Few Versus Many-Body Physics of an Impurity Immersed in a Superfluid of Spin 1/2 Attractive Fermions

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In this Letter we investigate the properties of an impurity immersed in a superfluid of strongly correlated spin 1/2 fermions and we calculate the beyond-mean-field corrections to the energy of a weakly interacting impurity. We show that these corrections are divergent and have to be regularized by properly accounting for three-body physics in the problem and that our approach naturally provides a unifying framework for Bose and Fermi polaron physics.

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The physics of an impurity immersed in a many-body ensemble is one of the simplest although non-trivial paradigms in many-body physics. One of the first examples of such a system is the polaron problem which was introduced by Landau and Pekar [1] to describe the interaction of an electron with the phonons of a surrounding crystal. Likewise, in magnetic compounds Kondo's Effect arises from the interaction of magnetic impurities with the background Fermi sea [2,3]. Similar situations occur in nuclear physics, e.g., in neutron stars to interpret the interaction of a proton with a superfluid of neutrons [4,5], or in quantum chromodynamics where the so-called Polyakov loop describes the properties of a test color charge immersed in a hot gluonic medium [6]. Finally, impurity problems can be used as prototypes for more complex many-body systems [7], as illustrated by the dynamical mean-field theory [8].

The recent advent of strongly correlated quantum gases permitted by the control of interactions in these systems has opened a new research avenue for the physics of impurities [9–12]. Experiments on strongly polarized Fermi gases [13–15] were interpreted by the introduction of the so-called Fermi polarons, a quasiparticle describing the properties of an impurity immersed in an ensemble of spin-polarized fermions and dressed by a cloud of particle-hole excitations of the surrounding Fermi sea [16–18]. More recently, the physics of Bose polarons (impurities immersed in a Bose-Einstein condensate) was explored using radio-frequency spectroscopy [19,20]. Contrary to the Fermi polaron, this system is subject to an Efimov effect [21] and three-body interactions play an important role in the strongly correlated regime [22,23]. Finally recent experiments on dual superfluids have raised the question of the behavior of an impurity immersed in a superfluid of spin 1/2 fermions [24–26]. In these experiments, the polaron was weakly coupled to the background superfluid and the interaction could be accurately modeled within mean-field approximation. Further theoretical works explored the strongly coupled regime using mean-field theory to describe the fermionic superfluid [27,28]. They highlighted the role of Efimov physics in the phase diagram of the system and as a consequence some results were plagued by unphysical ultraviolet divergences. In this Letter we address this problem without making any assumption on the properties of the superfluid component. We calculate the first beyond-mean-field corrections to the energy of the polaron and we show that the logarithmic divergence arising from three-body physics can be cured within an effective field theory approach introduced previously in the study of beyond mean-field corrections in Bose gases [29,30].

Qualitatively speaking, the phase diagram of the impurity can be decomposed in three different regions when the strength of the impurity-fermion interaction is varied (see Fig. 1). For a weak attraction, the impurity can be described as a polaronic quasiparticle. When attraction becomes resonant, the impurity and the fermions can form Efimov trimers. Earlier variational calculations suggest that this trimers can be interpreted as a bound state between the impurity and a Cooper pair and that the transition between the polaron and trimeron states is a smooth crossover [27,28]. Finally, in the strongly attractive regime, impurity-fermion attraction overcomes Cooper pairing leading to a dimeron state describing an impurity-fermion dimer immersed in a fermionic superfluid medium [31]. When fermion-fermion interactions are varied, the trimeron state vanishes for strongly attractive fermions [32].

Since the size of the ground-state Efimov trimer is typically much smaller than the interparticle spacing, its binding energy is much larger than the Fermi energy of the fermionic superfluid. As a consequence, except when the Efimov trimer becomes resonant with the atomic

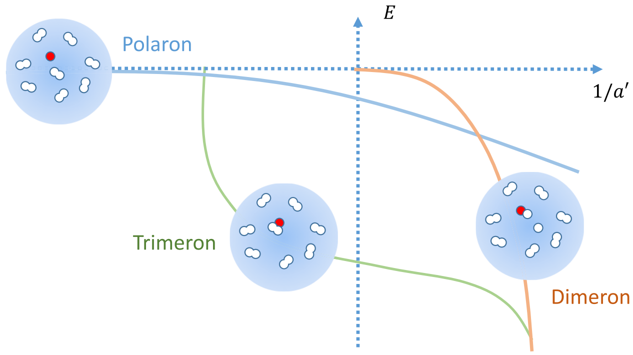

FIG. 1. Sketch of the energy branches of an impurity (red dot) immersed in an ensemble of Cooper-paired fermions when the impurity-fermion scattering length a' is varied. Blue, polaron branch; green, ground-state Efimov trimer branch; orange, dimer branch.

continuum, the internal structure of the trimer is only weakly affected by the many-body environment (see Ref. [32] for a semiquantitative description of the phase diagram).

