# Impurity immersed in a double Fermi sea

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(Received 25 April 2020; revised 16 August 2020; accepted 20 August 2020; published 14 September 2020)

We present a variational calculation of the energy of an impurity immersed in a double Fermi sea of noninteracting fermions. We show that in the strong-coupling regime, the system undergoes a first-order transition between polaronic and trimer states. Our result suggests that the smooth crossover predicted in previous literature for a superfluid background is the consequence of Cooper pairing and is absent in a normal system.

DOI: 10.1103/PhysRevA.102.033322

## I. INTRODUCTION

Introduced for the first time by Landau and Pekar to describe transport properties of electrons in semiconductors [1], polaron physics has become a prototype for other impurity problems in quantum many-body systems, from solid-state [2,3] to nuclear physics [4]. More recently, the crucial role played by polaronic properties in the performances of solar panels has revived the interest for this system in semiconductors, which is now an active field of research in both applied mathematics [5] and fundamental physics [6].

Thanks to the versatility of their experimental investigation tools, ultracold atoms have become over the past decade a remarkable playground for the exploration of quantum many-body physics [7–10]. In this context, polaron physics has been the subject of extensive research, starting from the so-called Fermi polaron, corresponding to an impurity immersed in a spin-polarized Fermi sea [11–17] (see also Ref. [18] for its realization in exciton-polariton systems), to the Bose polaron, where the impurity interacts with a weakly interacting Bose-Einstein condensate [19–21]. The study of dual superfluids of bosons and fermions recently paved the way to the study of a novel type of polaronic system where the impurity is immersed in a spin-1/2 fermionic superfluid [22–24]. This superfluid version of the Fermi polaron interpolates between aforementioned Fermi and Bose polarons, and like in this latter case, three-body physics, and most notably the existence of Efimov trimer states [25,26], play an important role in shaping the phase diagram of the system [27–29]. Using a mean-field description of the superfluid, the generalization of the Fermi-polaron wave function suggested the existence of a crossover between the polaron and trimeron states. In particular, Ref. [28] proposed a variational ansatz

$$|\psi\rangle = \left(\alpha\widehat{b}_0^\dagger + \sum_{\boldsymbol{k},\boldsymbol{k}'}\beta_{\boldsymbol{k},\boldsymbol{k}'}\widehat{b}_{\boldsymbol{k}'}^\dagger\widehat{\gamma}_{\boldsymbol{k},\uparrow}^\dagger\widehat{\gamma}_{-\boldsymbol{k}'-\boldsymbol{k},\downarrow}^\dagger\right)|\mathrm{BCS}\rangle, \tag{1}$$

where $|\mathrm{BCS}\rangle$ is the BCS mean-field ground state, $\widehat{b}_{\boldsymbol{k}}$ is the annihilation operator of an impurity of momentum $\boldsymbol{k}$, and $\gamma_{\boldsymbol{k},s}$ that of the Bogoliubov modes of the underlying superfluid. Under this assumption, the crossover arises from the fact that the $\gamma$'s are linear combinations of creation and annihilation operators of real fermions $\widehat{a}_{\boldsymbol{k},s=\uparrow,\downarrow}$. Indeed, the variational state (1) contains terms proportional to $\widehat{b}^\dagger\widehat{a}_{\boldsymbol{k},s}^\dagger\widehat{a}_{\boldsymbol{k}',-s}^\dagger$ and $\widehat{b}^\dagger\widehat{a}_{\boldsymbol{k},s}^\dagger\widehat{a}_{\boldsymbol{k}',s}$ that describe respectively a trimer made of fermions above the Fermi surface and a polaron dressed by a particle-hole pair. The crossover is here a direct consequence of the mixing between particles and holes induced by the quantum coherence of the superfluid state and trimers can be interpreted as bound states between the impurity and preexisting Cooper pairs. The question that naturally arises is then the existence of such a crossover in a normal system. Here, we analyze this question by considering the interaction of an impurity with an ideal gas of spin-1/2 fermions. By considering a variational ansatz incorporating two particle-hole excitations we suggest that the crossover is suppressed in the absence of Cooper pairing and is replaced by a sharp (first-order-like) transition between a polaron and a trimer branch. We show that this transition is driven by the onset of momentum correlations between holes of the background Fermi seas which can be associated with two subspaces that are uncoupled by the many-body Hamiltonian and leading to the suppression of the center of mass of the trimer.

## II. GENERAL FRAMEWORK

We consider an impurity of mass $m_i$ coupled to a Fermi sea of *noninteracting* spin-1/2 fermions of mass $m$. In the ultracold regime, matter waves do not resolve the microscopic details of the interatomic potential [30]. We therefore describe the system using an effective two-channel model known to

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give rise to Efimov trimers without requiring any additional physical ingredient [31]. Assuming periodic boundary conditions in a box of quantization volume $\Omega$, the Hamiltonian then takes the general form

$$\begin{aligned}\hat{H} = &\sum_{\boldsymbol{k},s}\frac{\hbar^2k^2}{2m}\hat{a}^\dagger_{\boldsymbol{k},s}\hat{a}_{\boldsymbol{k},s} + \sum_{\boldsymbol{k}}\frac{\hbar^2k^2}{2m_i}\hat{b}^\dagger_{\boldsymbol{k}}\hat{b}_{\boldsymbol{k}}\\ &+\sum_{\boldsymbol{k}}\left(\frac{\hbar^2k^2}{2M}+E_0\right)\hat{c}^\dagger_{\boldsymbol{k},s}\hat{c}_{\boldsymbol{k},s}\\ &+\frac{\Lambda}{\sqrt{\Omega}}\sum_{\boldsymbol{k},\boldsymbol{k}'}[\hat{a}_{\boldsymbol{k}s}\hat{b}_{\boldsymbol{k}'}\hat{c}^\dagger_{\boldsymbol{k}+\boldsymbol{k}',s}+\text{H.c.}],\end{aligned}\tag{2}$$

