Strong coupling Bose polarons in a two-dimensional gas

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We study the ground state properties of Bose polarons in a two dimensional geometry using quantum Monte Carlo techniques. Results for the binding energy, the effective mass and the quasiparticle residue are reported for a typical strength of interactions in the gas and for a wide range of impurity-gas coupling strengths. Two branches exist for any interaction strength. The lower branch corresponds to an attractive polaron and spans from the regime of weak interactions, where the size of the polaron is on the order of the healing length of the bath, to deeply bound states which involve many particles from the bath and extend far beyond the healing length. The upper branch corresponds to the ground state of a repulsive polaron or an excited state of an attractive polaron.

In the regime of strong interactions where many-body bound states are formed, we find that the energy is lower with respect to the two-body binding energy, the quasiparticle residue approaches zero and the effective mass of the impurity is significantly larger than its bare mass.

Impurities embedded in a quantum many-body environment can lead to the formation of quasiparticles coined polarons. The concept was first introduced by Landau and Pekar in the solid-state context to describe an electron coupled to an ionic crystal [1]. Polarons are fundamental ingredients in many different transport phenomena across condensed-matter physics. Electronic transport in polar crystals or semiconductors [2], charge and spin transport in organic materials [3, 4] can be understood in terms of polarons. Pairing between polarons is relevant in the physics of high-temperature superconductors [5] and polarons are also candidates for electronic transport in DNA and proteins [6]. Furthermore, polarons are used as probes of quantum many-body systems. For example, the low-energy excitations in a strongly-correlated superfluid such as \(^3\)He can be probed by \(^3\)He impurity atoms [7].

Unprecedented control and versatility of ultracold gases [8] made it possible to experimentally observe dressed impurities named Fermi and Bose polarons depending on whether they interact, respectively, with a degenerate Fermi gas [9,13] or a Bose-Einstein condensate (BEC). For Bose polarons, experiments have been carried out in three-dimensional (3D) [14,15] as well as one-dimensional (1D) [19,20] geometries. Observation of Bose polarons in ultracold gases has triggered an intense research activity aiming to describe the crossover from weak to strong-coupling regimes. In the former case the so-called Bogoliubov-Fröhlich Hamiltonian describes accurately the ground state properties of the polaron [21-30]. However, quantum fluctuations become relevant as interactions are increased, making the description in terms of the Fröhlich paradigm inadequate. By using the Gross-Pitaevskii equation strongly interacting Bose polarons were predicted to manifest exotic phenomena such as self-localization [31,32], but no experimental evidence has been found so far. More recently, properties of these strongly coupled impurities have also been addressed by techniques such as T-matrix, diagrammatic and variational approaches which go be-

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FIG. 1. Average over many snapshots of the particle positions around the impurity for for three characteristic values of the impurity-bath coupling constant \(\ln(k_F a)\). The impurity is located in the center and distances are in units of the healing length \(\xi\). The local density \(n(r)\) is estimated by summing particles over a square grid of size \(L/100\), where \(L\) is the size of the simulation box, and the color-bar indicates the ratio \(n(r)/n\) over the bulk density \(n\). At weak coupling impurities form polarons, having a size on the order of \(\xi\) (right and left upper panels). On the attractive branch (positive values of \(\ln(k_F a)\)), the impurity at strong coupling forms a many-body bound state whose size is significantly larger than the healing length (central upper panel).
beyond the single-phonon excitation scheme of the Fröhlich model \[30,32\]. These studies predict exotic out of equilibrium dynamics, non trivial quasiparticle splitting due to finite-temperature effects \[40,44,45\] as well as important few-body effects \[35,45\]. Furthermore, the regime of strong coupling should also feature the interchange of Bogoliubov modes between polarons via polaron-polaron interactions \[47,48\]. In the context of theoretical techniques suitable to investigate this regime, the quantum Monte-Carlo (QMC) method is based on a microscopic Hamiltonian which does not involve the Bogoliubov approximation thus providing exact (within controllable statistical errors) ground state properties of the polaron for arbitrary coupling strengths \[39,41,49,50\].

Physically, the two-dimensional (2D) geometry is appealing since the role of quantum fluctuations is enhanced while off-diagonal long-range order, responsible of BEC phenomena, still exists in the ground state. Polarons in 2D geometries have been extensively investigated in the context of Fermi polarons \[31,51\] and exciton impurities coupled to semiconductors \[55\]. Still, a precise theoretical description of Bose polarons in 2D is lacking while off-diagonal long-range order, responsible of BEC phenomena, still exists in the ground state. Polarons in 2D geometries have been extensively investigated in the context of Fermi polarons \[11,51–54\] and exciton impurities coupled to semiconductors \[55\].

