proposed in the strong coupling regime\cite{22, 23, 26, 27, 51, 52, 61}, where the impurity essentially binds with one fermion on the Fermi surface to form a dimer. In this sense, it has been pointed out that the polaron-molecule transition can be recognized as the energy competition between different $Q$-sectors\cite{30, 31}. Finally, by including higher-order p-h excitations, all the few-body correlations can be systematically incorporated. Specifically, the full $n$-body correlation effect has been contained in the $(n-1)$ p-h excitation terms in (2).

In this work, we will consider up to three p-h excitations, i.e., with $P_2(Q)$, which allow us to unify the dimer, trimer, and tetramer correlations in a single framework to examine their relations and competitions in-between. The integral equations from $|P_2(Q)|$ and the numerical details are presented in the supplementary material\cite{62}. Moreover, since the $P_2$ formulism can well cover the $P_3$ ones by neglecting the terms of three p-h excitations, in the regime where these excitations (or tetramer correlation) are negligible we shall work with $P_3$ for simplification. Finally, we remark that there are two important values of mass ratio to distinguish different few-body correlations in 2D Fermi polarons studied here, namely, the one to support a trimer in vacuum from the atom-dimer threshold $\eta_{tr} = 3.34$\cite{45} and the one to support a tetramer in vacuum from the atom-trimer threshold $\eta_{tr} = 3.38$\cite{49}. The effect of even larger cluster bound states will be discussed at the end of this paper.

RESULTS

I. Polaron-molecule transition for $\eta < \eta_{tr}$

We first briefly go through the regime with a small mass ratio $\eta < \eta_{tr}$. In this case, the three p-h excitations in $P_2$ take little effect and thus $P_3$ can serve as a good ansatz. In this regime the polaron-molecule transition persists, with the same nature as in equal mass case. Taking $\eta = 2$ for instance, we show in Fig.2(a) that as increasing the coupling strength, the ground state of Fermi polaron can switch from $Q = 0$ to $Q = k_F$, signifying the polaron to molecule transition. Nearby the transition, the dispersion curve displays a double well structure, indicating the polaron-molecule coexistence in realistic system with a finite impurity density and at finite temperature.

For comparison, we also consider the molecule ansatz

$$M_{2n+2}(Q_M) = \left(\sum_k \phi_k^{(0)} a_{Q_M-k}^\dagger f_k^\dagger + \sum_{i=1}^n \sum_{k, q_j} \phi_{kk, q_j}^{(0)} a_k^\dagger f_k^\dagger \prod_{l=1}^i f_{k_l}^\dagger \prod_{j=1}^i f_{q_j} \right) |FS\rangle_{N-1},$$

with $P = Q_M - k - \sum_{i=1}^n (k_i - q_j)$. As pointed out in Ref.\cite{30, 31}, $M_{2n+2}(0)$ expands a subset of the variational space of $P_{2n+3}(k_F)$, and thus the former is always energetically unfavorable as compared to the latter. However, in the strong coupling regime, $M_{2n+2}(0)$ can be a good approximation for $P_{2n+3}(k_F)$. As shown in Fig.2(b), at the transition between $Q = 0$ and $Q = k_F$, the energies from $M_{4}(0)$ and $P_{3}(k_F)$ are indistinguishable and thus it can be interpreted as the polaron-molecule transition. In Fig.1, we have mapped out the transition point and the coexistence region for polaron $(Q = 0)$ and molecule $(Q = k_F, Q_M = 0)$ in $(\eta, \ln(k_F a_{2d}))$ plane. It is found that as increasing $\eta$, the critical $\ln(k_F a_{2d})$ moves to strong coupling regime and saturates at $-\infty$ as $\eta \rightarrow \eta_{tr}$. This is consistent with the vacuum limit $(k_F \rightarrow 0)$ where the molecule (or dimer) gives way to a trimer ground state exactly at $\eta = \eta_{tr}$.

II. Smooth polaron-trimer crossover for $\eta_{tr} < \eta < \eta_{te}$

A remarkable difference between Fermi polarons with $\eta < \eta_{tr}$ and $\eta > \eta_{tr}$ is that the latter displays no sharp
By definition, a peak if their relative angle is \( \theta_{w_1} \), one p-h \( (w_1) \), and two p-h \( (w_2) \) terms in \( P_2(0) \) as functions of \( \ln(k_F a_{2d}) \). Clearly, (5) describes a trimer outside the Fermi sea dressed with p-h excitations. The polaron-trimer transition was drawn from an energy crossing between \( P_3(0) \) and \( T_{R5}(0) \)[51, 52]. Here, we remark that the polaron and trimer states are intimately related to each other. As indicated by Fig.3(c1,c2), the trimer ansatz \( T_{R2n+3}(0) \) (Eq.5) just corresponds to picking up a particular set of p-h excitations in the polaron ansatz \( P_{2n+5}(0) \) (Eq.2) where the two holes are right at the Fermi surface and with opposite directions. Therefore, \( T_{R2n+3} \) falls into the same \( Q \)-sector as \( P_{2n+5} \), and actually belongs to a subset of the latter. Because of this, \( T_{R2n+3}(0) \) should be always energetically unfavorable as compared to \( P_{2n+5}(0) \). This is to say, the polaron to trimer evolution can only be a crossover but