Since the trimeron and dimeron regimes are dominated by few-body physics, we focus on the energy of the polaronic branch that is more strongly affected by the presence of the superfluid, especially in the regime $a' \ll R_e$, where R_e is the resonance range [36]. When the fermion-fermion interaction is varied, the polaronic state evolves from a Fermi polaron when fermions are weakly interacting, to a Bose polaron in the BEC regime where fermions can be described as a Bose-Einstein condensate of molecules.

Consider thus an impurity of mass m_{i} immersed in a bath of spin 1/2 fermions of mass m_{f}. We write the Hamiltonian of the system as $\hat{H} = \hat{H}_{\mathrm{imp}} + \hat{H}_{\mathrm{mb}} + \hat{H}_{\mathrm{int}}$, where $\hat{H}_{\mathrm{imp}}$ ($\hat{H}_{\mathrm{mb}}$) is the Hamiltonian of the impurity (many-body background) alone, and $\hat{H}_{\mathrm{int}}$ describes the interaction between the two subsystems. We label the eigenstates of the impurity by its momentum $\boldsymbol{q}$ and its eigenvalues are $\varepsilon_q^{(\mathrm{i})} = \hbar^2 q^2/2m_{\mathrm{i}}$. The eigenstates and eigenvalues of $\hat{H}_{\mathrm{mb}}$ are denoted $|\alpha\rangle$ and E_α, where by definition $\alpha = 0$ corresponds to the ground state of the fermionic superfluid.

Assuming for simplicity an identical contact interaction between the impurity and each spin component of the many-body ensemble, we write

$$\hat{H}_{\mathrm{int}} = g_0' \sum_{\sigma=\uparrow,\downarrow} \int d^3\boldsymbol{r} \hat{\psi}_\sigma^\dagger(\boldsymbol{r}) \hat{\psi}_\sigma(\boldsymbol{r}) \hat{\phi}^\dagger(\boldsymbol{r}) \hat{\phi}(\boldsymbol{r}), \quad (1)$$

where $\hat{\psi}_\sigma$ and $\hat{\phi}$ are the field operators for spin σ particles of the many-body ensemble and of the impurity, respectively. In this expression, the bare and physical coupling constants g_0' and $g' = 2\pi\hbar^2 a'/m_r$, where m_r is the impurity-fermion reduced mass, are related through

$$\frac{1}{g_0'} = \frac{1}{g'} - \frac{1}{\Omega} \sum_{k<\Lambda} \frac{1}{\varepsilon_k^{(r)}}, \quad (2)$$

where Ω is the quantization volume, Λ is some ultraviolet cutoff and $\varepsilon_k^{(\mathrm{r})} = \hbar^2 k^2/2m_r$. Assuming that the contact interaction can be treated perturbatively, we have up to second order

$$g_0' = g' + \frac{g'^2}{\Omega} \sum_{k<\Lambda} \frac{1}{\varepsilon_k^{(r)}} + o(g'^2). \quad (3)$$

Calculating the energy ΔE of the polaron to that same order, we have

$$\Delta E_{\mathrm{pert}} = g' n + \frac{g'^2 n}{\Omega} \sum_{\boldsymbol{q}} \left(\frac{1}{\varepsilon_q^{(r)}} - \chi(\boldsymbol{q}, \varepsilon_q^{(i)}) \right). \quad (4)$$

where n is the particle density in the many-body medium and

$$\chi(\boldsymbol{q}, E) = \frac{1}{N} \sum_\alpha \frac{|\langle\alpha|\hat{\rho}_{-\boldsymbol{q}}|0\rangle|^2}{E_\alpha - E_0 + E}, \quad (5)$$

with $\hat{\rho}_{\boldsymbol{q}} = \sum_\sigma \int d^3\boldsymbol{r} \hat{\psi}_\sigma^\dagger(\boldsymbol{r}) \hat{\psi}_\sigma(\boldsymbol{r}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}}$ and N is the total number of fermions.