System and theory - We consider an impurity of mass \(m_I\) embedded in a 2D Bose gas consisting of \(N\) atoms of mass \(m_B\) at \(T = 0\) with overall density \(n = \frac{N}{L^2}\). In the first quantization formalism the Hamiltonian of the system reads

\[
H = -\frac{\hbar^2}{2m_B} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j} V_B(r_{ij}) - \frac{\hbar^2}{2m_I} \nabla^2 + \sum_{i=1}^{N} V_I(r_{i\alpha}) .
\]

Here, the first two terms represent the kinetic and the interaction energy of the bosonic bath where particles interact through the two-body potential \(V_B\), which depends on the distance \(r_{ij} = |r_i - r_j|\) between a pair of bosons. Furthermore, \(-\frac{\hbar^2\nabla^2}{2m_B}\) is the kinetic energy of the impurity denoted by the coordinate vector \(r_\alpha\) and \(V_I\) is the boson-impurity potential depending on the distance \(r_{i\alpha} = |r_i - r_\alpha|\) between the impurity and the \(i\)-th bath particle. Both interaction potentials \(V_B\) and \(V_I\) are short ranged and are parameterized by the scattering lengths \(a_B\) and \(a\), respectively.

Within perturbation theory, which treats the coupling between the impurity and the gas to the lowest order, the Hamiltonian \(H\) can be written as the sum of two terms

\[
H = H_0 + H_{\text{int}},
\]

where

\[
H_0 = \frac{\vec{p}^2}{2m_I} + E_B + \sum_k \epsilon_k \hat{a}_k^\dagger \hat{a}_k ,
\]

is the unperturbed Hamiltonian of a free impurity moving with momentum \(\vec{p}\) and a static host gas. The bath is described in terms of non-interacting Bogoliubov excitations with energy \(\epsilon_k = \sqrt{(\epsilon_k^0)^2 + 2g_B n^\frac{\epsilon_k^0}{\epsilon_k}}\), where \(\epsilon_k^0 = \frac{\hbar^2 k^2}{2m_B}\) is the dispersion of free particles and \(g_B = \frac{4\pi \hbar^2/m_B}{\ln(1/na_B^2)}\) is the 2D density-dependent coupling constant of the Bose gas. The ground state of the bath corresponds to the vacuum of excitations and has energy \(E_B\). The interaction Hamiltonian \(H_{\text{int}}\) is given by the sum of a mean-field shift and a term where the impurity is coupled to the creation and annihilation operators of single excitations in the Bose gas

\[
H_{\text{int}} = gn + \frac{g\sqrt{n}}{\sqrt{L^2}} \sum_q e^{i\vec{q}\cdot\vec{r}_\alpha} \sqrt{\frac{\epsilon_q^0}{\epsilon_q}} (a_q + a_q^\dagger) .
\]

Here, \(g = \frac{2\pi \hbar^2/m_B}{\ln(1/na^2)}\) is the 2D effective coupling constant which involves the reduced mass \(m_r = \frac{m_B m_I}{m_B + m_I}\). It describes the scattering processes between the impurity and the bath particles in terms of the scattering length \(a\) of the potential \(V_I\).

If one denotes by \(E(\vec{p})\) the energy of the impurity with momentum \(\vec{p}\) coupled to the bath, the low momentum expansion of the energy difference

\[
E(\vec{p}) - E_B = \mu + \frac{\vec{p}^2}{2m_I} + \ldots ,
\]

defines the binding energy \(\mu\) of the impurity and its effective mass \(m_I^*\). By using perturbation theory one finds the following results to the lowest order in the coupling strength \(g\) of the interaction Hamiltonian \(H_{\text{int}}\)

\[
\mu = \frac{2\pi \hbar^2 n/m_r}{\ln (1/na^2)} ,
\]

and

\[
\frac{m_B}{m^*} = \frac{m_I}{m_B} - \frac{1}{2} \frac{\ln(1/na_B^2)}{\ln^2(1/na^2)} .
\]