\[
T_{R2n+3}(0) = \sum_{k,k'} (\tau_{kk'}^{(0)} a_{k-k'}^\dagger f_{k}^\dagger f_{k'}^\dagger + \sum_{l=1}^n (\tau_{kk'}^{(l)} a_{p_{k,q} f_{k}^\dagger f_{k'}^\dagger \prod_{i=1}^l f_{k_i}^\dagger \prod_{j=1}^l f_{q_j}^\dagger) |FS \rangle_{N-2}.
\]

with \( P = -k-k'-\sum_{l=1}^n (k_i-q_i) \). Clearly, (5) describes a trimer outside the Fermi sea dressed with p-h excitations. The polaron-trimer transition was drawn from an energy crossing between \( P_3(0) \) and \( T_{R5}(0) \)[51, 52]. Here, we remark that the polaron and trimer states are intimately related to each other. As indicated by Fig.3(c1,c2), the trimer ansatz \( T_{R2n+3}(0) \) (Eq.5) just corresponds to picking up a particular set of p-h excitations in the polaron ansatz \( P_{2n+5}(0) \) (Eq.2) where the two holes are right at the Fermi surface and with opposite directions. Therefore, \( T_{R2n+3} \) falls into the same \( Q \)-sector as \( P_{2n+5} \), and actually belongs to a subset of the latter. Because of this, \( T_{R2n+3}(0) \) should be always energetically unfavorable as compared to \( P_{2n+5}(0) \). This is to say, the polaron to trimer evolution can only be a crossover but
not a sharp transition. Note that this is very different from the case of polaron-molecule competition, where\(P_{2n+2}(0)\) and \(M_{2n+2}(0)\) belong to different \(Q\)-sectors (taking |\(FS\rangle_N\) as reference) and there can be a transition between them[30, 31]. Moreover, we would like to clarify that the energy comparison between \(Tr_{2n+3}\) and \(P_{2n+1}\) with the same \(n\) is problematic in identifying a transition, as the former contains two more particles outside the Fermi sea and their additional scattering can easily produce a lower energy than the latter. A proper comparison is between \(Tr_{2n+3}\) and \(P_{2n+5}\), both having \(n+3\) particles outside the Fermi sea.

In Fig.3(d), we compare the energies from various ansatz for \(\eta = 3.35(\geq \eta_c)\). As expected, the energy of \(Tr_{5}(0)\) (or \(Tr_3(0)\)) is visibly higher than that of \(P_7(0)\) (or \(P_5(0)\)). Nevertheless, \(Tr_{5}(0)\) does have an energy crossing with \(P_3(0)\) and \(P_5(0)\), essentially because they are actually associated with different levels of p-h excitations on top of the Fermi sea \(|FS\rangle_N\). Such crossing cannot represent any transition in the system. Based on these analyses, we expect a similar polaron-trimer crossover instead of a transition in other Fermi polaron systems[55, 57].

III. Polaron-trimer-tetramer crossover and crystalline correlation for \(\eta > \eta_c\)

Continuously increasing mass ratio \(\eta\) beyond \(\eta_c\), the four-body (tetramer) correlation can become dominant and lead to even intriguing physics. To capture the physics here, we have worked with \(P_7\) ansatz which includes up to three p-h excitations and thus covers all the dimer, trimer and tetramer correlations. We have confirmed the absence of phase transition in this case and the ground state is always at \(Q = 0\), similar to the case of \(\eta \in (\eta_t, \eta_c)\). However, here a crucial difference is that as increasing the coupling strength, the system undergoes a sequence of crossover from polaron to trimer, and then from trimer to tetramer states.

To understand the relation between the tetramer and the general ansatz in (2), we write down the tetramer ansatz according to the same strategy as in writing (3,5):

\[
Te_{2n+4}(0) = \sum_{kk'k''\ell} (v_{kk'k''\ell}^{(0)} a_{k-k'}^\dagger f_{k}^\dagger f_{k''}^\dagger) +
\sum_{l=1}^{n} \sum_{k,q} (v_{kk'k''q,l}^{(l)} a_{p}^\dagger f_{k}^\dagger f_{k''}^\dagger \prod_{i=1}^{l} f_{k_i}^\dagger \prod_{j=1}^{l} f_{q_j}^\dagger |FS\rangle_{N-3},
\]

with \(P = -k-k'k''-\sum_{i=1}^{n} (k_i-q_i)\). Eq.6 describes a tetramer bound state that is on top of the Fermi sea and dressed with p-h excitations. Then, following a similar analysis as in the trimer case, we can immediately see that \(Te_{2n+4}\) belongs to a special case of \(P_{2n+7}\) by only considering the p-h excitations with three holes pinning at the Fermi surface. By manipulating the directions of three holes, these two ansatz can even belong to the same \(Q\)-sector and thus there exists no sharp transition between them but just a crossover. We have numerically verified this in Fig.4, and showed that the crossover is accompanied with the emergence of intriguing crystalline correlation of majority fermions.