In the sum, the presence of the two terms allows for a UV cancellation of their $1/q^2$ asymptotic behaviors. Indeed, for large q the eigenstates of the many-body Hamiltonian excited by the translation operator $\hat{\rho}_{\boldsymbol{q}}$ correspond to free-particle excitations of momentum $\boldsymbol{q}$ and energy $\varepsilon_q^{(f)} = \hbar^2 q^2/2m_{\mathrm{f}}$. We therefore have

$$\chi(\boldsymbol{q}, E) \simeq \frac{S(q)}{\varepsilon_q^{(f)} + E}, \quad (6)$$

where $S(q) = \sum_\alpha |\langle\alpha|\hat{\rho}_{\boldsymbol{q}}|0\rangle|^2/N$ is the static structure factor of the many-body system. At large momenta, we have $S(q) = 1 + C_2/4Nq + \cdots$, where C_2 is Tan's contact parameter of the fermionic system and characterizes its short-range two-body correlations [39,40]. From this scaling we see that the UV-divergent $1/q^2$ contributions in Eq. (4) cancel out. However, the next-to-leading order term in $S(q)$ suggests that this cancellation is not sufficient to regularize the sum that is still log-divergent. This logarithmic behavior is supported by a directed calculation of χ using BCS mean-field theory [32] and is characteristic of a singularity in the three-body problem for particles with contact interactions that was pointed out first by Wu for bosons [41] and was more recently investigated in the context of nuclear physics [4] or cold atoms (see, for instance, Refs. [28,29,42,43]).

To get a better insight on the origin of this singularity, we analyze first the scattering of an impurity with a pair of free fermions. Within Faddeev's formalism [44], the corresponding three-body T matrix is written as a sum of three contributions, $\hat{T}_{i=1,2,3}$ solutions of the set of coupled equations

$$\begin{pmatrix} \hat{T}_1 \\ \hat{T}_2 \\ \hat{T}_3 \end{pmatrix} = \begin{pmatrix} \hat{t}_1 \\ \hat{t}_2 \\ \hat{t}_3 \end{pmatrix} + \begin{pmatrix} 0 & \hat{t}_1 & \hat{t}_1 \\ \hat{t}_2 & 0 & \hat{t}_2 \\ \hat{t}_3 & \hat{t}_3 & 0 \end{pmatrix} \hat{G}_0 \begin{pmatrix} \hat{T}_1 \\ \hat{T}_2 \\ \hat{T}_3 \end{pmatrix}, \quad (7)$$

where $\hat{G}_0 = 1/(z - \hat{H}_0)$ is the free resolvant operator and $\hat{t}_i$ is the two-body T matrix leaving particle i unaffected. The solutions of this equation can be expressed as a series of diagrams where a given two-body t-matrix never acts twice in a row and $\hat{T}_i$ corresponds to the sum of all diagrams finishing by $\hat{t}_i$. Assuming that the impurity is labeled by the index $i = 3$ and that its interaction with the other two atoms ($i = 1,\ 2$) is weak, we can expand the solutions of Faddeev's equation with $\hat{t}_1$ and $\hat{t}_2$. To be consistent with the polaron-energy calculation outlined in the previous section, we proceed up to second order in $\hat{t}_{1,2}$.

When the full two-body T matrices $t_{1,2} = g'/\Omega/(1 + ia'k + a'R_e k^2)$ are used, all terms of the expansion are finite. However, when treating them within second order Born's approximation [i.e., taking simply $t_{1,2} = g'(1 - ika')/\Omega$ and stopping the expansion of the T matrix at second order in a'], some diagrams are logarithmically divergent. The singular diagrams are listed in Fig. 2: they all start and end with t_3 and their contribution can be written as $(t_3)_{\rm out}\Gamma(t_3)_{\rm in}$. In Born's approximation the sums over inner momenta are divergent and the integrals are therefore dominated by the large-k behavior of t_3 and G_0. After a straightforward calculation, we obtain that

$$\Gamma_{\rm Born} \underset{\Lambda\to\infty}{\sim} \frac{m_f^3}{\hbar^6} g'^2 \kappa(\eta = m_i/m_f) \ln(\Lambda|a|), \quad (8)$$

with

$$\kappa(\eta) = \frac{\sqrt{\eta^3(\eta+2)}}{2\pi^3(\eta+1)^2} - \frac{\eta}{2\pi^3}\arctan\left(\frac{1}{\sqrt{\eta(\eta+2)}}\right) - \frac{4}{\pi^3}\sqrt{\frac{\eta}{\eta+2}}\arctan\left(\sqrt{\frac{\eta}{\eta+2}}\right)^2. \quad (9)$$