Within the same approximation scheme, the polaron state can be written as \(|0\rangle_{\text{int}} = \sqrt{Z_\alpha}|0\rangle - \ldots\)
\[
\frac{g \sqrt{\pi}}{\sqrt{2m}} \sum_{\mathbf{q} \neq 0} \sqrt{\frac{\epsilon_i^{2}}{\epsilon_q}} e^{-\frac{\epsilon_i^{2}}{\epsilon_q}} |\mathbf{q}|. \]
Here \( |\mathbf{q}| \) denotes the eigenstates of the Hamiltonian (2) corresponding to the energies \( E_0(\mathbf{q}) = \left( \frac{p + h \mathbf{q}}{2m} \right)^2 + E_B + \epsilon_q \) and \( \mathbf{q} \) is the exchanged momentum between the impurity and the bath. The coefficient \( Z_0 \) defines the quasiparticle residue, i.e. the fraction of the free impurity state present in the interacting polaron state. For the impurity at rest (\( \mathbf{p} = 0 \)) one finds

\[
Z_0 = 1 - \frac{m_B + m_I}{2m_I} \frac{\ln \left( 1/na_B^2 \right)}{\ln^2 \left( 1/na^2 \right)}. \tag{7}
\]

Notice that results [6] and [7] hold under the weak-coupling condition \( \frac{\ln(\alpha \gamma)}{\ln(a^2)} \ll 1 \), which requires that the interaction strength between the impurity and the bath is much smaller than the one between bath particles.

**Strong-coupling regime** - In order to determine the properties of the polaron beyond the weak-coupling limit we resort to the QMC technique. Details on the method can be found in Refs. [39, 59, 68]. Simulations are performed for a gas of \( N \) identical particles and a single impurity in a square box of length \( L \) with periodic boundary conditions. For simplicity, we consider only the case where impurity and particles in the bath have the same mass: \( m_B = m_I = m \).

Boson-boson interactions are modelled via a repulsive soft-disk potential \( V_B(r) = V_0 \Theta(R_0 - r) \), where \( \Theta(x) \) is the Heaviside function. The scattering length \( a_B \) is related to the range \( R_0 \) and the height \( V_0 > 0 \) of the potential by \( a_B = R_0 \exp \left[ -\frac{1}{\kappa_0 R_0} \ln \frac{I_0(k_0 R_0)}{I_1(k_0 R_0)} \right] \). Here, \( k_0 = \sqrt{V_0 m_B/\hbar^2} \) and \( I_k \) is the modified Bessel function of zeroth (\( k = 0 \)) and first order (\( k = 1 \)). In our calculations we use \( nR_0^2 = 0.01 \), thus ensuring that \( R_0 \) is small compared to the mean interparticle distance. The value of the 2D scattering length \( a_B \) is exponentially suppressed and allows us to describe typical experimental conditions where the 3D s-wave scattering length is much smaller than the transverse length of the 2D confinement [5]. In particular, we choose the height \( V_0 \) of the repulsive potential such that the 2D gas parameter is given by \( na_B^2 \approx 10^{-40} \). This corresponds to a dimensionless coupling constant of the bath \( \tilde{g}_B = \frac{m_B g_B}{\hbar a_B^2} \approx 0.136 \), quite close to the experimental conditions of Ref. [57] (see Supplementary Materials [?]).

The impurity-boson interaction is modelled by a contact pseudopotential. In this case the interaction potential is replaced by an appropriate boundary condition on the many-body wave function when a particle of the bath approaches the impurity. These contact conditions are imposed on the guiding function which is also used for importance sampling. Its general form is given by

\[
\psi_T(\mathbf{R}) = \prod_{i<j} f_B(r_{ij}) \prod_{i=1}^{N} f_I(r_{ia}), \tag{8}
\]
where \( \mathbf{R} = (\mathbf{r}_a, \mathbf{r}_1, \ldots, \mathbf{r}_N) \) is the multidimensional vector containing the spatial coordinates of the impurity and of the bath particles and \( f_B \) and \( f_I \) are two-body Jastrow terms accounting, respectively, for correlations between the bosons and between the impurity and the bosons. In both cases the explicit functional form of the Jastrow function is obtained by matching the solution of the two-body scattering problem at short distances with an appropriate tail at large distances (see Supplementary Materials [?]). In particular, the short-distance behavior of the function \( f_I \) is chosen as \( f_I(r) \propto K_0(2e^{-\gamma r/\hbar a}) \) for the attractive branch of the polaron and \( f_I(r) \propto \text{ln}(r/\hbar a) \) for the repulsive branch. Here, \( K_0 \) is the modified Bessel function of the second kind and \( \gamma = 0.577 \) is Euler’s constant. For both branches, the pair wavefunction satisfies the 2D Bethe-Feierls contact condition of a pseudopotential with scattering length \( a \) which read

\[
|f_I| e^{-\text{ln}(qa)} = -\frac{e^{-\text{ln}(qa)}}{\text{ln}(qa)}, \quad q \text{ is an arbitrary wave vector. Furthermore, for any value of the scattering length } a, \text{ a two-body bound state exists with binding energy } \epsilon_b = -\frac{4\hbar^2}{me^2a^2}. \]