In Fig.4, we take the \(^{40}\)K\(^{6}\)Li Fermi polaron with \(\eta = 40/6\) and demonstrated the polaron-trimer-tetramer crossover therein. Fig.4(a) shows that as increasing the coupling strength, the system undergoes a continuous evolution from a polaronic state (where \(w_9\) dominates), to trimer (\(w_2\) dominates) and finally to tetramer state (\(w_3\) dominates). To look into the inner structure of these states, we compute the hole-hole and particle-particle correlation functions of majority fermions in momentum space, which are defined as

\[
D_h(q_0, q) \equiv \langle (1-n_{q_0}^\dagger)(1-n_{q}^\dagger) \rangle,
\]

\[
D_p(k_0, k) \equiv \langle n_{k_0}^\dagger n_{k}^\dagger \rangle,
\]

with all \(q\) (\(k\)) staying below (above) the Fermi surface. In Fig.4(b1-b3), we plot \(D_h\) and \(D_p\) together in momentum space (as varying \(q\) and \(k\)), while keeping \(q_0\) and \(k_0\) fixed nearby the Fermi surface. In the polaron regime (b1), we can see that both \(D_h\) and \(D_p\) are extensively distributed in a broad angular range near the Fermi surface. In comparison, the correlation develops a visible crystalline feature in the trimer and tetramer regimes. Specifically, the crystalline correlation displays as a diagonal structure in trimer regime (b2) and a regular triangle in tetramer regime (b3). To trace the evolution, we further examine the particle-particle angular correlation, i.e., \(\sum_{k,k',\ell} D_p(k, k')\delta_{\theta_h^k-\theta_h^{k'}}\delta_{\theta_h^{k'}},\) as a function of relative angle \(\theta_h^{kk'},\) see Fig.4(c1, c2). We can see that during the polaron-trimer crossover (c1), the angular dependence of \(D_p\) becomes gradually pronounced at \(\theta_h^{kk'} = \pi\), signifying a diagonal correlation (similar to Fig.3(c1, c2)); while during the trimer-tetramer crossover (c2), the peaks of \(D_p\) gradually deviate from \(\pi\) and finally end up at \(2\pi/3\) and \(4\pi/3\), signifying the emergence of triangular correlation. All these processes can be well captured by the general ansatz \(P_7(0)\), which produces a considerably lower variational energy than \(Tr_{5}(0)\) and \(Te_{4}(0)\), see Fig.3(d). Again, the energy crossing between \(Tr_{5}(0)\) and \(Te_{4}(0)\) does not exist for any real transition.

In above, we have shown that the emergent crystalline correlations in trimer and tetramer regimes all display high symmetries, i.e., either with a diagonal or a regular triangular structure. Physically, it is because these highly symmetric structures are associated with a large degeneracy manifold, in which they can be scattered freely to other similar configurations to minimize the energy. As shown schematically in Fig.5 (a) and (b), from a given p-h configuration with a diagonal or triangular structure near the Fermi surface, it can be coupled to another p-
FIG. 4. (Color Online). Polaron-trimer-tetramer crossover at mass ratio \( \eta = 40/6 \).

(a) Weights of the bare term and various p-h excitation terms (see the \( w_n \) definition in (4)) in \( \mathcal{P}_7(0) \) as functions of \( \ln(k_Fa_{2d}) \).

(b1-b3) Contour plots of hole-hole correlation \( D_h(q_0, q) \) and particle-particle correlation \( D_p(k_0, k) \) for different \( \ln(k_Fa_{2d}) = 1.972(\text{b1}), 0.172(\text{b2}), -0.428(\text{b3}) \), which, respectively, belong to the polaron, trimer and tetramer regime as labeled by different stars in (a). Here we take \( q_0 = -k_F\mathbf{e}_x \) and \( k_0 = -1.08k_F\mathbf{e}_x \), as marked by white and red points in the plots. The white circle denotes the Fermi surface.

(c1,c2) Particle-particle angular correlation during the crossover from polaron to trimer (c1), and from trimer to tetramer (c2).

(d) Energy comparison between \( \mathcal{P}_7(0) \), \( \mathcal{T}_5(0) \) and \( \mathcal{T}_4(0) \).