where $\hat{a}_{\boldsymbol{k},s}$ is the annihilation operator of a fermion of spin $s$ and momentum $\hbar\boldsymbol{k}$, $\hat{b}_{\boldsymbol{k}}$ is the annihilation operator of an impurity, and $\widehat{c}_{\boldsymbol{k},s}$ is the annihilation operator of a molecule made of an impurity and a spin-$s$ atom. $E_0$ and $M = m + m_i$ are the binding energy and the mass of the bare molecules. For the sake of simplicity, we match the experimental parameters of Re. [22] where a mixture of fermionic $^6$Li and bosonic $^7$Li was used. In this system, the interactions between the impurity and each spin component are the same and $m_i \simeq m$. The coupling $\Lambda$ does not depend on momentum [32,33], but a UV cutoff $k_c$ is introduced to match the scattering length $a$ and the effective range $R_e$ of the true potential using the following relations [31]:

$$\frac{1}{a} = \frac{2k_c}{\pi} - \frac{2\pi\hbar^2E_0}{m^*\Lambda^2}, \qquad R_e = \frac{\pi\hbar^4}{m^{*2}\Lambda^2},\tag{3}$$

where $m^*$ is the reduced mass of the impurity-fermion pair.

We search for the ground-state energy within a variational space spanned by the states depicted in Fig. 1. This space can be divided into two sectors. The polaron sector is spanned by state $|0\rangle$, which corresponds to the impurity sitting at the center of the two unperturbed Fermi seas, and single particle-hole states $|\boldsymbol{q}_1\rangle_s$ and $|\boldsymbol{q}_1, \boldsymbol{k}_1\rangle_s$ where a hole of spin $s$ and momentum $\boldsymbol{q}_1$ is accompanied by either a bound or unbound impurity-fermion pair. The Efimov sector is characterized by states $|\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{k}_1\rangle_s$ and $|\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{k}_1, \boldsymbol{k}_2\rangle$ containing both one hole in each Fermi sea.

The general structure of a variational state is therefore

$$\begin{aligned}|\psi\rangle = &A|0\rangle + \sum_{\boldsymbol{q}_1,s}B_s(\boldsymbol{q}_1)|\boldsymbol{q}_1\rangle_s + \sum_{\boldsymbol{q}_1,\boldsymbol{k}_1,s}C_s(\boldsymbol{q}_1,\boldsymbol{k}_1)|\boldsymbol{q}_1,\boldsymbol{k}_1\rangle_s\\ &+\sum_{\boldsymbol{q}_1,\boldsymbol{q}_2,s}D_s(\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{k}_1)|\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{k}_1\rangle_s\\ &+\sum_{\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{k}_1,\boldsymbol{k}_2}E(\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{k}_1,\boldsymbol{k}_2)|\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{k}_1,\boldsymbol{k}_2\rangle\end{aligned}\tag{4}$$

with $q_i < k_F$ and $k_i > k_F$ and where $k_F$ is the Fermi wave vector of the background fermions. For spin-balanced Fermi seas, the interactions of the impurity with the two spin components are identical. We can thus assume that the amplitudes $B_s$, $C_s$, and $D_s$ do not depend on $s$ and within this subspace we explore two families of variational states.

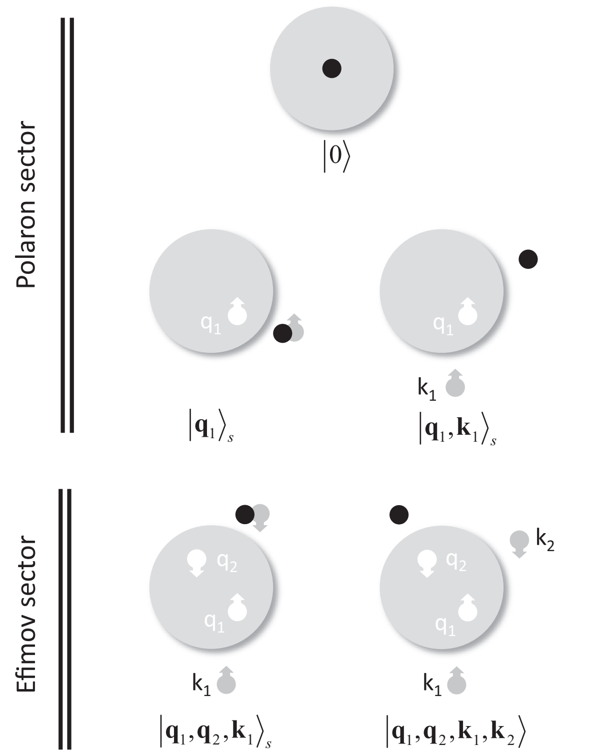


FIG. 1. Structure of the variational Hilbert space. In the first two rows, the polaronic state is created by the impurity and one particle-hole excitation; in the third row, a second particle-hole excitation allows for the trimer to exist.

### III. POLARON SECTOR

The polaronic sector corresponds to $D = E = 0$. The corresponding ansatz generalizes the approach successfully used to describe the Fermi polaron problem, i.e., an impurity immersed in a spin-polarized Fermi sea [11]. In particular this trial wave function recovers the exact perturbative expansion of the energy of the polaron up to second order in scattering length. In the following, we assume that the impurity has the same mass as the fermions: $m_i = m$.

