Bipolarons in a Bose-Einstein Condensate

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Mobile impurities in a Bose-Einstein condensate form quasiparticles called polarons. Here, we show that two such polarons can bind to form a bound bipolaron state. Its emergence is caused by an induced nonlocal interaction mediated by density oscillations in the condensate, and we derive using field theory an effective Schrödinger equation describing this for an arbitrarily strong impurity-boson interaction. We furthermore compare with quantum Monte Carlo simulations finding remarkable agreement, which underlines the predictive power of the developed theory. It is found that bipolaron formation typically requires strong impurity interactions beyond the validity of more commonly used weak-coupling approaches that lead to local Yukawa-type interactions. We predict that the bipolarons are observable in present experiments, and we describe a procedure to probe their properties.

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The notion of quasiparticles is a powerful concept that is indispensable for our understanding of a wide range of problems from helium mixtures and condensed matter systems to nuclear matter [1–3]. Quasiparticles can experience induced interactions mediated by their surroundings. The induced interaction is inherently attractive and can therefore lead to the formation of bound states. This is the origin of Cooper pairing in conventional superconductors [4] where the size of the Cooper pairs typically is much larger than the average distance between unbound quasiparticles. Bipolarons stand out as an important example of the opposite limit, where two quasiparticles, so-called polarons, form a bound state much smaller than the average distance between the unbound polarons. The formation of bipolarons is suggested to be the mechanism behind electrical conduction in polymer chains [5,6], organic magnetoresistance [7], and even high temperature superconductivity [8,9].

The recent experimental realization of polarons in ultracold quantum gases [10–16] has opened up unique opportunities to study quasiparticle physics in a highly controlled manner. So far, experimental and theoretical efforts have focused on single-polaron properties in degenerate Fermi [10–14] and Bose gases [15,16], for which we now have a good understanding. Bipolarons in Bose-Einstein condensates (BECs) have been explored within the Fröhlich model [2], which is valid only for weak interactions [17]. Yet, their observability hinges on sufficiently strong binding, and the formation of bipolarons in atomic gases remains an outstanding question that requires a new theoretical framework for strong interactions.

In this Letter, we present such a theory and demonstrate that two impurities immersed in a BEC can indeed form bound states for sufficiently strong interactions between the impurities and the condensate atoms. Based on field theory, we derive an effective Schrödinger equation with a *nonlocal* polaron-polaron interaction that describes the emergence of bipolarons. This effective description provides an intuitive and feasible approach to account for arbitrarily strong impurity-boson interactions, and it is furthermore shown to be in remarkable agreement with first-principle quantum Monte Carlo results. Our theory allows us to reliably predict the existence of bipolarons under realistic conditions, and it demonstrates that it is possible to realize bipolarons with sufficiently strong binding to enable their observation.

We consider two impurities of mass m immersed in a zero-temperature BEC of bosons with mass m_B and density n_B. As is typical for cold-atom experiments, the BEC features weak interactions with $n_B^{1/3} a_B \ll 1$, so that it is accurately described by the Bogoliubov theory. Here, a_B is the scattering length for the zero-range boson-boson interaction. The interaction of a single impurity with the BEC is characterised by the scattering length a, and it leads to the formation of the Bose polaron [18–28], which was recently observed experimentally [15,16].

Two polarons can interact strongly by exchanging density fluctuations in the BEC, even when there is no significant direct interaction between the actual impurities. This induced interaction is inherently attractive and can therefore facilitate bound dimer states, as illustrated in Fig. 1(a). Within a field-theoretical formulation, two-body bound states in a quantum many-body system can be identified as poles of the generalized scattering matrix Γ. Considering the scattering of two impurities from states with energy momenta (k_1, k_2) to (k_3, k_4), the Bethe-Salpeter equation for the scattering matrix reads in the ladder approximation [29] [see Fig. 2(a)]

