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Mediated interactions between two impurities immersed in a Bose–Einstein condensate

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We consider two pointlike static impurities without direct interaction immersed in a three-dimensional Bose–Einstein condensate (BEC) at zero temperature. By solving the Gross–Pitaevskii (GP) equation in a perturbative manner, we calculate the ground state energy in the region where the atom–impurity interaction is assumed to be weak. We obtain an analytical expression for the spatial distribution of atom number density and the effective force between these two impurities. The effective force is found to be closely related to the strength of the atom–impurity interaction and the relative distance between these two impurities. Two critical relative distances are found between the two impurities. The first one corresponds to the vanishing of the perturbed energy with impurities, although the effective force between the two impurities still exists. At the second critical value, the energy of the impurities changes linearly with the atom–impurity interaction; otherwise, it changes quadratically with the atom–impurity interaction.

Keywords: quantum gases, Bose–Einstein condensate, Bose polaron, mediated interaction

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1. Introduction

Since Landau and Pekar first proposed that the coupling between electrons and lattice phonons leads to the existence of quasiparticles termed polarons,[1] this idea has proven useful in understanding a variety of physical systems such as semiconductors,[2] along with conventional and high-temperature superconductivity.[3,4] Later research found that the description of an impurity atom in a Bose–Einstein condensate (BEC) can be cast in the form of Fröhlich's polaron Hamiltonian.[5] The concept of the polaron can be generalized to a system where an impurity interacts with its surrounding medium. Indeed, even elementary particles in the Standard Model acquire their masses by coupling to the bosonic Higgs particle.[6] It is also important to understand the effective interaction between two polarons due to the key role it plays in Landau's theory, where it determines both thermodynamic and dynamical properties.[7] For example, in conventional and high-temperature superconductivity, the interaction is mediated by lattice vibrations and spin fluctuations, respectively.[8,9] Also, in particle physics, the fundamental interaction is regarded as the exchange of gauge bosons.[6]

The experimental realization of impurity atoms through ultracold atoms mainly exploits highly population-imbalanced atomic gases,[10] where the minority forms impurity atoms. The interaction between the impurity atoms and the majority atoms can be tuned using Feshbach resonances.[11] Impurity atoms were first realized experimentally in degenerate Fermi gases, where they form quasiparticles called Fermi polarons.[12–17] We now have a good understanding of the Fermi polaron, even for strong interactions between the impurity and the Fermi gas.[18–25] For an impurity immersed in a BEC, impurity–boson interactions are expected to dress the impurity into a Bose polaron. The Bose polaron has been explored not only in the weakly interacting regime[26–30] but also in the strongly interacting regime.[31–36]

Most of the research into atomic gases has focused on systems with a single impurity, and much less is known about the interaction between impurities. Although the Landau effective interactions between Bose polarons have been systematically investigated using diagrammatic schemes[7] and variational techniques,[37,38] exploration of the physical mechanism underlying this interaction remains intriguing. In this work, we study Bose condensates with two fixed impurities. We assume that the impurity–boson interaction is weak such that we can apply the perturbation method. We investigate the ground-state energy in terms of the relative distance between impurities and the impurity–boson scattering length. From the ground-state energy, we also obtain the effective force, which

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turns out to be attractive, regardless of whether the impurity–boson interaction is attractive or repulsive. Finally, we map out the condensate density to illustrate this interesting effect.

The rest of the paper is structured as follows. In Section 2, we describe the theoretical model and the methods we will use based on the mean-field approximation at zero temperature. In Section 3, we discuss the effects of impurities on the energy and analyze the effective interaction between two impurities mediated by the background BEC. Finally, we summarize these results in Section 4.