The minimization of the energy $W$ with respect to $A$, $B$, and $C$ in the polaronic sector can be reduced to a single scalar equation $P_W = 0$ with

$$P_W = W - \frac{2}{\Omega}\sum_{q<k_F}\frac{1}{\Delta_{\boldsymbol{q}}(W)}\tag{5}$$

and

$$\begin{aligned}\Delta_{\boldsymbol{q}}(W) = \frac{m}{4\pi\hbar^2}\Bigg\{&a^{-1} - R_e\left(\lambda^2 - \frac{q^2}{4}\right) - \frac{2}{\pi}k_F\\ &+\frac{4\pi}{\Omega}\sum_{k>k_F}\frac{1}{\lambda^2+k^2-\boldsymbol{k}\cdot\boldsymbol{q}} - \frac{1}{k^2}\Bigg\},\end{aligned}\tag{6}$$

where $W = -\hbar^2\lambda^2/m$ is the ground-state energy.

In the perturbative regime $k_Fa \to 0^-$, the energy of the polaron can be expanded as

$$W = \frac{8\pi\hbar^2a}{m}n_F\left(1 + \frac{3}{2\pi}k_Fa + \cdots\right).\tag{7}$$

At this order, the variational result recovers the exact perturbative expansion and amounts to twice the interaction energy with a single spin component. Because of the dependence of $\Delta_q$ with respect to the energy $W$, this coincidence does not extend beyond that order though. For instance, at the unitary limit $|a| = \infty$, we know that for a single component Fermi sea, the energy of the polaron is $W_{\rm FP} \simeq -0.606\,E_F$ [11–13], where $E_F = \hbar^2 k_F^2/2m$ is the Fermi energy of the background fermions, while for a two-component system, we find $|W| \simeq 1.026 E_F < 2|W_{\rm FP}|$, meaning that, contrary to the perturbative expression, the interaction energy of the polaron with the two Fermi seas is not additive in the strong-coupling regime.

## IV. EFIMOV SECTOR

We now consider the opposite limit $A = B = C = 0$ corresponding to the formation of a ground-state Efimov trimer above the Fermi surface.

As a reference, we first consider the energy of the trimer in the absence of a Fermi sea that is obtained as a solution of Skornyakov and Ter-Martirosyan's equation [26]

$$\left[\frac{1}{4\pi}\left\{a^{-1} - R_e\left(\lambda^2 + \frac{3}{4}k^2\right)\right\} + \frac{1}{\Omega}\sum_{k'}\left(\frac{1}{\lambda^2 + k^2 + k'^2 + \boldsymbol{k}\cdot\boldsymbol{k}'} - \frac{1}{k'^2}\right)\right]D(k) + \frac{1}{\Omega}\sum_{k'}\frac{D(k')}{\lambda^2 + k^2 + k'^2 + \boldsymbol{k}\cdot\boldsymbol{k}'} = 0. \quad (8)$$

In this case, the only relevant dimensionless parameter is $R_e/a$ and we observe that the trimer merges with the atomic continuum for a scattering length $a_-$ such that $R_e/a_- = -2 \times 10^{-4}$. It means that in our situation, where only the impurity-fermion interactions are resonant, the three-body bound states essentially exist only in a regime where an impurity-fermion bound state is also stable. This is to be contrasted with the more traditional three-boson problem for which all three interactions are resonant and Efimov trimers are stable deep in the domain where two-body bound states are unstable [31] (in this case we have indeed $R_e/a_- \simeq -0.1$).

We consider next the effect of the Fermi sea on the energy of the trimer. In a first approach we simply assume that its role is to prevent the fermions above the Fermi surface from occupying states below $k_F$, in a manner very similar to the celebrated Cooper pairing problem for pairs of fermions in superconductors. These "Cooper-like" trimer states correspond to locating hole momenta $\boldsymbol{q}_{1,2}$ on the Fermi surface, and having $\boldsymbol{q}_1 + \boldsymbol{q}_2 = 0$ to cancel the center-of-mass momentum of the trimer. The energy of the trimer state is then the solution of

$$\left[\frac{1}{4\pi}\left\{a^{-1} - \frac{2}{\pi}k_F - R_e\left(\lambda^2 - k_F^2 + \frac{3}{4}k^2\right)\right\} + \frac{1}{\Omega}\sum_{k'>k_F}\left(\frac{1}{\lambda^2 - k_F^2 + k^2 + k'^2 + \boldsymbol{k}\cdot\boldsymbol{k}'} - \frac{1}{k'^2}\right)\right]D(k) + \frac{1}{\Omega}\sum_{k'>k_F}\frac{D(k')}{\lambda^2 - k_F^2 + k^2 + k'^2 + \boldsymbol{k}\cdot\boldsymbol{k}'} = 0. \quad (9)$$