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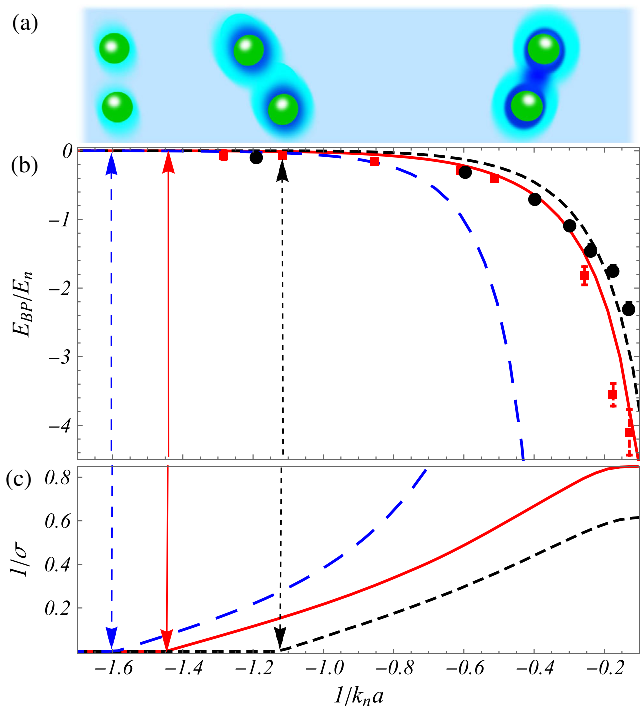

FIG. 1. (a) The cartoon shows Bose polarons forming a bipolaron as a consequence of a mediated interaction. (b) Binding energy E_{BP} of the bipolaron as a function of the impurity-boson interaction strength for two bosonic impurities with $m = m_B$. The solid red and dashed black lines are solutions to Eq. (3) with the induced interaction given by Eq. (4) for the gas parameters $n_B a_B^3 = 10^{-6}$ and $n_B a_B^3 = 10^{-5}$. The red squares and black circles are the results of the DMC calculations for the same two gas parameters. The long dashed blue line is the ground state energy of the Yukawa interaction Eq. (5) for $n_B a_B^3 = 10^{-6}$. (c) The corresponding inverse size $1/\sigma = \xi_B/\sqrt{\langle r^2 \rangle}$ of the bipolaron wave function, where $\xi_B = 1/\sqrt{8\pi n_B a_B}$, is the BEC coherence length. Vertical arrows denote the critical strength to form a bound state.

$$\Gamma(k_1, k_2; k_1 - k_3) = V(k_1, k_2; k_1 - k_3) + \sum_q V(k_1, k_2; q) \times G(k_1 - q) G(k_2 + q) \times \Gamma(k_1 - q, k_2 + q; k_1 - q - k_3). \tag{1}$$

Here $G(k)$ is the impurity Green's function, $k = (\mathbf{k}, z)$ is the four-momentum vector, and $V(k_1, k_2; q)$ is the induced interaction between two impurities. We calculate this interaction using the diagrammatic scheme illustrated in Fig. 2(b), which simultaneously accounts for arbitrarily strong boson-impurity scattering and the propagation of density waves in the BEC [30,31].

In order to derive an effective Schrödinger equation for the bipolaron, we change our description from bare impurities to polarons by approximating the impurity Green's functions in Eq. (1) by their value around the polaron poles; i.e., $G(k) \simeq Z_{\mathbf{k}}/(z - \omega_{\mathbf{k}})$. Here $\omega_{\mathbf{k}}$ is the energy of a polaron with momentum $\mathbf{k}$ and quasiparticle residue $Z_{\mathbf{k}}$. We furthermore multiply the Bethe-Salpeter equation (1) by $Z_{\mathbf{k}_1} Z_{\mathbf{k}_2}$ so that it gives the scattering matrix Γ_P of two polarons instead of two impurities. This gives

$$V_{\mathrm{eff}}(k_1, k_2; q) = Z_{\mathbf{k}_1} Z_{\mathbf{k}_2} V(k_1, k_2; q) \tag{2}$$

for the effective polaron-polaron interaction. Since it depends on the incoming k_1 and k_2, as well as the transferred four-momentum q, a direct solution of the Bethe-Salpeter equation is very difficult. We therefore neglect retardation effects and take the static limit of the interaction setting all energies to zero in V_{eff}. This is a good approximation if the binding energy $|E_{\mathrm{BP}}|$ of the bipolaron is smaller than the typical energies of the Bogoliubov modes exchanged between the polarons, i.e., if $\sqrt{|E_{\mathrm{BP}}|/m} \ll c$ with $c = 2\sqrt{\pi n_B a_B}/m_B$ the speed of sound in the BEC. Neglecting the frequency dependence of V_{eff} means that the frequency sum involving the two impurity Green's functions in Eq. (1) can be performed analytically. The Bethe-Salpeter equation (1) then reduces to the Lippmann-Schwinger equation, which in turn is equivalent to the Schrödinger equation for two polarons interacting via an instantaneous interaction. It reads in the center of mass frame

$$E_{\mathrm{BP}} \psi(\mathbf{k}) = 2\omega_{\mathbf{k}} \psi(\mathbf{k}) + \sum_{\mathbf{k}'} V_{\mathrm{eff}}(\mathbf{k}, \mathbf{k}') \psi(\mathbf{k}'), \tag{3}$$

where $\psi(\mathbf{k})$ is the relative wave function of the bipolaron with energy E_{BP}. The effective interaction for two polarons with momenta $(\mathbf{k}, -\mathbf{k})$ scattering into $(\mathbf{k}', -\mathbf{k}')$ is