2. Model and method

We consider two pointlike impurities without direct interaction, immersed in a uniform three-dimensional BEC. We assume the masses of the impurities are much larger than the masses of the atoms in the condensate, so that these two impurities always stay at fixed locations during scattering with the atoms in the condensate. According to the mean-field theory, at zero temperature, the Gross–Pitaevskii (GP) energy functional of such a system can be written as follows:

$$E = \int \mathrm{d}^3\boldsymbol{r}\left[\frac{\hbar^2}{2m}|\nabla\phi(\boldsymbol{r})|^2+\frac{g}{2}|\phi(\boldsymbol{r})|^4 + g_{\mathrm{i}}\sum_{j=1,2}\delta(\boldsymbol{r}-\boldsymbol{r}_j)|\phi(\boldsymbol{r})|^2\right], \tag{1}$$

where $\phi(\boldsymbol{r})$ is the condensate wave function and m is the mass of an atom in the condensate. Here, $\delta(\boldsymbol{r}-\boldsymbol{r}_j)$ represents the contact interaction potential between the atom and the impurity, and $\boldsymbol{r}$ and $\boldsymbol{r}_j$ with $j=1,2$ are the coordinates of the atom and the impurities, respectively. $g=4\pi\hbar^2 a_{\mathrm{BB}}/m$ and $g_{\mathrm{i}}=2\pi\hbar^2 a_{\mathrm{IB}}/m$ are the strengths of the atom–atom and atom–impurity interactions, respectively, with a_{BB} and a_{IB} being the respective scattering lengths, where we have assumed the two different impurities have the same coupling strengths with the atoms of the condensate for the sake of simplicity. Furthermore, to avoid the collapse of the BEC, the atom–atom interaction is assumed to be repulsive with $a_{\mathrm{BB}}>0$, while the atom–impurity interaction can be taken as repulsive or attractive, corresponding to $a_{\mathrm{IB}}>0$ or $a_{\mathrm{IB}}<0$, respectively. Consequently, the stationary properties of the system are governed by the time-independent GP equation

$$\mu\phi = \left[-\frac{\hbar^2}{2m}\nabla^2+g|\phi|^2+g_{\mathrm{i}}\sum_{j=1,2}\delta(\boldsymbol{r}-\boldsymbol{r}_j)\right]\phi, \tag{2}$$

where μ is the chemical potential of the BEC.

In this paper, to highlight the effects of impurities, we consider a dilute BEC that satisfies the condition $na_{\mathrm{BB}}^3\ll 1$, with n denoting the total density. All atoms are assumed to be condensed into the zero-momentum state in the absence of impurities. In particular, the fluctuation caused by the atomic interaction can be neglected; thus, the ground-state wave function is a real constant denoted by ϕ_0, and we have $\mu=gn_0$ with $n_0=\phi_0^2$. In the presence of two impurities, we treat the impurities as perturbations by considering the very weak atom–impurity interaction, so we can decompose the wave function into a sum of the unperturbed solution ϕ_0 and a small correction $\delta\phi(\boldsymbol{r})$ only caused by the impurities, that is $\phi(\boldsymbol{r})=\phi_0+\delta\phi(\boldsymbol{r})$. After inserting this into GP equation (2) and retaining terms to the first order in the perturbed wave function, we obtain

$$\frac{\hbar^2}{2m}\nabla^2\delta\phi-gn_0(\delta\phi+\delta\phi^*)=g_{\mathrm{i}}\sqrt{n_0}\sum_{j=1,2}\delta(\boldsymbol{r}-\boldsymbol{r}_j), \tag{3}$$

where we have also neglected the terms $g_{\mathrm{i}}n_0\delta\phi$ and $g_{\mathrm{i}}n_0\delta\phi^*$ as second-order small quantities due to the very weak atom–impurity interaction. Now, the approximated energy function corresponding to the linear GP equation (3) is

$$\begin{aligned}E = &\int \mathrm{d}^3\boldsymbol{r}\Big\{-\frac{\hbar^2\sqrt{n_0}}{2m}\nabla^2\delta\phi-\frac{\hbar^2}{2m}\delta\phi^*\nabla^2\delta\phi \\ &+\frac{g}{2}n_0[\sqrt{n_0}+2\mathrm{Re}(\delta\phi)]^2+gn_0|\delta\phi|^2\Big\}+2g_{\mathrm{i}}n_0 \\ &+g_{\mathrm{i}}\sqrt{n_0}\{2\mathrm{Re}[\delta\phi(\boldsymbol{r}_1)]+2\mathrm{Re}[\delta\phi(\boldsymbol{r}_2)]\},\end{aligned} \tag{4}$$

where Re denotes the real part.