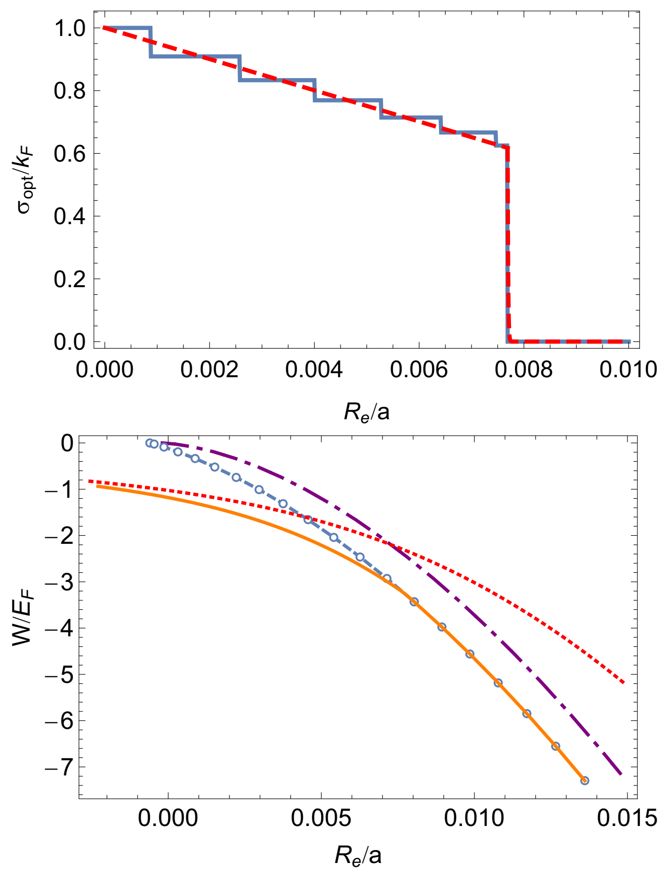


FIG. 2. Variational ground state in the polaron-trimeron space for $k_F R_e = 10^{-2}$. Top: Optimal value of the width $\sigma$ of the hole-pair wave function (solid blue line). $\sigma$ was varied over a finite set of values between between zero and 1 (see text). For $R_e/a \lesssim 0.0077$, each step corresponds to a jump from one value of $\sigma$ to the next and is therefore an artifact of the discretization of $\sigma$. The red dashed line corresponds to a smooth interpolation. For $R_e/a \simeq 0.0077$, we observe a jump of the value of $\sigma$ which straddles several consecutive values of $\sigma$ and thus marks a discontinuity between a Cooper-like trimer and a polaron-trimeron crossover state. Bottom: Energy of the variational state. Cooper-like trimer ($\sigma = 0$, open blue circles), compared to the energy of an Efimov trimer in vacuum (purple dash-dotted line). The ground state associated with the optimal value of $\sigma$ is the solid orange line. The purely orange section of the line corresponds to finite width hole pair wave functions $F$ while the dotted section corresponds to Cooper-like trimers ($\sigma = 0$).

This equation is very similar to Eq. (8), the main difference stemming from the sums over momenta that are now restricted to $k > k_F$ and the shift of the energy associated with the chemical potential of the two fermions that were removed from the Fermi seas to create the trimer. The corresponding ground-state energy is plotted in Fig. 2 for an experimentally relevant value $k_F R_e \simeq 10^{-2}$ ($k_F \approx 10^7\ \mathrm{m}^{-3}$ typically and we take $R_e$ on the order of $50 a_0$, where $a_0$ is the Bohr radius, that corresponds to a typical van der Waals length for alkali-metal atoms [34]). We observe that like for traditional Cooper pairing the presence of the Fermi sea stabilizes the trimer.

We can generalize this result by considering trimer amplitudes $D_s$ and $E$ of the form

$$D_s(\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{k}_1)=F(\boldsymbol{q}_1,\boldsymbol{q}_2)\tilde{D}(\boldsymbol{k}_1), \tag{10}$$

$$E(\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{k}_1,\boldsymbol{k}_2)=F(\boldsymbol{q}_1,\boldsymbol{q}_2)\tilde{E}(\boldsymbol{k}_1,\boldsymbol{k}_2), \tag{11}$$

where the Cooper-like trimer corresponds to $F(\boldsymbol{q}_1,\boldsymbol{q}_2)=\delta_{\boldsymbol{q}_1,-\boldsymbol{q}_2}\widetilde{F}(q_1)$, where $\widetilde{F}$ is peaked near the Fermi surface. We choose the following normalization for the function $F(\boldsymbol{q}_1,\boldsymbol{q}_2)$: $\sum_{q_1,q_2}|F(\boldsymbol{q}_1,\boldsymbol{q}_2)|^2=N_F^2$, where $N_F$ is the total number of fermions per spin state.

Once again, we can eliminate $E$ and we see that at fixed $F$, $\tilde{D}$ is a solution of a Skornyakov–Ter-Martirosyan-like equation:

$$\begin{aligned}&\left[\frac{1}{4\pi}\left\{a^{-1}-\frac{2}{\pi}k_F-R_e\left(\lambda^2+\frac{3}{4}k^2-\frac{\langle(\boldsymbol{q}_1-\boldsymbol{q}_2)^2\rangle}{4}\right)\right\}\right.\\&\left.+\frac{1}{\Omega}\sum_{k'>k_F}\left(\frac{1}{\lambda^2+\langle\boldsymbol{q}_1\cdot\boldsymbol{q}_2\rangle+k^2+k'^2+\boldsymbol{k}\cdot\boldsymbol{k}'}-\frac{1}{k'^2}\right)\right]\tilde{D}(k)\\&+\frac{1}{\Omega}\sum_{k'>k_F}\frac{\tilde{D}(k')}{\lambda^2+\langle\boldsymbol{q}_1\cdot\boldsymbol{q}_2\rangle+k^2+k'^2+\boldsymbol{k}\cdot\boldsymbol{k}'}=0\end{aligned} \tag{12}$$

with $\langle f(\boldsymbol{q}_1,\boldsymbol{q}_2)\rangle=\sum_{q_i}|F(\boldsymbol{q}_1,\boldsymbol{q}_2)|^2f(\boldsymbol{q}_1,\boldsymbol{q}_2)/N_F^2$, and where we assumed that the distribution $|F|^2$ is an even function of $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$. Comparing Eqs. (9) and (12) we see that their respective energies are simply translated one with respect to the other since we have

$$\begin{aligned}W_F(R_e/a)=W_C\big(R_e/a+R_e^2\langle(\boldsymbol{q}_1+\boldsymbol{q}_2)^2\rangle/4\big)\\-\frac{\hbar^2}{m}\big(k_F^2+\langle\boldsymbol{q}_1\cdot\boldsymbol{q}_2\rangle\big).\end{aligned} \tag{13}$$

This mapping corresponds to a translation of both the argument and the value of $W_c$ and in practice we observe that the latter dominates. Since $q_1$ and $q_2$ are bounded by the Fermi wave vector $k_F$, we see that $k_F^2+\langle\boldsymbol{q}_1\cdot\boldsymbol{q}_2\rangle$ is always positive and the Cooper-like ansatz is always the optimal choice.