The important difference between attractive and repulsive branches is that in the former case the function \( f_I \) is nodeless and properly describes the ground state of the polaron. In the latter case, instead, \( f_I \) has a node at \( r = a \) and its short-distance behavior corresponds to an excited state of the two-body problem orthogonal to the bound state with energy \( \epsilon_b \). We point out that we also employed a square-well potential with fixed (short) radius to model the boson-impurity interaction. We find results that only depend on the interaction strength \( \text{ln}(kB) \) and not on the details of the potential.

We determine the polaron binding energy \( \mu \) from the direct calculation of the ground state energy of the bath with and without the impurity, \( \mu = E(N,1) - E(N) \), where \( N \) is the number of particles in the gas. In Fig. 2 we
report the QMC results for $\mu$ in units of $\mu_0 = \hbar^2 k_F^2 / 2m$ as a function of the coupling strength $\ln(k_F a)$, where $k_F = \sqrt{2\pi n}$ is the Fermi momentum of a system having the same density $n$ of the gas. In analogy with the 2D Fermi polaron, we find two branches: one corresponds to the ground state of the attractive polaron with $\mu < 0$ and the second to an excited state of the quasiparticle with $\mu > 0$. Notice that the latter branch also corresponds to the ground state of the impurity coupled to the bath via purely repulsive interactions. Here a two-body bound state with energy $\epsilon_b$ exists for any value of the coupling constant $\ln(k_F a)$. This is in contrast with the 3D polaron where the dimer state only appears as the s-wave scattering length turns positive, on one side of the scattering resonance. In Fig. 2 we report the polaron energy obtained by the QMC method and compare it with the mean-field prediction $\tilde{\mu}_0 = 0.136$ of the interaction strength in the gas. In the weakly interacting regime, $\ln(k_F a) \gg 1$, the mean-field prediction and the QMC results are in good agreement, whereas deviations become evident as one approaches the strongly interacting regime $\ln(k_F a) \approx 1$. We notice that, due to many-body effects, the polaron energy $\mu$ along the attractive branch is always much larger, in absolute value, than the dimer binding energy $\epsilon_b$. In the vicinity of $\ln(k_F a) \approx 0$ large fluctuations occur in our QMC simulations due to the formation of many-body bound states (clusters) which make it very hard to follow further both the attractive and the repulsive branch of the polaron. This situation differs from what happens in a 2D Fermi polaron, where a transition to a molecular state is expected, as only one fermion can be deeply bound to the impurity and the other fermions experience repulsion due to the Pauli exclusion principle.

We study the mobility of the impurity by calculating its effective mass $m^*$ as a function of the coupling strength $\ln(k_F a)$. The effective mass is determined by computing the mean-square displacement of the impurity in imaginary time

$$m^* = \lim_{\tau \to \infty} \frac{\langle |\Delta r_\alpha(\tau)|^2 \rangle}{4 D \tau},$$

where $D = \hbar^2 / (2m_B)$ is the diffusion constant of a free particle and $\langle |\Delta r_\alpha(\tau)|^2 \rangle = \langle |r_\alpha(\tau) - r_\alpha(0)|^2 \rangle$, being $\tau = it$ the imaginary time of the QMC simulation. The effective mass is found by fitting the slope of $\langle |\Delta r_\alpha(\tau)|^2 \rangle$ for large values of $\tau$. The quasiparticle residue $Z_0$ of the polaron is obtained from the one-body density matrix associated to the impurity

$$\rho(\mathbf{r}) = \begin{pmatrix} \psi_T(\mathbf{r}_\alpha + \mathbf{r}, \mathbf{r}_1, \cdots, \mathbf{r}_N) \\ \psi_T^\dagger(\mathbf{r}_\alpha, \mathbf{r}_1, \cdots, \mathbf{r}_N) \end{pmatrix}.$$  

This quantity is normalized to unity for $\mathbf{r} \to 0$, whereas its long-range limit gives the residue

$$\lim_{\mathbf{r} \to \infty} \rho(\mathbf{r}) \to Z_0.$$  

In Fig. 3 we show the QMC results for the effective mass as a function of $\ln(k_F a)$ and we compare them with the perturbative prediction from Eq. (6). We notice that in the strongly interacting regime the effective mass becomes much larger than the bare mass, signalling that the polaron gets dressed by a significant number of bosons and carries them as the impurity moves.