To solve Eq. (3), we further apply the Fourier transformation $\delta\phi_{\boldsymbol{k}}=\frac{1}{\sqrt{V}}\int \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\delta\phi(\boldsymbol{r})\,\mathrm{d}^3\boldsymbol{r}$ with $\boldsymbol{k}$ being the momentum; then, in the momentum representation, equation (3) can be written as

$$\begin{pmatrix}\mathcal{E}_{\boldsymbol{k}} & gn_0\\ gn_0 & \mathcal{E}_{\boldsymbol{k}}\end{pmatrix}\begin{pmatrix}\delta\phi_{\boldsymbol{k}}\\ \delta\phi^*_{-\boldsymbol{k}}\end{pmatrix}=-\frac{g_{\mathrm{i}}\sqrt{n_0}}{\sqrt{V}}\sum_{j=1,2}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_j}\begin{pmatrix}1\\1\end{pmatrix}, \tag{5}$$

where $\mathcal{E}_{\boldsymbol{k}}=\varepsilon_{\boldsymbol{k}}+gn_0$ with $\varepsilon_{\boldsymbol{k}}=\hbar^2\boldsymbol{k}^2/2m$, and V denotes the volume of the system. Therefore, in momentum space, the matrix equations (5) can easily be solved:

$$\delta\phi_{\boldsymbol{k}}=-\frac{g_{\mathrm{i}}\sqrt{n_0}\left(\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_1}+\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_2}\right)}{\sqrt{V}(\varepsilon_{\boldsymbol{k}}+2gn_0)}, \tag{6}$$

which indicates that the perturbed wave function depends on the locations of the two impurities. In the rest of this paper, we mainly work in coordinate space; thus, we further apply an inverse Fourier transformation to get the perturbed wave function in coordinate space:

$$\delta\phi(\boldsymbol{r})=-\frac{\sqrt{n_0}mg_{\mathrm{i}}}{2\pi\hbar^2\xi}\left[\frac{\mathrm{e}^{-\sqrt{2}\frac{|\boldsymbol{r}-\boldsymbol{r}_1|}{\xi}}}{\frac{|\boldsymbol{r}-\boldsymbol{r}_1|}{\xi}}+\frac{\mathrm{e}^{-\sqrt{2}\frac{|\boldsymbol{r}-\boldsymbol{r}_2|}{\xi}}}{\frac{|\boldsymbol{r}-\boldsymbol{r}_2|}{\xi}}\right], \tag{7}$$

where $\xi=\hbar/\sqrt{2mgn_0}$ is the healing length of the BEC.

Solution (7) contains the full information about the system. To extract the underlying physics, in what follows, we perform a detailed analysis by calculating the atomic density distribution, perturbed energy, and effective forces between the two impurities.

3. Results and discussion

The perturbed wave function in Eq. (7) depends on the atom–impurity interaction, which implies that the repulsive and attractive atom–impurity interactions give rise to different effects on the BEC and the impurities. To illustrate this point, the following expression gives the atomic density distribution of the BEC:

$$\frac{n}{n_0}=\left[1-\frac{a_{\rm IB}}{\xi}\left(\frac{\mathrm{e}^{-\sqrt{2}\frac{|\boldsymbol{r}-\boldsymbol{r}_1|}{\xi}}}{\frac{|\boldsymbol{r}-\boldsymbol{r}_1|}{\xi}}+\frac{\mathrm{e}^{-\sqrt{2}\frac{|\boldsymbol{r}-\boldsymbol{r}_2|}{\xi}}}{\frac{|\boldsymbol{r}-\boldsymbol{r}_2|}{\xi}}\right)\right]^2. \tag{8}$$