## V. POLARON-TRIMERON COUPLING

We now study the hybridization of the polaronic and Efimov sectors by minimizing the energy with respect to all five amplitudes $A$, $B$, $C$, $D$, and $E$. From the previous analysis, we would expect that the optimal choice would be to mix the polaron wave function with the Cooper-like trimer. However, as we show below, these two sectors are not coupled at the thermodynamic limit. Indeed, the normalization of the state of a Cooper-like trimer requires that

$$\begin{aligned}|A|^2&+2\sum_{\boldsymbol{q}_1}|B(\boldsymbol{q}_1)|^2+2\sum_{\boldsymbol{q}_1,\boldsymbol{k}_1}|C(\boldsymbol{q}_1,\boldsymbol{k}_1)|^2\\&+2\sum_{\boldsymbol{q}_1,\boldsymbol{k}_1}|D(\boldsymbol{q}_1,-\boldsymbol{q}_1,\boldsymbol{k}_1)|^2\\&+\sum_{\boldsymbol{q}_1,\boldsymbol{k}_1,\boldsymbol{k}_2}|E(\boldsymbol{q}_1,-\boldsymbol{q}_1,\boldsymbol{k}_1,\boldsymbol{k}_2)|^2=1.\end{aligned} \tag{14}$$

For large quantization volumes, the sums are turned into integrals and in the normalization each sum gives rise to a density-of-states prefactor $\Omega/(2\pi)^3$. To recover results that do not depend on $\Omega$, we see that $A$ should not depend on $\Omega$ and $B$, $C$, $D$, and $E$ should respectively scale like

$$\begin{aligned}B&=\frac{b(\boldsymbol{q}_1)}{\sqrt{\Omega}},\quad D(\boldsymbol{q}_1,-\boldsymbol{q}_1,\boldsymbol{k}_1)=\frac{d(\boldsymbol{q}_1,\boldsymbol{k}_1)}{\Omega},\\C&=\frac{c(\boldsymbol{q}_1,\boldsymbol{k}_1)}{\Omega},\quad E(\boldsymbol{q}_1,-\boldsymbol{q}_1,\boldsymbol{k}_1,\boldsymbol{k}_2)=\frac{e(\boldsymbol{q}_1,\boldsymbol{k}_1,\boldsymbol{k}_2)}{\Omega^{3/2}},\end{aligned} \tag{15}$$

where $b$, $c$, $d$, and $e$ do not depend on the size of the system. (For unrestricted hole momenta $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$, $C$ and $D$ would scale as $1/\Omega^{3/2}$ and $1/\Omega^2$, respectively.) Under this assumption, the interaction term of the Hamiltonian can be recast as

$$\begin{aligned}\langle\widehat{H}_{\rm int}\rangle=\Lambda&\left[\int\frac{d^3\boldsymbol{q}_1}{(2\pi)^3}A^*b(\boldsymbol{q}_1)+\int\frac{d^3\boldsymbol{q}_1d^3\boldsymbol{k}_1}{(2\pi)^6}b(\boldsymbol{q}_1)^*c(\boldsymbol{q}_1,\boldsymbol{k}_1)\right.\\&+\int\frac{d^3\boldsymbol{q}_1d^3\boldsymbol{k}_1}{(2\pi)^6\sqrt{\Omega}}c(\boldsymbol{q}_1,\boldsymbol{k}_1)^*d(\boldsymbol{q}_1,\boldsymbol{k}_1)\\&\left.+\int\frac{d^3\boldsymbol{q}_1d^3\boldsymbol{k}_1d^3\boldsymbol{k}_2}{(2\pi)^9}d(\boldsymbol{q}_1,\boldsymbol{k}_1)^*e(\boldsymbol{q}_1,\boldsymbol{k}_1,\boldsymbol{k}_2)\right]\\&+\text{c.c.}\end{aligned} \tag{16}$$

In this expression, we see that the energy does not depend on the quantization volume, except for the term coupling the amplitudes $c$ and $d$ which vanishes as $1/\sqrt{\Omega}$ for diverging $\Omega$ thus showing that, in this limit, the polaron and Cooper-like trimer sectors are decoupled.

To explore a possible polaron-trimeron crossover we therefore need to relax the constraint on the vanishing center-of-mass momentum characterizing the Cooper-like trimer state. For this purpose we consider a trial wave function $F(\boldsymbol{q}_1,\boldsymbol{q}_2)=F_0e^{-\boldsymbol{q}_1\cdot\boldsymbol{q}_2/2\sigma^2}$, where $F_0$ is a normalization constant. Just like for the Cooper-like trimer, this amplitude is maximum when $\boldsymbol{q}_1+\boldsymbol{q}_2=0$ and when both momenta are on the Fermi surface. The parameter $\sigma$ allows us to tune continuously the width of the hole wave function between a uniform distribution and the Cooper-like trimer configuration. The Cooper-like trimer corresponds to $\sigma=0$ while the opposite limit ($\sigma=\infty$) corresponds to a uniform distribution $F$.