FIG. 5. (Color Online). Schematics of the crystalline particle-hole configurations and their mutual scattering. The blue and white points denote, respectively, the particle and hole of majority fermions, and the orange point denotes the impurity. In the trimer or tetramer regime, the scattering between different diagonal configurations (a) or between different triangular ones (b) is allowed by multiple scattering processes. All configurations in (a,b) are with the same total momentum \( Q = 0 \) (taking the Fermi sea \( |FS\rangle_N \) as reference). This is in contrast to the molecule case with \( |Q| = k_F \) (c), where different p-h configurations cannot be scattered freely due to the conservation of total \( Q \).

h configuration with the same structure via interactions, without changing the total momentum or costing any energy. This is quite similar to the facilitated three-body scattering between an impurity and two fermions with Rashba spin-orbit coupling[63]. With such high symmetry, the scattering phase space is maximized and the variational energy is expected to be significantly reduced. This is why the full \( \mathcal{P}_7(0) \) ansatz can produce reasonably lower energy than the trimer or tetramer ansatz, as shown in Figs.3(d) and 4(d). Note that the trimer or tetramer ansatz corresponds to a specific hole configuration in Fig.5 (a,b), while with particles scattering freely outside the Fermi sea. Moreover, given the final state (\( \mathcal{P}_7(0) \)) a superposition of all these degenerate configurations, the rotational invariance of the whole system can be recovered. Therefore, the crystalline correlation can only be reflected in the two- and higher-body correlation functions, but not in the one-body density profile.

In addition, it is important to note that the diagonal and regular triangular p-h distributions guarantee the system remain in \( Q = 0 \) sector (take \( |FS\rangle_N \) as reference). This is quite different from the molecule state which belongs to the \( |Q| = k_F \) sector. In this case, different hole configurations cannot be scattered freely due to the conservation of total \( Q \), see also Fig.5(c). Such forbidden scattering is a crucial reason why the molecule ansatz (corresponding to a specific hole configuration in Fig.5(c)) can energetically well approximate the full \( |Q| = k_F \) state in strong coupling regime, see Fig.2(b).

To conclude, when the two-body (dimer) correlation dominates, the system undergoes a first-order transition from polaron (\( Q = 0 \)) to molecule (\( |Q| = k_F \)); while when the three-body (trimer), four-body (tetramer) and
even higher-body correlations dominate, the system just evolves smoothly between different regimes since all these correlations can be harbored within the same $Q = 0$ sector.

Finally, we comment on the difference between the crystalline correlation in Fermi polarons and that in purely few-body systems. In the latter case, the emergence of crystalline correlation only relies on the values of $\eta$ as compared to $\eta_{tr}$, $\eta_{tet}$, etc, with the crystalline radius changing solely with the scattering length[49]. In contrast, in Fermi polaron system, the crystalline correlation gradually emerges near the Fermi surface when the coupling is strong enough. For instance, the triangular correlation appears only after a polaron-trimer-tetramer crossover (Fig.4), but not exists for arbitrary couplings as in the four-body system. In this sense, the majority Fermi sea serves as a many-body reservoir to output few-body correlations required for the Fermi polaron. Moreover, the crystallization in Fermi polarons first appears near the Fermi surface, where the particle-hole excitations play an important role in its emergence. More details can be found in supplementary material[62].

**SUMMARY AND DISCUSSION**

In summary, we have demonstrated the dominant three- and four-body correlations in the mass-imbalanced Fermi polarons in 2D. As increasing the mass ratio or attraction strength between fermions and the impurity, the system is found to evolve smoothly from a polaronic to dressed trimer and tetramer states. Such a crossover is accompanied by the emergence of momentum-space crystallization of majority fermions, as featured by the diagonal or regular triangular structure of $p\cdot h$ excitations nearby the Fermi surface. The emergent crystallization can be detected through the density-density correlation function of majority fermions in momentum space, as having been successfully implemented in cold atoms systems using the atom noise in absorption images[64–69] or the single atom resolved images[70, 71]. Since all the Fermi-Fermi mixtures realized so far, including $^{40}$K-$^6$Li[37–39], $^{16}$Dy-$^{40}$K[40, 41] and $^{53}$Cr-$^6$Li[42], have the mass ratio $\eta > \eta_r = 3.38$[49], we expect that the polaron-trimer-tetramer crossover and its associated crystalline correlations can be readily observed in these Fermi polaron systems once confined in 2D.

Given the robust intrinsic relation between polaron, trimer and tetramer, the conclusion in this work can be generalized to Fermi polaron systems with arbitrarily high-order correlations and in higher dimension. For instance, the $(1+4)$ pentamer bound state can emerge in 2D at a larger $\eta$[49], which is expected to drive a smooth crossover of Fermi polarons further from the dressed tetramer to pentamer regime as increasing the coupling strength. Similar physics is also expected for 3D, where a smooth polaron-trimer crossover and a diagonal crystallization would occur at $\eta > \eta_r = 8.2$[44] and a promising system for its observation is $^{53}$Cs-$^6$Li mixture[42]. Surely, the emergence of crystalline tetramer and pentamer correlations would be even more intriguing on a 3D Fermi sphere, but that would require a larger $\eta$ that is to be achieved in laboratories in future.