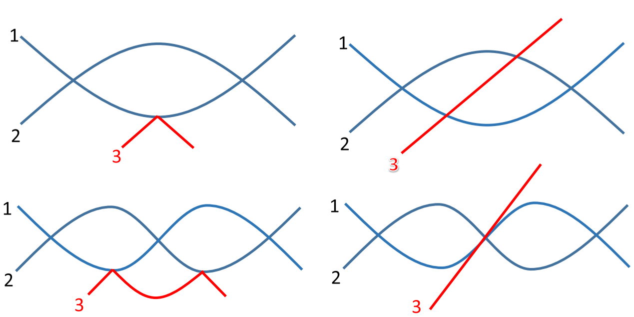

FIG. 2. Singular diagrams at second order of Born's approximation. The red line corresponds to the impurity.

In the case of equal mass particles ($\eta = 1$), we obtain, for instance, $\kappa(1) = (\sqrt{3}/8\pi^3) - (1/12\pi^2) - (1/9\pi\sqrt{3}) \simeq -0.0219$.

Since Γ is finite when the full two-body physics is taken into account, we introduce a three-body characteristic length R_3 such that

$$\Gamma_{\rm Born} - \Gamma_{\rm Faddeev} \underset{\Lambda\to\infty}{=} \frac{m_f^3}{\hbar^6} g'^2\kappa(\eta)\ln(\Lambda R_3) + o(1), \quad (10)$$

where $\Gamma_{\rm Faddeev}$ corresponds to the value of Γ obtained by using the full two-body T matrices $t_{1,2}$ to calculate the first three diagrams of Fig. 2. In this perturbative approach, R_3/a' depends on η and R_e/a', but does not depend on a in the experimentally relevant regime $a' \lesssim R_e \ll a$. It can be computed numerically [32], and for a ^{6}Li-^{7}Li mixture for which $R_e \simeq a'$, we obtain $R_3 \simeq 3.1a'$. Since we work in a regime where the polaron is the ground state and Efimov trimers are absent, we do not have to use nonperturbative approaches compatible with Efimov physics and leading to a log-periodic dependence of Γ [45].

Following the effective field theory approach discussed in Ref. [43], divergences plaguing Born's expansion can be cured by introducing an explicit three-body interaction described by a Hamiltonian

$$\hat{H}_{3b} = g_3(\Lambda)\int d^3\boldsymbol{r}\hat{\psi}_\uparrow^\dagger(\boldsymbol{r})\hat{\psi}_\downarrow^\dagger(\boldsymbol{r})\hat{\phi}^\dagger(\boldsymbol{r})\hat{\phi}(\boldsymbol{r})\hat{\psi}_\downarrow(\boldsymbol{r})\hat{\psi}_\uparrow(\boldsymbol{r}). \quad (11)$$

The contribution of this three-body interaction to Γ corresponds to the fourth diagram of Fig. 2 and yields the following expression:

$$\Gamma_{\rm 3b} = g_3(\Lambda)\left(\frac{1}{\Omega}\sum\nolimits_{k<\Lambda}\frac{1}{2\epsilon_k^{\rm (f)}}\right)^2. \quad (12)$$

Using this three-body interaction to cure Born's approximation, we must have $\Gamma_{\rm Born} + \Gamma_{\rm 3b} = \Gamma_{\rm Faddeev}$, hence the following expression for the three-body coupling constant

$$g_3(\Lambda)\left(\frac{1}{\Omega}\sum\nolimits_{k<\Lambda}\frac{1}{2\epsilon_k^{(f)}}\right)^2 = -\frac{m_f^3}{\hbar^6}g'^2\kappa(\eta)\ln(\Lambda R_3). \quad (13)$$