The minimization of the energy with respect to the amplitudes $A,B,\ldots,E$ yields the following set of coupled equations (see Appendix B for derivation) on $\tilde{A}=A/(\sqrt{\Omega}N_F\Lambda)$ and $\tilde{D}$ generalizing Eqs. (5) and (12):

$$P_W\tilde{A}=\frac{2}{\Omega}\sum_{\mathbf{k}}h(k)\tilde{D}(k), \tag{17}$$

$$\mathcal{T}[\tilde{D}](k)=h(k)\tilde{A}+f(k)\tilde{D}(k)+\frac{1}{\Omega}\sum_{\mathbf{k}'}g(\mathbf{k},\mathbf{k}')\tilde{D}(k'), \tag{18}$$

where $\mathcal{T}$ is the operator from Eq. (12) (times $m/\hbar^2$), and the coupling functions $h$, $f$, and $g$ are

$$h(k)=-\frac{m}{\hbar^2\Omega}\sum_{\mathbf{q}}\frac{\beta(q)}{(\lambda^2+k^2-\boldsymbol{q}\cdot\boldsymbol{k})\Delta_{\boldsymbol{q}}},$$

$$f(k)=-\frac{m}{\hbar^2\Omega}\sum_{\mathbf{q}}\frac{\beta(q)^2}{\lambda^2+k^2-\boldsymbol{q}\cdot\boldsymbol{k}},$$

$$g(\mathbf{k},\mathbf{k}') = \frac{m^2}{\hbar^4\Omega}\sum_{\mathbf{q}}\frac{\beta(q)^2}{(\lambda^2+k^2-\boldsymbol{q}\cdot\boldsymbol{k})(\lambda^2+k'^2-\boldsymbol{q}\cdot\boldsymbol{k}')\Delta_{\boldsymbol{q}}},$$
$$\beta(q) = \frac{1}{N_F}\sum_{\mathbf{q}'}F(\mathbf{q},\mathbf{q}'), \quad (19)$$

and where $\Delta_{\boldsymbol{q}}$ is defined in Eq. (6). Functions $f$, $g$, and $h$ describe the coupling between the polaron and trimer sectors. If we set them equal to zero then Eqs. (17) and (18) simply yield the equations of the polaron and trimeron sectors obtained earlier.

The results of the minimization are displayed in Fig. 2 (see Appendix A for details on the numerical calculation). For each value of $R_e/a$ we solve Eqs. (17) and (18) for a fixed set of values of $\sigma$ ($\sigma \in \{0, 0.1, 0.125, 0.2, 0.25, 0.4, 0.5, 0.625, 0.67, 0.71, 0.77, 0.83, 0.91, 1\}$, $\sigma = 0$ corresponding to the Cooper-like trimer). For each value of $R_e/a$ we search for the optimal value of $\sigma_{\rm opt}$ that minimizes the energy of the impurity. The corresponding values of $\sigma_{\rm opt}$ are displayed in Fig. 2. For $R_e/a \lesssim 7.7 \times 10^{-3}$, we observe that the optimum value decreases smoothly (in this regime the steps are just due to the discrete values of $\sigma$) and drops to $\sigma_{\rm opt} = 0$ (corresponding to the Cooper-like trimer) at $R_e/a \simeq 7.7 \times 10^{-3}$ that suggests a sharp transition to the Cooper-like trimer state. The variational ground-state energy corresponding to $\sigma = \sigma_{\rm opt}$ is displayed in the lower panel of Fig. 2, as well as the energy of the polaron state, and of the Cooper-like trimer. On this graph, we clearly see that for weak attractive interactions ($R_e/a \to -\infty$), the variational states converge to the polaron energy and that the ground-state abruptly jumps to the Cooper-like trimer state in the vicinity of $R_e/a \simeq 7.7 \times 10^{-3}$. Note that this critical value depends on $k_F R_e$ and should converge to $R_e/a_-$ for vanishing fermionic density.

## VI. CONCLUSION

From our variational approach, we conclude that the ground state of an impurity immersed in a noninteracting mixture of spin-1/2 fermions undergoes a first-order transition between a polaronic and a trimer state. This is different from the case of superfluid background where the presence of Cooper pairs allows for a crossover between these two states. We attribute this difference to the absence of coupling at the thermodynamic limit between the vector space spanned by the polaron and that of the trimer state. In the strongly attractive limit, the energy of the Cooper-like trimer is lowered thanks to the exact cancellation of its center-of-mass motion. A similar situation seems to occur in the Fermi polaron for the transition between the polaron and dimer [35–38] and trimer [17] states. More generally our approach can help in understanding the transition between few-body states in a many-body environment, such as the recently reported trimer and dimer avoided crossing for the Efimov ground state [39]. Finally, a natural extension of this work would be to study the existence of such a transition in the case of the *normal* state of an interacting fermionic background to understand the relative role of pairing and superfluidity in this problem.

## ACKNOWLEDGMENTS

The authors thank F. Werner, K. van Houcke, S. Giorgini, C. Lobo, L. Khaykovich, and C. Salomon for helpful discussions. F. Chevy and R. Alhyder acknowledge support from ERC (advanced grant CritiSup2) and Fondation Simone et Cino del Duca.

## APPENDIX A: NUMERICAL CALCULATION

The energy spectrum of Eq. (18) can be obtained numerically. In the following we put $\hbar$ and $m$ to unity for simplicity. We use the following parameters:

$$x = \lambda R_e, \quad y = k_F/\lambda,$$
$$k = \lambda\sinh(\xi), \quad \phi(\xi) = \lambda\sinh(\xi)D(\lambda\sinh(\xi)). \quad (A1)$$