Our results shed light on the quantum phases of highly polarized Fermi-Fermi mixtures with mass imbalance. First, the results suggest that if the majority fermions have a much heavier mass than the minorities, the dominant correlation can switch from two-body to three- and even higher-body sectors. As a result, the ground state is no longer a pairing superfluid as extensively studied in literature, but a new quantum state dominated by $n$-body$(n \geq 3)$ correlation. Such a state could be called as a trimer $(n = 3)$ or tetramer $(n = 4)$ superfluid. Secondly, the results suggest the absence of sharp phase transition or phase separation in the highly polarized Fermi-Fermi mixtures with large mass imbalance, where the evolution from the normal to the trimer or tetramer superfluid phases is a smooth crossover. This is in contrast to the equal mass case which supports a first-order transition from the normal to pairing superfluid as well as a phase separation between them[34]. In future, a precise description of such polarized trimer or tetramer superfluid requires the knowledge of effective interactions within trimers, tetramers, and between trimer/tetramer and majority fermions. Finally, the regime with intermediate polarization may exhibit even richer physics due to various competing orders associated with different few-body correlations. Our study thus opens an avenue for searching novel quantum phases beyond the traditional pairing superfluids in the mass-imbalanced fermion systems.

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[1] A. Altland and B. Simons, *Condensed matter field theory* (Cambridge University Press, 2006).
[2] A. N. Wenz, G. Zürn, S. Murmann, I. Brouzos, T. Lompe, S. Jochnim, *From Few to Many: Observing the Formation of a Fermi Sea One Atom at a Time*, Science 342, 457 (2013).
[3] P. Massignan, M. Zaccanti and G. M. Bruun, *Polaron, dressed molecules and itinerant ferromagnetism in ultracold Fermi gases*, Rep. Prog. Phys. 77, 034401 (2014).
[4] L. D. Landau, *Über Die Bewegung der Elektronen in Kristallgitter*, Phys. Z. Sowjetunion 3, 664 (1933).
[5] A. Schirotzek, C.-H. Wu, A. Sommer, and M. W. Zwier-
lein, Observation of Fermi Polarons in a Tunable Fermi Liquid of Ultracold Atoms, Phys. Rev. Lett. 102, 230402 (2009).

[6] S. Nascimbène, N. Navon, K. J. Jiang, L. Tarruell, M. Teichmann, J. McKeever, F. Chevy, and C. Salomon, Collective Oscillations of an Imbalanced Fermi Gas: Axial Compression Modes and Polaron Effective Mass, Phys. Rev. Lett. 103, 170402 (2009).

[7] C. Kohstall, M. Zaccanti, M. Jag, A. Trenkwalder, P. Massignan, G. M. Bruun, F. Schreck, R. Grimm, Metastability and coherence of repulsive polarons in a strongly interacting Fermi mixture, Nature 485, 615 (2012).

[8] M. Koschorreck, D. Pertot, E. Vogt, B. Frölich, M. Feld, M. Köhl, Attractive and repulsive Fermi polarons in two dimensions, Nature 485, 619 (2012).

[9] M. Cetina, M. Jag, R. S. Lous, I. Fritsche, J. T. M. Wal-raven, R. Grimm, J. Levinsen, M. M. Parish, R. Schmidt, M. Knap, E. Demler, Ultrafast many-body interferometry of impurities coupled to a Fermi gas, Science 354, 96 (2016).

[10] F. Scazza, G. Valtolina, P. Massignan, A. Recati, A. Amico, A. Burchianti, C. Fort, M. Inguscio, M. Zaccanti, G. Roati, Repulsive Fermi Polarons in a Resonant Mixture of Ultracold $^6$Li Atoms, Phys. Rev. Lett. 118, 083602 (2017).

[11] Z. Yan, P. B. Patel, B. Mukherjee, R. J. Fletcher, J. Struck, M. W. Zwierlein, Boiling a Unitary Fermi Liquid, Phys. Rev. Lett. 122, 093401 (2019).

[12] G. Ness, C. Shkedrov, Y. Floshaim, O. K. Diesel, J. von Milczewski, R. Schmidt, and Y. Sagi, Observation of a Smooth Polaron-Molecule Transition in a Degenerate Fermi Gas, Phys. Rev. X 10, 041019 (2020).

[13] H. S. Adlong, W. E. Liu, F. Scazza, M. Zaccanti, N. D. Oppong, S. Fölling, M. M. Parish, and J. Levinsen, Quasiparticle Lifetime of the Repulsive Fermi Polaron, Phys. Rev. Lett. 125, 133401 (2020).

[14] N. B. Jørgensen, L. Wacker, K. T. Skalmstang, M. M. Parish, J. Levinsen, Quasiparticle Lifetime of the Repulsive Fermi Polaron in a Bose-Einstein Condensate, Phys. Rev. Lett. 117, 055302 (2016).

[15] M.-G. Hu, M. J. Van de Graaff, D. Kedar, J. P. Corson, E. A. Cornell, D. S. Jin, Bose Polarons in the Strongly Interacting Regime, Phys. Rev. Lett. 117, 055303 (2016).

[16] F. Schmidt, D. Mayer, Q. Bouton, D. Adam, T. Lausch, N. Spethmann, A. Widera, Quantum Spin Dynamics of Individual Neutral Impurities Coupled to a Bose-Einstein Condensate, Phys. Rev. Lett. 121, 130403 (2018).