As shown in Fig. 1, for the attractive atom–impurity interaction with $a_{\rm IB}<0$, the impurities serve as an effective trapping potential that traps the atoms in the BEC, causing the atoms to gather around the two impurities, just as in the so-called Anderson localization. Conversely, for the repulsive atom–impurity interaction with $a_{\rm IB}>0$, the impurities serve as an effective infinite-potential barrier for atoms in the BEC; hence, the atomic density near the impurities is lower.

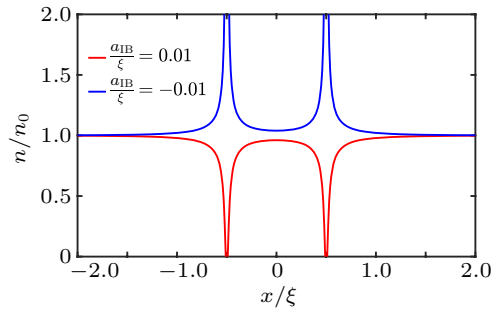


Fig. 1. The atomic density for attractive and repulsive atom–impurity interactions, where the two impurities are assumed to be located on the x-axis with $x_1=-x_2=0.5\xi$.

Upon substituting the perturbed wave function (7) into Eq. (4) and performing the integration, we obtain the total energy of the system

$$E=\frac{1}{2}Vgn_0^2+2g_{\rm i}n_0-\frac{1}{V}\sum_{\boldsymbol{k}}\frac{2g_{\rm i}^2n_0}{\varepsilon_{\boldsymbol{k}}+2gn_0}-\frac{mg_{\rm i}^2n_0}{\pi\hbar^2}\frac{\mathrm{e}^{-\sqrt{\frac{4mgn_0}{\hbar^2}}|\boldsymbol{r}_1-\boldsymbol{r}_2|}}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}. \tag{9}$$

The first term in Eq. (9) is nothing but the unperturbed ground state energy of the BEC in the absence of impurities. The other terms correspond to the correction energy δE generated by the impurities, which is related to the strength of the atom–impurity interaction and the relative distance between the two impurities. We remark that the total energy is not simply a linear superposition of two independent single-impurity results, since the presence of both impurities modifies the condensate wavefunction and the energy in a nontrivial way due to their collective effects on the condensate.

To remove the ultraviolet divergence from the third term of the energy equation (9), we replace $g_{\rm i}$ in the second term with the renormalization relation

$$g_{\rm i}=g_{\rm i}\left(1+\frac{g_{\rm i}}{V}\sum_{\boldsymbol{k}}\frac{1}{\varepsilon_{\boldsymbol{k}}}\right). \tag{10}$$

Then, after converting the sum over momentum into an integral, the perturbed energy can be expressed exactly as follows:

$$\frac{\delta E}{gn_0}=\frac{a_{\rm IB}}{a_{\rm BB}}+\frac{\sqrt{2}a_{\rm IB}^2}{\xi a_{\rm BB}}-\frac{a_{\rm IB}^2}{\xi a_{\rm BB}}\frac{\mathrm{e}^{-\sqrt{2}R}}{R}, \tag{11}$$

where $R=|\boldsymbol{r}_1-\boldsymbol{r}_2|/\xi$. The first two terms in Eq. (11) are the asymptotic energy of the separated impurities. The last term represents the so-called Yukawa potential, which depends on the relative distance between the two impurities. This potential describes the effective interaction between impurities mediated by the exchange of excitations in a BEC, similar to the solid-state physics of electron–electron interactions mediated by lattice phonons. Therefore, the effective force between two impurities mediated by a background BEC is given by $F=-\frac{\partial E}{\xi\partial R}$, that is,

$$\frac{Fa_{\rm BB}}{gn_0}=-\frac{a_{\rm IB}^2}{\xi^2}\left(\frac{\sqrt{2}}{R}+\frac{1}{R^2}\right)\mathrm{e}^{-\sqrt{2}R}, \tag{12}$$

which is a short-range attraction with a strength related to $a_{\rm IB}$, like the nuclear force mediated by the mesons in high-energy physics.