With this we can write Eq. (18) as follows:

$$\mathcal{M}(x,y,a)\tilde{\phi} = 0, \quad (A2)$$

where $\mathcal{M}$ is a nonsymmetric square matrix. Its elements have the following form:

$$\mathcal{M}_i(\xi,\xi',x,y,a) = \delta(\xi,\xi')\mathcal{M}_D(\xi,x,y,a) + \epsilon\int_0^{2\pi}d\phi\int_0^{\pi}d\theta\,\sin(\theta)\cosh(\xi') \times \sinh^2(\xi')\mathcal{M}_N(\xi,\xi',x,y,a), \quad (A3)$$

where $\epsilon$ is a discretization step we choose in order to have a convergent value of the unknown variable. We note that $\epsilon = \xi'_{\rm max}/N_p$ where $\xi'$ is the cutoff of the integral over $\xi'$ and $N_p$ is the number of points per row. Note also that $\xi, \xi' > {\rm asinh}(y)$. We define the two functions $\mathcal{M}_D$ and $\mathcal{M}_N$ as follows:

$$\mathcal{M}_N(\xi,\xi',x,y,a) = \frac{1}{\lambda^2 I(\xi,\xi')} + \frac{2h(\xi)h(\xi')}{P_W} + g(\xi,\xi') \quad (A4)$$

and

$$\mathcal{M}_D(\xi',x,y,a) = f(\xi) - \frac{\lambda}{4\pi}\left\{\left(1+\frac{3}{4}\sinh(\xi)^2 - \langle(\boldsymbol{q}_1-\boldsymbol{q}_2)^2\rangle/(4\lambda^2)\right)\lambda R_e - \frac{1}{\lambda a} + \frac{2k_F}{\pi\lambda}\right\} - \frac{1}{\lambda^2\Omega}\sum_{\xi'>{\rm asinh}(y)}\frac{1}{I(\xi,\xi')}, \quad (A5)$$

where

$$I(\xi,\xi') = 1 + \langle\boldsymbol{q}_1\cdot\boldsymbol{q}_2\rangle/\lambda^2 + \sinh^2(\xi) + \sinh^2(\xi') + \sinh(\xi)\sinh(\xi')\cos(\theta) \quad (A6)$$

and $g$ and $h$ are functions defined in Eq. (19), after the proper variable change. By fixing the value of $k_F R_e$ and for each value of $x = x_c$, we search the smallest value of $1/\lambda a$ which verifies the equation

$$\det[\mathcal{M}(x_c,y_c,a)] = 0. \quad (A7)$$

Note that the results in Fig. 2 are obtained using a total number of points $N_p = 350$ and $\xi'_{\rm max} = 10$.

## APPENDIX B: DERIVATION OF POLARON-TRIMERON COUPLED EQUATIONS

We minimize $\langle\psi|\hat{H}|\psi\rangle$ with the condition that we keep $\langle\psi|\psi\rangle$ constant, and for that we use a Lagrange multiplier which is the energy $W$ in this case. We write this formally:

$$\delta\langle\psi|\hat{H}|\psi\rangle - W\delta\langle\psi|\psi\rangle = 0. \tag{B1}$$

Since we have a wave function with five parameters $A$, $B$, $C$, $D$, and $E$, we need to solve a system of five equations resulting from deriving Eq. (B1) with respect to each of the parameters. In the following we take $\hbar = 1$; we take also the masses of the impurity and the fermions to be equal to 1.

With respect to $E^*(\boldsymbol{k}_1, \boldsymbol{k}_2)$,

$$\begin{aligned}\big(W - k_1^2 - k_2^2 - \boldsymbol{k}_1\cdot\boldsymbol{k}_2 - \langle\boldsymbol{q}_1\cdot\boldsymbol{q}_2\rangle\big)E(\boldsymbol{k}_1,\boldsymbol{k}_2)\\ = \frac{\Lambda}{\sqrt{\Omega}}(D(\boldsymbol{k}_1) + D(\boldsymbol{k}_2)).\end{aligned} \tag{B2}$$

With respect to $D^*(\boldsymbol{k}_1)$,

$$\begin{aligned}\left(W - E_0 - \frac{3k_1^2}{4} + \frac{1}{4}\langle(\boldsymbol{q}_1 - \boldsymbol{q}_2)^2\rangle\right)D(\boldsymbol{k}_1)\\ = \frac{\Lambda}{\sqrt{\Omega}N_F}\sum_{\boldsymbol{q}_1}\beta(\boldsymbol{q}_1)C(\boldsymbol{q}_1,\boldsymbol{k}_1) + \frac{\Lambda}{\sqrt{\Omega}}\sum_{\boldsymbol{k}_2}E(\boldsymbol{k}_1,\boldsymbol{k}_2).\end{aligned} \tag{B3}$$

We can plug the expression of $E(\boldsymbol{k}_1, \boldsymbol{k}_2)$ from Eq. (B2) to have a single expression for $C$ and $D$:

$$\begin{aligned}&\Bigg(W - E_0 - \frac{3k_1^2}{4} + \frac{1}{4}\langle(\boldsymbol{q}_1 - \boldsymbol{q}_2)^2\rangle\\ &- \frac{\Lambda^2}{\Omega}\sum_{\boldsymbol{k}_2}\frac{1}{W - k_1^2 - k_2^2 - \boldsymbol{k}_1\cdot\boldsymbol{k}_2 - \langle\boldsymbol{q}_1\cdot\boldsymbol{q}_2\rangle}\Bigg)D(\boldsymbol{k}_1)\\ &- \frac{\Lambda^2}{\Omega}\sum_{\boldsymbol{k}_2}\frac{D(\boldsymbol{k}_2)}{W - k_1^2 - k_2^2 - \boldsymbol{k}_1\cdot\boldsymbol{k}_2 - \langle\boldsymbol{q}_1\cdot\boldsymbol{q}_2\rangle}\\ &= \frac{\Lambda}{N_F\sqrt{\Omega}}\sum_{\boldsymbol{q}_1}\beta(\boldsymbol{q}_1)C(\boldsymbol{q}_1,\boldsymbol{k}_1).\end{aligned} \tag{B4}$$

When $C = 0$ this equation describes three particles with zero center-of-mass momentum, which represents the trimer (Efimov problem).