[17] Z. Z. Yan, Y. Ni, C. Robens, M. W. Zwierlein, Bose polarons near quantum criticality, Science, 368, 190 (2020).

[18] I. Fritsche, C. Barioni, E. Dobler, E. Kirilov, B. Huang, R. Grimm, G. M. Bruun, and P. Massignan, Stability and breakdown of Fermi polarons in a strongly interacting Fermi-Bose mixture, Phys. Rev. A 103, 053314 (2021).

[19] M. Sidler, P. Back, O. Cotlet, A. Srivastava, T. Fink, M. Kroner, E. Demler and A. Imamoglu, Fermi polaron-polaritons in charge-tunable atomically thin semiconductors, Nat. Phys. 13, 255 (2017).

[20] M. Navadeh-Toupci, N. Takemura, M. D. Anderson, D. Y. Oberli, and M. T. Portella-Oberli, Polaritonic Cross Feshbach Resonance, Phys. Rev. Lett. 122, 047402 (2019).

[21] N. V. Prokofev and B. V. Svistunov, Bold diagrammatic Monte Carlo: A generic sign-problem tolerant technique for polaron models and possibly interacting many-body problems, Phys. Rev. B 77, 125101 (2008); Phys. Rev. B 77, 020408 (R) (2008).

[22] R. Combescot, S. Giraud, and X. Leyronas, Analytical theory of the dressed bound state in highly polarized Fermi gases, Europhys. Lett. 88, 60007 (2009).

[23] M. Punk, P. T. Dumitrescu, and W. Zwerger, Polaron-to-molecule transition in a strongly imbalanced Fermi gas, Phys. Rev. A 80, 053605 (2009).

[24] G. M. Bruun and P. Massignan, Decay of Polarons and Molecules in a Strongly Polarized Fermi Gas, Phys. Rev. Lett. 105, 020403 (2010).

[25] R. Schmidt and T. Enss, Excitation spectra and rf response near the polaron-to-molecule transition from the functional renormalization group, Phys. Rev. A 83, 063620 (2011).

[26] C. Trefzger and Y. Castin, Impurity in a Fermi sea on a narrow Feshbach resonance: A variational study of the polaronic and dimeronic branches, Phys. Rev. A 85, 053612 (2012).

[27] M. M. Parish, Polaron-molecule transitions in a two-dimensional Fermi gas, Phys. Rev. A 83, 051603(R) (2011).

[28] J. Vlietinck, J. Ryckebusch, and K. van Houcke, Diagrammatic Monte Carlo study of the Fermi polaron in two dimensions, Phys. Rev. B 89, 055119 (2014).

[29] P. Kroiss and L. Pollet, Diagrammatic Monte Carlo study of quasi-two-dimensional Fermi polarons, Phys. Rev. B 90, 104510 (2014).

[30] X. Cui, Fermi polaron revisited: Polaron-molecule transition and coexistence, Phys. Rev. A 102, 061301(R) (2020).

[31] C. Peng, R. Liu, W. Zhang and X. Cui, Nature of the polaron-molecule transition in Fermi polarons, Phys. Rev. A 103, 063312 (2021).

[32] J.-G. Chen, T.-S. Deng, W. Y. and W. Zhang, Polarons and molecules in a Fermi gas with orbital Feshbach resonance, Phys. Rev. A 94, 053627 (2016).

[33] M. M. Parish, H. S. Adlong, W. E. Liu, J. Levinsen, Thermodynamic signatures of the polaron-molecule transition in a Fermi gas, Phys. Rev. A 103, 023312 (2021).

[34] S. Pilati and S. Giorgini, Phase Separation in a Polarized Fermi Gas at Zero Temperature, Phys. Rev. Lett. 100, 030401 (2008).

[35] G. B. Partridge, W. Li, R. I. Kamar, Y. Xiao, and R. G. Hulet, Pairing and Phase Separation in a Polarized Fermi Gas, Science 311, 503 (2006).

[36] Y. Shin, M. W. Zwierlein, C. H. Schunck, A. Schirotzek, and W. Ketterle, Observation of Phase Separation in a Strongly Interacting Imbalanced Fermi Gas, Phys. Rev. Lett. 97, 030401 (2006).

[37] M. Taglieber, A.-C. Voigt, T. Aoki, T. W. Hänsch, and K. Dieckmann, Quantum Degenerate Two-Species Fermi-Matter Mixture Coexisting with a Bose-Einstein Condensate, Phys. Rev. Lett. 100, 010401 (2008).

[38] E. Wille, F. M. Spiegelhalder, G. Kerner, D. Naik, A. Trenkwalder, G. Hendl, F. Schreck, R. Grimm, T. G. Tiecke, J. T. M. Walraven, S. J. J. M. F. Kokkelmans, E. Tiesinga, and P. S. Julienne, Exploring an Ultracold Fermi-Fermi Mixture: Interspecies Feshbach Resonances and Scattering Properties of $^6$Li and $^{40}$K, Phys. Rev. Lett. 100, 053201 (2008).