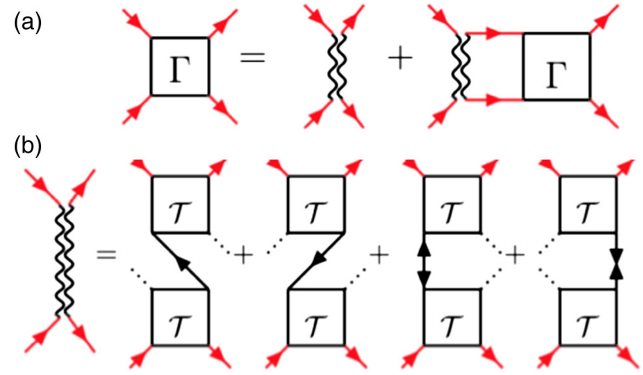

FIG. 2. (a) Diagrammatic representation of the Bethe-Salpeter equation for impurity-impurity scattering. The red lines are the impurity Green's function, and the double wavy line is the induced interaction. (b) The induced interaction. The black lines are normal and anomalous BEC Green's functions, the dashed lines are condensate bosons, and $\mathcal{T}$ is the impurity-boson scattering matrix in the ladder approximation.

$$V_{\rm eff}(\mathbf{k},\mathbf{k}') = Z^2 n_B[2\mathcal{T}(\mathbf{k},0)\mathcal{T}(\mathbf{k}',0)G_{11}(\mathbf{k}-\mathbf{k}',0) + \mathcal{T}^2(\mathbf{k},0)G_{12}(\mathbf{k}-\mathbf{k}',0) + \mathcal{T}^2(\mathbf{k}',0)G_{12}(\mathbf{k}-\mathbf{k}',0)], \quad (4)$$

where $G_{11}(\mathbf{k},0)$ and $G_{12}(\mathbf{k},0)$ are the normal and anomalous Green's functions for the bosons and $\mathcal{T}(\mathbf{k},0)$ is the boson-impurity scattering matrix, all evaluated at momentum $\mathbf{k}$ and zero energy. Note that $\mathcal{T}$ is distinct from Γ_P, which describes the scattering of two polarons. We calculate the polaron energy $\omega_\mathbf{k}$ and residue $Z_\mathbf{k}$ using an extended ladder scheme with the effective mass approximation $\omega_\mathbf{k} = \mathbf{k}^2/2m^* + \omega_0$, where ω_0 is the energy of a zero-momentum polaron, and assuming that $Z_\mathbf{k} \approx Z_{\mathbf{k}=0}$. This scheme agrees well both with experimental data and with Monte Carlo calculations for the single-polaron properties. More details are given in the Supplemental Material [32].

With Eq. (3), we have arrived at an effective Schrödinger equation for the bipolaron. In addition to providing an intuitive picture, it is much simpler to solve than the full Bethe-Salpeter equation (1), yet it gives accurate results even for strong coupling as we shall demonstrate shortly. The fact that Eq. (3) is a two-body effective description of an underlying many-body problem is reflected in the energy dispersion $\omega_\mathbf{k}$ and by the fact that the interaction is *nonlocal*; i.e., $V_{\rm eff}(\mathbf{k},\mathbf{k}') \neq V_{\rm eff}(\mathbf{k}-\mathbf{k}')$. It becomes local only for weak coupling $|k_n a| \ll 1$ with $k_n^3/6\pi^2 = n_B$, where the boson-impurity scattering matrix reduces to the constant $\mathcal{T}_v = 2\pi a/m_{\rm BI}$ with $m_{\rm BI} = m m_B/(m+m_B)$. Equation (4) then simplifies to the well-known second order (in a) Yukawa expression

$$V_{\rm eff}(\mathbf{k},\mathbf{k}') = -\mathcal{T}_v^2 \chi(\mathbf{k}-\mathbf{k}',0), \quad (5)$$

where $\chi(\mathbf{k},z) = n_B k^2/[m_B(z^2 - E_k^2)]$ describes density-density correlations in the BEC. Our theory extends this result into strong coupling by including multiple impurity-boson scattering.