With respect to $C^*(\boldsymbol{q}_1, \boldsymbol{k}_1)$,

$$C(\boldsymbol{q}_1,\boldsymbol{k}_1) = \frac{\Lambda}{\sqrt{\Omega}}\frac{B(\boldsymbol{q}_1) + N_F\beta(\boldsymbol{q}_1)D(\boldsymbol{k}_1)}{W - k_1^2 + \boldsymbol{q}_1\cdot\boldsymbol{k}_1}. \tag{B5}$$

With respect to $B^*(q_1)$,

$$B(\boldsymbol{q}_1) = \frac{\Lambda}{\sqrt{\Omega}}\frac{A + \sum_{\boldsymbol{k}_1}C(\boldsymbol{q}_1,\boldsymbol{k}_1)}{W - E_0 + \frac{q_1^2}{4}}. \tag{B6}$$

We can plug in the expression of $C$ from Eq. (B5):

$$B(\boldsymbol{q}_1) = \frac{1}{\Lambda\sqrt{\Omega}}\frac{A}{\Delta(\boldsymbol{q}_1)} + \frac{1}{\Omega}\frac{N_F}{\Delta(\boldsymbol{q}_1)}\sum_{\boldsymbol{k}_1}\frac{\beta(\boldsymbol{q}_1)D(\boldsymbol{k}_1)}{W - k_1^2 + \boldsymbol{q}_1\cdot\boldsymbol{k}_1}. \tag{B7}$$

With respect to $A^*$,

$$WA = 2\frac{\Lambda}{\sqrt{\Omega}}\sum_{\boldsymbol{q}_1}B(\boldsymbol{q}_1) \tag{B8}$$

We plug in $B$ from Eq. (B7):

$$\begin{aligned}\underbrace{\left(W - 2\frac{1}{\Omega}\sum_{\boldsymbol{q}_1}\frac{1}{\Delta(\boldsymbol{q}_1)}\right)A}_{\mathcal{P}_W}\\ = 2\frac{\Lambda N_F}{\Omega^{3/2}}\sum_{\boldsymbol{q}_1,\boldsymbol{k}_1}\frac{1}{\Delta(\boldsymbol{q}_1)}\frac{\beta(\boldsymbol{q}_1)D(\boldsymbol{k}_1)}{W - k_1^2 + \boldsymbol{q}_1\cdot\boldsymbol{k}_1}.\end{aligned} \tag{B9}$$

If $D = 0$ this would be the equation of the polaron. We can call

$$\tilde{A} = \frac{A}{\Lambda\sqrt{\Omega}N_F}, \quad h(k_1) = \frac{1}{\Omega}\sum_{\boldsymbol{q}_1}\frac{\beta(\boldsymbol{q}_1)}{\Delta(\boldsymbol{q}_1)(W - k_1^2 + \boldsymbol{q}_1\cdot\boldsymbol{k}_1)}.$$

Then we can write Eq. (B9) as

$$\mathcal{P}_W\tilde{A} = \frac{2}{\Omega}\sum_{\boldsymbol{k}_1}h(k_1)D(\boldsymbol{k}_1), \tag{B10}$$

which is Eq. (17) in the main text.

Now that we have an equation which relates $A$ with $D$, we will try to have another equation from Eq. (B4); we write the right-hand side of Eq. (B4) with the goal of writing it in terms of $A$ and we obtain after writing

$$f(\boldsymbol{k}_1) = \frac{1}{\Omega}\sum_{\boldsymbol{q}_1}\frac{\beta(\boldsymbol{q}_1)^2}{W - k_1^2 + \boldsymbol{q}_1\cdot\boldsymbol{k}_1},$$

$$g(\boldsymbol{k}_1,\boldsymbol{k}_2) = \frac{1}{\Omega}\sum_{\boldsymbol{q}_1}\frac{\beta(\boldsymbol{q}_1)^2}{\Delta(\boldsymbol{q}_1)\big(W - k_1^2 + \boldsymbol{q}_1\cdot\boldsymbol{k}_1\big)\big(W - k_2^2 + \boldsymbol{q}_1\cdot\boldsymbol{k}_2\big)},$$

$$\begin{aligned}I(\boldsymbol{k}_1) = \frac{1}{\Lambda^2}\Bigg(&W - E_0 - \frac{3k_1^2}{4} + \frac{1}{4}\langle(\boldsymbol{q}_1 - \boldsymbol{q}_2)^2\rangle\\ &- \frac{\Lambda^2}{\Omega}\sum_{\boldsymbol{k}_2}\frac{1}{W - k_1^2 - k_2^2 - \boldsymbol{k}_1\cdot\boldsymbol{k}_2 - \langle\boldsymbol{q}_1\cdot\boldsymbol{q}_2\rangle}\Bigg).\end{aligned}$$

With this Eq. (B4) becomes

$$\begin{aligned}I(\boldsymbol{k}_1)D(\boldsymbol{k}_1) - \frac{1}{\Omega}\sum_{\boldsymbol{k}_2}\frac{D(\boldsymbol{k}_2)}{W - k_1^2 - k_2^2 - \boldsymbol{k}_1\cdot\boldsymbol{k}_2 - \langle\boldsymbol{q}_1\cdot\boldsymbol{q}_2\rangle}\\ = h(k_1)\tilde{A} + \frac{1}{\Omega}\sum_{\boldsymbol{k}_2}g(\boldsymbol{k}_1,\boldsymbol{k}_2)D(\boldsymbol{k}_2) + f(\boldsymbol{k}_1)D(\boldsymbol{k}_1),\end{aligned} \tag{B11}$$

which corresponds to Eq. (18) from the main text.

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