[39] A.-C. Voigt, M. Taglieber, L. Costa, T. Aoki, W. Wieser,
SUPPLEMENTARY MATERIAL

In this supplementary material we provide more details for the integral equation and numerical details from \(P_7\) ansatz, as well as the comparison of crystalline correlations in Fermi polarons and few-body systems.

Integral equation and numerical details from \(P_7\) ansatz

Given the \(P_7(\mathbf{Q})\) ansatz (Eq.(2) in the main text), we rescale the coefficients as \(\alpha^{(l)} \equiv \psi^{(l)}/\psi^{(0)}\) and define three auxiliary functions:

\[
f(q) = \frac{g}{S}(1 + \sum_k \alpha^{(1)}_{kq}),
\]

\[
G(k, q', q) = \frac{g}{S} \sum_{k'} (\alpha^{(2)}_{k'kq'q} + \alpha^{(1)}_{kq'} - \alpha^{(1)}_{kq}),
\]

\[
h(k', k, q'', q', q) = \frac{g}{S} \sum_{k''} \alpha^{(3)}_{k''k'kq'q}. \tag{9}
\]

We arrive at the following equations for these functions:

\[
E - \epsilon^{(f)}_\mathbf{q} = \sum_q f(q), \tag{10}
\]

\[
\left[\frac{1}{g} - \sum_{k} \frac{1}{E_{k, q_1}}\right]f(q) = \frac{\sum_q f(q)}{E - \epsilon^{(f)}_\mathbf{q}} - \sum_{k_1 q_1} \frac{G(k_1, q, q_1)}{E_{k_1, q_1}}, \tag{11}
\]

\[
\left[\frac{1}{g} - \sum_{k_1} \frac{1}{E_{k_1, k_2, q_1, q_2}}\right]G(k_2, q_1, q_2) = \alpha^{(1)}_{k_2q_1} - \alpha^{(1)}_{k_2q_2} - \sum_{k_1} \frac{1}{E_{k_1, k_2, q_1, q_2}} G(k_1, q_1, q_2) + \sum_{k_1 q_1 q_2} \frac{h(k_1, k_2, q_1, q_2, q)}{E_{k_1, k_2, q_1, q_2}} \tag{12}
\]

\[
\left[\frac{1}{g} - \sum_{k_1} \frac{1}{E_{k_1, k_2, k_3, q_1, q_2, q_3}}\right]h(k_2, k_3, q_1, q_2, q_3) = \alpha^{(2)}_{k_2k_3q_1, q_2} - \alpha^{(2)}_{k_2k_3q_2, q_3} + \alpha^{(2)}_{k_2k_3q_1, q_3}
\]

\[ + \sum_{k_1} \frac{1}{E_{k_1, k_2, k_3, q_1, q_2, q_3}} [h(k_1, k_2, q_1, q_2, q_3) - h(k_1, k_3, q_1, q_2, q_3)]. \tag{13}
\]

Here the energies are defined as \(E_{k_1 \ldots k_i, q_1 \ldots q_i} = E - \epsilon^{(f)}_\mathbf{P} + \sum_{j=1}^i (\epsilon^{(f)}_{q_j} - \epsilon^{(f)}_{k_j})\), with \(\mathbf{P} = \mathbf{Q} + \sum_{j=1}^i (\mathbf{q}_j - \mathbf{k}_j)\). The scaled coefficients can be represented by the auxiliary functions via

\[
\alpha^{(1)}_{k_1 q_1} = \frac{f(q_1) - \sum_q G(k_1, q, q_1)}{E_{k_1, q_1}}, \tag{14}
\]

\[
\alpha^{(2)}_{k_2 k_3 q_1, q_2} = \frac{1}{E_{k_1, k_2, q_1, q_2}} [G(k_2, q_1, q_2) - G(k_1, q_1, q_2) + \sum_q h(k_1, k_2, q_1, q_2, q)], \tag{15}
\]

\[
\alpha^{(3)}_{k_1 k_2 k_3 q_1, q_2, q_3} = \frac{1}{E_{k_1, k_2, k_3, q_1, q_2, q_3}} [h(k_1, k_2, q_1, q_2, q_3) - h(k_1, k_3, q_1, q_2, q_3) + \sum_q h(k_2, k_3, q_1, q_2, q_3)]. \tag{16}
\]

It is noted that above equations can well reproduce the trimer and tetramer bound states in vacuum by sending \(k_F\) to zero. For instance, by only keeping \(G(k, q_1, q_2) \to G(k)\) terms, Eq.(12) can be reduced to the equation of trimer bound state. Similarly, the tetramer binding energy can be extracted from Eq.(13) by only keeping \(h(k_1, k_2, q_1, q_2, q_3) \to h(k_1, k_2)\) terms.