The introduction of the three-body Hamiltonian implies a new contribution to the second-order energy shift (4). This new term amounts to $\Delta E_{3b} = g_3(\Lambda)\langle 0|\hat{\psi}_\uparrow^\dagger(\boldsymbol{r})\hat{\psi}_\downarrow^\dagger(\boldsymbol{r})\hat{\psi}_\downarrow(\boldsymbol{r})\hat{\psi}_\uparrow(\boldsymbol{r})|0\rangle$. Using Hellman-Feynman's theorem, we can recast this correction as

$$\Delta E_{3b} = g_3(\Lambda)\frac{\partial E_0}{\partial g_0}, \quad (14)$$

where E_0 is as before the energy of the ground state of the fermionic ensemble and g_0 is the bare fermion-fermion coupling constant. Expressing g_0 using the physical coupling constant $g = 4\pi\hbar^2 a/m_{\rm f}$ yields

$$\Delta E_{3b} = -\frac{g_3(\Lambda)}{g_0^2}\frac{\partial E_0}{\partial 1/g} \tag{15}$$

$$\underset{\Lambda\to\infty}{\sim} -g_3(\Lambda)\left(\frac{1}{\Omega}\sum\nolimits_{k<\Lambda}\frac{1}{2\varepsilon_k^{(f)}}\right)^2\frac{\partial E_0}{\partial 1/g}, \tag{16}$$

where we have used the fact that for large Λ, $1/g_0$ diverges as $-(1/\Omega)\sum[1/2\varepsilon_k^{(f)}]$. Using Eq. (13) as well as Tan's adiabatic sweep theorem, we then obtain after a straightforward calculation

$$\Delta E_{3b} = -g'^2\kappa(\eta)\frac{m_f C_2}{\hbar^2\Omega}\ln(\Lambda R_3). \tag{17}$$

Adding this contribution to Eq. (4), we obtain for the polaron energy $\Delta E = \Delta E_{\rm pert} + \Delta E_{3b}$:

$$\Delta E = g' n\left[1 + k_F a' F\left(\frac{1}{k_F a}\right) - 2\pi\frac{m_f}{m_r}\kappa(\eta)\frac{a' C_2}{N}\ln(k_F R_3) + \cdots\right], \tag{18}$$

with

$$F\left(\frac{1}{k_F a}\right) \underset{\Lambda\to\infty}{=} \frac{2\pi}{k_F}\left[\frac{\hbar^2}{m_r}\int_{q<\Lambda}\frac{d^3\boldsymbol{q}}{(2\pi)^3}\left(\frac{1}{\varepsilon_q^{(\mathrm{r})}} - \chi(q,\varepsilon_q^{(\mathrm{i})})\right) - \frac{m_f}{m_r}\kappa(\eta)\frac{C_2}{N}\ln(\Lambda/k_F)\right]. \tag{19}$$

Equations (18) and (19) are the main results of this Letter. They show that the second order correction of the polaron energy is the sum of two terms: a regular term characterized by the function F defined by Eq. (18), as well as a second term, characterized by a logarithmic singularity and proportional to the fermionic contact parameter.

The function F is in general hard to compute exactly but we can obtain its exact asymptotic expression in the BEC and BCS limits. When the fermions of the background ensemble are weakly interacting, we must recover the Fermi-polaron problem. For the mass-balanced case $\eta = 1$, we obtain $F(-\infty) = 3/2\pi$. In the strongly attractive limit, the fermionic ensemble behaves as a weakly interacting Bose-Einstein condensate of dimers and the polaron energy takes a general mean-field form $g_{\rm ad}n/2$, where $g_{\rm ad}$ is the impurity-dimer s-wave coupling constant and $n/2$ is the dimer density. Since in the BEC limit, $C_2/N = 4\pi/a$, identifying Eq. (18) with the mean-field impurity-dimer interaction implies that

$$F\left(\frac{1}{k_F a}\right) \underset{a\to 0^+}{=} 8\pi^2\kappa(\eta)\frac{m_f}{m_r}\frac{\ln(k_F a)}{k_F a} + \cdots \tag{20}$$

and

$$g_{\rm ad} = 2g'\left[1 - 8\pi^2\kappa(\eta)\frac{m_f}{m_r}\frac{a'}{a}[\ln(R_3/a) + C_{\rm ad}]\cdots\right], \tag{21}$$

where the constant $C_{\rm ad}$ can be obtained from the direct analysis of the atom-dimer scattering problem [32].