We notice that in real space, the nonlocal interaction term in Eq. (3) reads $\int d^3 r_2 V_{\rm eff}(\mathbf{r}_1,\mathbf{r}_2)\psi(\mathbf{r}_2)$. To quantify the nonlocality, we write $V_{\rm eff}(\mathbf{r}_1,\mathbf{r}_2)$ as a function of $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, where $\mathbf{r}_1$ and $\mathbf{r}_2$ denote the relative distances between the in- and outgoing polarons. The local Yukawa interaction Eq. (5) can then be written as $V_{\rm eff}(\mathbf{R},\mathbf{r}) = \delta(\mathbf{r})\alpha\exp(-\sqrt{2}R/\xi_B)/R$ in real space, where $\alpha = \mathcal{T}_v^2 n_B m_B/\pi$. We define the "local" and "nonlocal" parts of the interaction as $U(\mathbf{R}) = \int d^3 r V_{\rm eff}(\mathbf{R},\mathbf{r})$ and $u(\mathbf{r}) = \int d^3 R V_{\rm eff}(\mathbf{R},\mathbf{r})$. For the Yukawa interaction, we have $U(\mathbf{R}) = \alpha\exp(-\sqrt{2}R/\xi_B)/R$ and $u(\mathbf{r}) \propto \delta(\mathbf{r})$. Figure 3 plots $U(\mathbf{R})$ for $n_B a_B^3 = 10^{-6}$ and $1/k_n a = -0.4$. We see that whereas $U(\mathbf{R})$ approaches the Yukawa form for large distances, it differs significantly for $R/\xi_B \lesssim 1$. In particular, $U(\mathbf{R})$ is finite for $R \to 0$. We also plot the wave

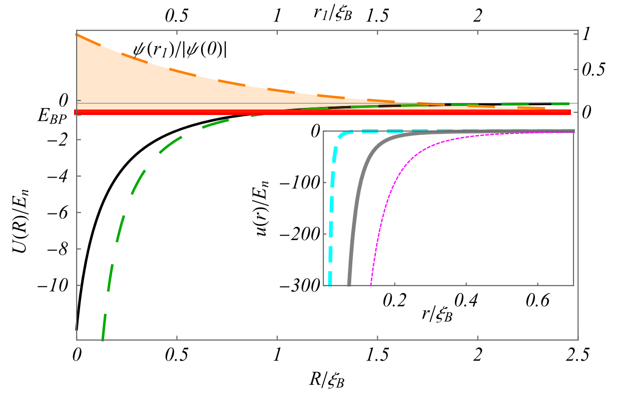

FIG. 3. The local part $U(R)$ of $V_{\rm eff}(\mathbf{r}_1,\mathbf{r}_2)$ (solid black) and the Yukawa interaction (dashed green) for $n_B a_B^3 = 10^{-6}$ and $1/k_n a = -0.4$. The corresponding s-wave binding energy $E_{\rm BP}$ and wave function are shown by solid red and dashed orange lines. Inset: the nonlocal part $u(r)$ for $1/k_n a = -10$ (dashed blue), -1.5 (solid gray), and -0.4 (short dashed purple).

function $\psi(\mathbf{r}_1)$ of the lowest bound state offset vertically by its binding energy $E_{\rm BP}$, to illustrate that it extends well beyond the classical turning point $U(R) = E_{\rm BP}$. This is a consequence of the nonlocal character of the interaction. The inset of Fig. 3 plots $u(\mathbf{r})$, which shows that the nonlocality given by the width of $u(\mathbf{r})$ increases with increasing interaction. This nonlocality is a characteristic sign of the underlying many-body physics, which is analogous to the case of the nuclear force [33].

In order to verify the accuracy of our theory and the involved approximations, we also perform diffusion Monte Carlo (DMC) simulations [27,32], which in principle takes into account all possible impurity-boson correlations. To this end, we determine the ground state energy E_0 for a BEC of N particles in a box with periodic boundary conditions. We then obtain the bipolaron binding energy $E_{\rm BP} = E - 2\omega_0 = E_2 - 2E_1 + E_0$ from the ground state energies E_1 and E_2 of the same condensate but containing one impurity and two impurities, respectively. Details of the DMC calculations are given in the Supplemental Material [32].