In principle, the coupled Eqs.(10-13) can be transformed as matrix equation by discretizing each momentum \(\mathbf{q}\) and \(\mathbf{k}\). The energy and wavefunction can then be obtained by directly solving the matrix equation. However, the numerical cost can be very large. For example, when perform the discretization \(7 - 13 - 8 - 13\) with respect to \(q - \theta q - k - \theta k\) in the polar coordinates, the dimension of the corresponding matrix will be \(\sim 10^{10} \times 10^{10}\). Though the dimension can be reduced by utilizing the antisymmetry (due to Fermi statistics) and rotational symmetry of the wavefunctions, the direct solution of the matrix equation is still out of reach.

Instead of solving a large matrix equation, we obtain the energy and wavefunctions using the successive over-relaxation method by iteratively solving the coupled Eqs.(10-13). Specifically, we first set the initial wavefunctions...
Then by substituting them into the right-hand side of the coupled (10-13), we can obtain new wavefunctions $f_i$, $g_i$, $h_i$ and energy $E_i$. Then by substituting them into the right-hand side of the coupled (10-13), we can obtain new wavefunctions $f_i$, $g_i$, $h_i$ and energy $E_i$, which will be treated as the updated initial inputs. In addition, to avoid divergence during the iteration, we introduce a step factor $s$ to control the changes between successive iterations, i.e., we take $(1 - s)f_i + sf_j \rightarrow f_i$, $(1 - s)g_i + sg_j \rightarrow g_i$, $(1 - s)h_i + sh_j \rightarrow h_i$ and $(1 - s)E_i + sE_j \rightarrow E_i$. The iterations stop once the changes of wavefunctions and energies between successive iterations are smaller than the criterions we set. In Fig.(6), we show an example for the numerical process of the iteration.

![Fig. 6](image)

**FIG. 6.** Details of the iterations for mass ratio $\eta = 3$ and interaction strength $\ln(k_F a_{2d}) = -1.15$. (a) Changes of wavefunctions between successive iterations. (b) Energy evolution during the iteration. The discretization is taken as $7 - 13 - 8 - 13$ with respect to $q - \theta_q - k - \theta_k$ in the polar coordinates and the cutoff of momentum is taken as $k_c = 50k_F$.

In our numerics, we have also ensured the convergence of the results with respect to different momentum cutoffs ($k_c$) and discretization scheme. In Fig.(7), we show the energy and weight distributions for mass ratio $\eta = 3$ by choosing different $k_c$ and different momentum discretizations, which show agreement to a good extent.

![Fig. 7](image)

**FIG. 7.** Convergency of the results for mass ratio $\eta = 3$. (a) Energies obtained from discretization $7 - 13 - 8 - 13$ and $7 - 7 - 14 - 19$ with respect to $q - \theta_q - k - \theta_k$ in the polar coordinates. The cutoff of momentum is taken as $k_c = 50k_F$ and $k_c = 180k_F$, respectively. (b) Weight distributions with discretization and momentum cutoff the same as in (a). Lines: $7 - 13 - 8 - 13$ and $k_c = 50k_F$; Symbols: $7 - 7 - 14 - 19$ and $k_c = 180k_F$.

Comparison of crystalline correlation between Fermi polarons and few-body systems

The crystalline correlation in Fermi polarons is very different from that in pure few-body systems. As a concrete example, in Fig.8 we take the mass ratio $\eta = 40/6$ and show the difference of tetramer correlations in Fermi polaron and in 1 + 3 system.

As show in Fig.8 (a1-a4) for the few-body system, the crystalline triangular correlation of heavy fermions exists for all couplings, with the crystalline radius changing solely with $a_{2d}$. In comparison, the triangular correlation in Fermi
polaron gradually emerges after the polaron-trimer-tetramer crossover as increasing the coupling strength, see Fig.8 (b1-b4). Moreover, the triangular structure first shows up near the Fermi surface, indicating an important role of the Fermi sea background and the particle-hole excitations therein for its emergence. All these features are distinct from the few-body case. However, for extremely strong coupling, such as in Fig.8(a4,b4), the correlation profiles are essentially identical between the few-body and polaron systems, due to the very deep tetramer bound state and a much larger crystalline radius ($\gg k_F$). In this case the Fermi sea plays little roles in affecting the correlation profiles.

FIG. 8. (Color Online). Comparison of particle-particle correlation, $D_p(k_0, k)$, between the pure four-body system (a1-a4) and the Fermi polaron system (b1-b4) at mass ratio $\eta = 40/6$. The coupling strengths are $\ln(k_Fa_{2d}) = 1.272(a1,b1), 0.172(a2,b2), -0.328(a3,b3), -0.728(a4,b4)$. Here we take a fixed $k_0 = -1.08k_F$ (as marked by red circle) and show the contour plot of $D_p$ in $k$ space. In (a1-a4), $k_F$ is just a constant momentum unit without any physical meaning; the triangular correlation appears for all couplings and its radius is solely determined by the scattering length. In (b1-b4), the white round area denotes the Fermi sea; the triangular correlation is absent for weak couplings and shows up gradually from the polaron(b1)-trimer(b2)-tetramer(b3) crossover.