Equation (18) can be used to benchmark approximation schemes used to address this problem. Using a purely BCS approach yields a similar form but with a value of κ where the third term of Eq. (9) is missing [32]. This discrepancy is easily understandable. Indeed, this term corresponds to the third diagram of Fig. 2, where the two fermions interact between their interaction with the impurity, which contradicts the BCS assumption of noninteracting Bogoliubov excitations. For $\eta = 1$, $\kappa/\kappa_{\rm MF} \simeq 15$, showing that BCS approximation underestimates strongly beyond mean-field contributions. This contribution was recovered in Ref. [28] whose numerical results agree with Eq. (18) albeit with a mean-field value for the contact parameter C_2.

Equation (21) can also be compared to the numerical calculation of the atom-dimer scattering length reported in Ref. [46]. The comparison between numerics and our analytical result for experimentally relevant mass ratios is shown in Fig. 3 which demonstrates a very good agreement between the two approaches [47]. Note also that Eq. (21) clarifies the range of validity of the perturbative expansion. In addition to the diluteness assumption $k_F|a'| \ll 1$, the validity of Born's expansion requires the additional condition $|a'|/a \ll 1$ when $a > 0$.

Finally, the convergence of Eq. (19) entails that χ must obey the large momentum asymptotic behavior

$$\chi(q,\varepsilon_q^{(i)}) \underset{q\to\infty}{=} \frac{1}{\varepsilon_q^{(r)}}\left[1 - \pi^2\kappa(\eta)\frac{m_f}{m_r}\frac{C_2}{Nq} + \cdots\right]. \tag{22}$$

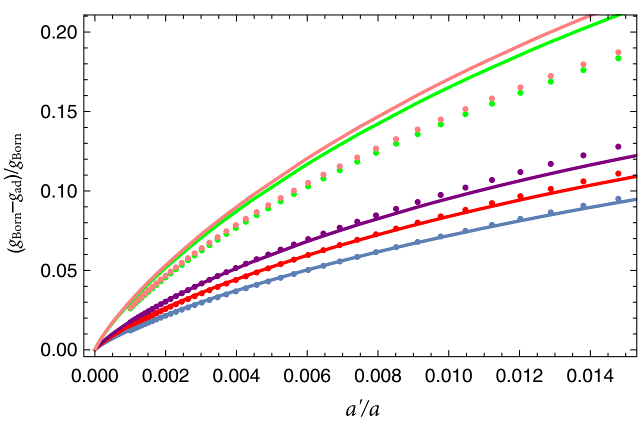

FIG. 3. Atom-dimer s-wave coupling constant relatively to Born's approximation prediction $g_{\rm Born} = 2g'$. Dots: numerical resolution of the three-body problem from Ref. [46]. From bottom to top: $\eta = 7/40$ (blue), $23/40$ (red), $7/6$ (purple), $87/6$ (orange), $133/6$ (green). Solid line: Asymptotic result Eq. (21) where R_3 and $C_{\rm ad}$ are computed numerically and are given in Ref. [32]. Here R_3 and $C_{\rm ad}$ are computed taking $R_e = 0$ and the slight discrepancy observable at large η is probably due to the finite range $R_e \lesssim a'$ used in Ref. [46] to regularize the three-body problem.

For $m_\mathrm{i} \to \infty$, $\varepsilon_q^{(\mathrm{i})} = 0$, we have $\kappa(\infty) = -1/4\pi$ and we recover the asymptotic result derived in Ref. [48] using operator product expansion. Note that mean-field theory predicts $\kappa_{\mathrm{MF}}(\infty) = 0$, and therefore disagrees with this independent result.

In conclusion, we have shown that by encapsulating three-body interactions within a field theoretical approach, we could obtain an expression for the beyond mean-field corrections of the polaron energy unifying within the same framework the Fermi and Bose polarons problems, as well as the scattering properties of an atom with a halo dimer. Using the mean-field estimate for F at unitarity, we see that the second-order correction to the polaron energy [Eq. (18)] is dominated by the logarithmic contribution. In the case of the polaron oscillation experiments reported in Ref. [24], the predicted correction amounts to a 5% shift of the oscillation frequency. Although small, this correction is within the reach of current experimental capabilities and shows that the results presented in this work are necessary to achieve the percent-level agreement between experiment and theory targeted by state of the art precision quantum many-body physics.

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[31] Note that since we are only dealing with the ground state of the system, we do not consider the so-called upper-branch polaron which describes an unbound impurity with $a' > 0$ and corresponds to a metastable excited state of the system.
[32] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.123.080403 for a sketch of the phase diagram of the system and an explicit proof of the logarithmic singularity within BCS frameworks, including Refs. [33–35].
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