Equations (11) and (12) show that the effective interaction between two impurities is attractive, irrespective of whether the impurity–boson interaction is attractive or repulsive. The underlying mechanism is illustrated by the density distortion shown in Fig. 1. When the impurity–boson interaction is repulsive ($a_{\rm IB}>0$, red line), the condensate density is depleted between the two impurities compared to the bulk density. This density depletion creates a pressure imbalance, effectively pushing the impurities together and resulting in an attractive mediated force. Conversely, for an attractive impurity–boson interaction ($a_{\rm IB}<0$, blue line), condensate density accumulates between the impurities. Since attractive impurities are drawn to regions of higher density, they are pulled toward the area between them. Thus, the effective interaction between two attractive impurities is also attractive. However, when one impurity is repulsive ($a_{\rm IB}>0$) and the other is attractive ($a_{\rm IB}<0$), their combined effect on the density differs. The repulsive impurity repels bosons, creating a region of lower density around it. The attractive impurity is drawn to regions of higher density. Therefore, the attractive impurity is pulled away from the low-density region near the repulsive impurity, toward the higher-density bulk condensate. This effectively leads to a repulsive force between the two impurities.

Equation (11) indicates that the perturbed energy depends on the strength of the atom–impurity interaction and the relative distance between the two impurities. We find the critical value R_c of the relative distance between two impurities as follows:

$$R_c = \frac{1}{\sqrt{2}}\text{LambertW}\left(\frac{\sqrt{2}a_{IB}}{\sqrt{2}a_{IB}+\xi}\right), \tag{13}$$

at which the perturbed energy vanishes even for $a_{IB} \neq 0$. Here, LambertW is a short name for the Lambert W function, which is the inverse function of $f(W) = W\,e^W$. As shown in Fig. 2(a), as long as $a_{IB}/\xi < -1/\sqrt{2}$ and $a_{IB} \geq 0$ due to $R_c \geq 0$, the perturbed energy is negative for $R < R_c$; however, it is positive for $R > R_c$, no matter whether the atom–impurity interaction is attractive or repulsive. For the intermediate case with $-1/\sqrt{2} < a_{IB}/\xi < 0$, the perturbed energy is always negative. In particular, although the perturbed energy vanishes for $R = R_c$, the effective force between two impurities still exists, as shown in Fig. 2(b).

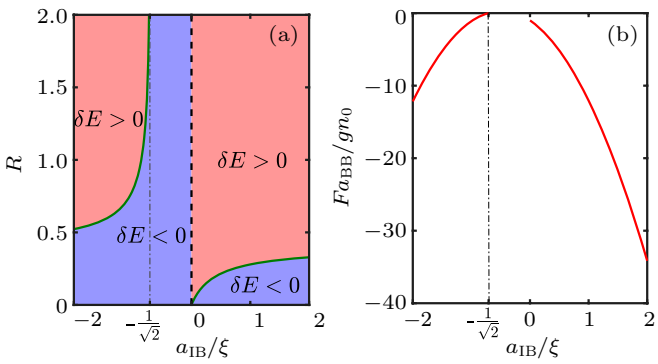


Fig. 2. (a) The change in perturbed energy δE versus the atom–impurity interaction and the relative distance between two impurities. The green lines denote the critical value R_c of the relative distance between two impurities, the dashed line represents $\delta E = 0$ at $a_{IB} = 0$, and the dashed–dotted line denotes $a_{IB}/\xi = -1/\sqrt{2}$. (b) The change in effective force between two impurities versus the atom–impurity interaction when the relative distance between the two impurities is R_c.