Figure 1(b) shows the bipolaron binding energy $E_{\rm BP}$ in units of $E_n = k_n^2/2m$ as a function of the impurity-boson scattering length a. We consider the case of bosonic impurities, so that the bipolaron wave function is symmetric under particle exchange (s-wave symmetry). Results obtained from our DMC simulations and the effective Schrödinger equation using the interaction Eq. (4) as well as Eq. (5) are compared for two different BEC gas parameters. We keep $a < 0$ here and in the following. For both interactions, we find that bound bipolaron states with $E_{\rm BP} < 0$ emerge beyond a critical interaction strength $k_n a_c$ which is marked by the vertical lines in Fig. 1. Beyond this critical value, the binding energy initially increases very slowly since the polaron-polaron interaction is at least a second order effect in a. For stronger coupling $k_n|a| \gtrsim 1$, the binding energy crucially becomes significant compared to the single-polaron energy ω_0, which is maximally of order E_n [19,22,34]. We moreover find that a smaller gas parameter leads to deeper binding, reflecting that the BEC becomes more compressible and hence induces a stronger effective interaction.

The predictions of our effective theory are in remarkably good agreement with the numerical DMC results for the entire considered range of coupling strengths $k_n a$. This level of agreement is particularly striking in the strong-interaction regime $k_n a \gtrsim 1$, which does not offer a small parameter to develop a controlled many-body theory. Yet, the predictive power of our description arises from the systematic combination of two reliable theories. First, the boson-impurity scattering is treated within the ladder approximation, which has turned out to be surprisingly accurate for cold atomic gases [35]. Second, the BEC density oscillations that mediate the interaction are described by the Bogoliubov theory, which is accurate for the typical situation of a small gas parameter. Respectively, our approach presents a rare instance of an intuitively simple yet accurate theory for a strongly interacting many-body system.

In Fig. 4, we compare the resulting bipolaron energy for the two cases of bosonic and fermionic impurities. We have chosen the mass ratio $m/m_B = 40/23$ corresponding to the experimentally relevant case of ^{40}K fermionic atoms in a ^{23}Na BEC [36,37]. While both cases promote the formation of bipolaron states beyond a critical interaction strength, Fig. 4 clearly illustrates that fermionic impurities are more weakly bound than their bosonic counterparts. This is simply because their wave function must have p-wave symmetry.

To accurately determine the critical coupling strength $k_n a_c$ for bipolaron formation, we consider the size $\sigma = \sqrt{\langle r^2 \rangle}/\xi_B$ of the dimer state with $\langle r^2 \rangle = \int d^3 r |\psi(\mathbf{r})|^2 r^2$. Since $\langle r^2 \rangle$ diverges when the polarons unbind, the inverse $1/\sigma$ provides a clear indicator of the critical interaction strength. Indeed, its dependence on $1/k_n a$ depicted in Fig. 1(c) features a kink at $k_n a_c$ beyond which $1/\sigma$ increases abruptly from zero. Our theory recovers the classic results for the critical coupling strength $\sqrt{2}/\alpha\xi_B m_r = 1.1905$ and $\sqrt{2}/\alpha\xi_B m_r = 0.2202$ for bound s- and p-wave states in the Yukawa potential [38–40]. This demonstrates the accuracy of our approach.

The Yukawa interaction Eq. (5), which results from a second order treatment within the Fröhlich model, is accurate only for weak interactions $k_n|a| \ll 1$. Indeed, it predicts critical interaction strengths $k_n a_c$ and binding energies E_{BP} substantially different from our strong coupling theory in Figs. 1 and 4. This is because second order theory approximates $\mathcal{T}(\mathbf{k}, 0) \approx \mathcal{T}_\nu$, which is a significant overestimation for $k_n a \gtrsim 1$. Since the bipolaron is observable only for not too small interaction strengths, the Fröhlich model is insufficient to analyze bipolarons in atomic gases. This is further illustrated in Fig. 5, where we show the critical interaction strength $k_n a_c$ as a function of the gas parameter $n_B a_B^3$, obtained using both Eq. (4) and the Yukawa potential Eq. (5). As can clearly be seen, the Yukawa potential is reliable only for weak impurity-boson interaction whereas the BEC has to be very compressible in order for the induced interaction to bind two polarons.

The two Bose polaron experiments so far, which had the gas parameters $n_B a^3 \approx 2 \times 10^{-8}$ [15] and $n_B a^3 \approx 2 \times 10^{-5}$ [16], both used radio-frequency (rf) spectroscopy to observe the polaron. The same technique can in fact be employed to detect bipolarons, whereby the rf field induces photoassociation of polaron dimers leading to a resonantly enhanced atom-loss signal. In both measurements, the observed polaron spectrum had a typical line width of $\sim E_n$. The bipolarons found in our strong coupling theory should thus be observable for strong interactions, where we predict a bipolaron resonance to emerge well separated

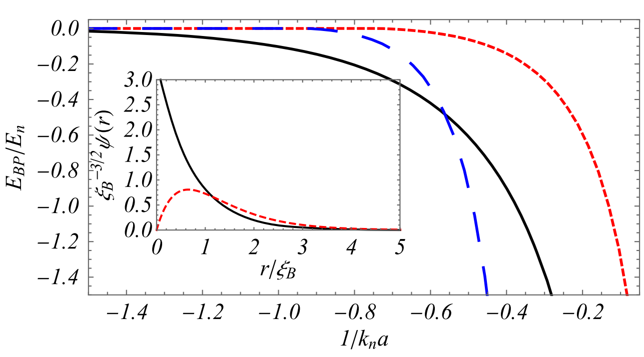

FIG. 4. Binding energy E_{BP} of two bosonic (solid black line) and fermionic (dashed red line) impurities with the mass ratio $m/m_B = 40/23$ for $n_B a_B^3 = 10^{-6}$. The dashed blue line is to the Yukawa binding energy for the p-wave bipolaron. Inset: the radial parts of the s- and p-wave functions (solid black and dashed red, respectively) for $1/k_n a = -0.4$.

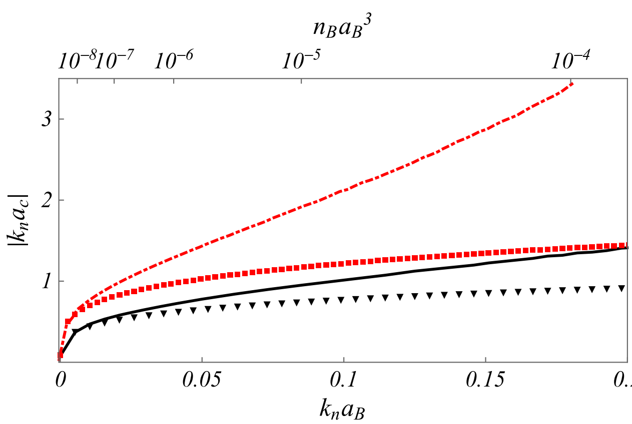

FIG. 5. The critical interaction strength $k_n a_c$ for the formation of bipolarons as a function of $k_n a_B$ (or $n_B a_B^3$) for bosonic (solid black line) and fermionic impurities (dashed red line). The black triangles and red squares are the Yukawa result for bosonic and fermionic impurities, respectively.

from the single-polaron signal. A natural question arises whether there are bound states of more than two polarons, e.g., tripolarons consisting of three polarons. Indeed, it was found for the Yukawa potential that tripolarons can be stable, but only for a narrow range of coupling strengths and with a small binding energy: at the threshold $k_n a_c$ for bipolaron formation, the binding energy of the tripolaron is $-0.29 k_n a_B E_n$ [41] making them very hard to observe for $k_n a_B \ll 1$. We note that the attractive interaction mediated by Bogoliubov modes also can give rise to superfluid pairing in Bose-Fermi mixtures [42–47].

In summary, we showed that two polarons formed by impurities in a BEC can merge into a bipolaron state that is bound by a nonlocal interaction mediated by phonons in the BEC. The bipolaron states are a pure many-body effect arising from the surrounding BEC. They are therefore distinct from three-body Efimov states of two impurities and one boson, which are stable in a vacuum [48]. The theory described in this Letter opens the door for a number of future investigations. For example, the nonlocal nature of the effective interaction suggests exotic and interesting many-body physics of multiple interacting polarons. This question as well as the potentially profound effects of different system dimensions should be addressable in future work by the presented theoretical framework. We finally note that the induced interaction between Fermi polarons is rather weak [49], which has made the observation of bipolarons in degenerate Fermi gases challenging [14]. On the other hand, the results of this Letter show that the observation of bipolarons should now be possible in currently available BECs [15], presenting an exciting positive outlook on future experiments.

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