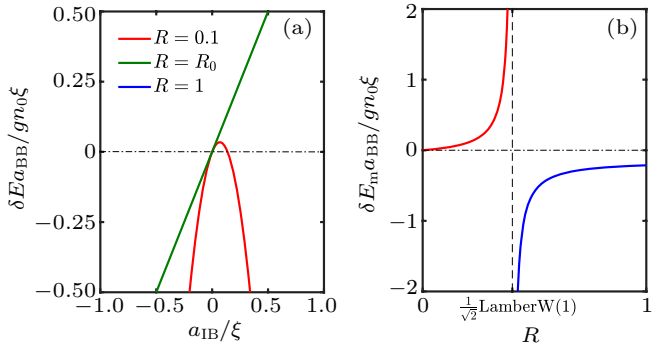


Fig. 3. (a) The change in perturbed energy versus a_{IB}/ξ for different distances between the two impurities; (b) the change in the extreme value of perturbed energy versus the relative distance between the two impurities. Here $R_0 = \frac{1}{\sqrt{2}}\text{LambertW}(1) \approx 0.4$.

On the other hand, as shown in Fig. 3(a), if $R = \frac{1}{\sqrt{2}}\text{LambertW}(1) \approx 0.4$, then we have $\delta E/gn_0 = a_{IB}/a_{BB}$, which indicates that the perturbed energy grows linearly with a_{IB}. While $R \neq \frac{1}{\sqrt{2}}\text{LambertW}(1)$, the perturbed energy changes quadratically with a_{IB} and has an extreme value of $\delta E_m/gn_0 = -\xi R/\left[4\left(\sqrt{2}R - e^{-\sqrt{2}R}\right)a_{BB}\right] = a_{IB}/2a_{BB}$ at $a_{IB}/\xi = -R/\left[2\left(\sqrt{2}R - e^{-\sqrt{2}R}\right)\right]$. For $R < \frac{1}{\sqrt{2}}\text{LambertW}(1)$, the perturbed energy changing with a_{IB} is a downward parabola; thus, it has a maximum value. However, for $R > \frac{1}{\sqrt{2}}\text{LambertW}(1)$, since the perturbed energy changing with a_{IB} is an upward parabola, the perturbed energy has a minimum value. Furthermore, the extreme value of the perturbed energy also depends on the relative distance between the two impurities, as shown in Fig. 3(b).

4. Conclusions

We have investigated the effective interactions between two impurities caused by exchanging an atom in a uniform BEC within the mean-field approximation at zero temperature. By considering the two impurities as a perturbation and solving the GP equation in a perturbative manner, we have analytically derived the density fluctuation of atoms and the perturbed energy caused by these two impurities. Our results show that the effective interaction between two impurities caused by exchanging an atom in a BEC can be accurately mapped to the Yukawa potential. Two critical values of the relative distance between two impurities are found, namely, $\frac{1}{\sqrt{2}}\text{LambertW}\left[\sqrt{2}a_{IB}/\left(\sqrt{2}a_{IB}+\xi\right)\right]$ and $\frac{1}{\sqrt{2}}\text{LambertW}(1)$. The former corresponds to the zero correction energy generated by the impurities, at which the effective interaction between the two impurities still exists. At the second critical value, the perturbed energy changes linearly with the atom–impurity interaction; otherwise, the perturbed energy changes quadratically with the atom–impurity interaction.

Experimental verification of our predictions will contribute to a better understanding of the physics of the Bose polaron and mediated interaction in a general context. Additionally, the inclusion of direct interactions between impurities could qualitatively influence the results, suggesting that this extension constitutes an interesting direction for future studies. Furthermore, investigating the dynamics of two impurities immersed in a non-equilibrium BEC[39–41] would also be of interest. We sincerely hope this work will stimulate further research along these lines.

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