In Fig. 4 we report results of the quasiparticle residue. We notice that, similarly to the effective mass in Fig. 3, in the range of $\ln k_F a$ considered the residue $Z_0$ is larger than the perturbative result from Eq. (7). Moreover, it approaches zero in the strongly interacting regime. A

![Figure 3: Effective mass $m^*$ of the polaron as a function of the coupling strength $\ln(k_F a)$. The coupling constant of the Bose gas is $\tilde{\mu}_0 = 0.136$.

![Figure 4: Quasiparticle residue $Z_0$ of the polaron as a function of the coupling strength $\ln(k_F a)$. The coupling constant of the gas is $\tilde{\mu}_0 = 0.136$.](image-url)
finite quasiparticle residue indicates that the polaron is delocalized within the bath and maintains a finite overlap with the non interacting plane-wave state of the impurity. When the coupling is strong, instead, the interacting and non interacting polaron state approach full orthogonality and the impurity has a tendency to become more and more localized. Along the attractive branch this behavior of the quasiparticle residue is a consequence of the formation of a many-body bound state between the impurity and particles in the bath.

Conclusions - We investigated the properties of Bose polarons in two dimensions. The polaron energy, effective mass and quasiparticle residue have been calculated using QMC techniques for arbitrary coupling strength. We study the properties of the attractive and repulsive branch which correspond to the ground state and to a metastable state of the impurity. For the polaron ground state we find an energy that is much lower than the one of a many-body bound state between the impurity and particles in the bath.

- We investigated the properties of Bose polarons in two dimensions. The polaron energy, effective mass and quasiparticle residue have been calculated using QMC techniques for arbitrary coupling strength. We study the properties of the attractive and repulsive branch which correspond to the ground state and to a metastable state of the impurity. For the polaron ground state we find an energy that is much lower than the one of the two body bound state, always present in two dimensions. By approaching the strongly interacting regime, many particles from the bath form a many-body bound state around the impurity. This is in contrast to the Fermi-polaron where Pauli exclusion principle only allows for the formation of a molecular state involving just one particle from the bath. Our findings are supported by the calculation of the effective mass which greatly exceeds the value of the bare atomic mass as well as the quasiparticle residue that drops to zero. Our system may serve to pave the way for quantum simulations of several intriguing systems in two dimensions such as layered manganites and atomically thin semiconductors. The role of many impurities, in particular the possible formation of bipolarons, as well as the role of temperature are future perspectives for our work.

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I. SUPPLEMENTARY MATERIAL

A. Experimental implementation

In Ref. [59] a gas of $^{87}$Rb atoms in the hyperfine state $|F = 1, m = 0\rangle$ is confined in a 2D rectangular box with dimensions $L_x \approx L_y = 30 \mu m$, at temperatures much below the Berezinskii-Kosterlitz-Thouless critical temperature. In the transverse direction a strong harmonic confinement is applied with frequency $\omega_z/(2\pi) \approx 4.6$ kHz and by changing the number of trapped atoms the 2D density can be varied in the range $n \approx 10 - 80 \mu m^{-2}$. The 2D scattering length is given by $a_B = 1.863 \ell_z \exp \left( -\frac{\pi}{2} \ell_z/a_B^{(3D)} \right)$ (see Ref. [8]), in terms of the 3D s-wave scattering length $a_B^{(3D)}$ and the transverse length $\ell_z = \sqrt{\hbar/m_B \omega_z}$. With the typical ratio of lengths $\ell_z/a_B^{(3D)} \approx 30 - 50$ reached in experiments the interaction strength is in the range $\tilde{g}_B \approx 10 - 0.16$, where $\tilde{g}_B$ is the dimensionless parameter $\tilde{g}_B = \frac{mg \phi_0}{\pi z} = \sqrt{8\pi a_B^{(3D)} / \ell_z}$. Due to the exponential dependence of $a_B$ on the ratio $\ell_z/a_B^{(3D)}$, the 2D gas parameter takes on very small values: $na_B^2 \approx 10^{-30} - 10^{-50}$. In our purely 2D simulations we use the value $na_B^2 = 10^{-40}$ for the gas parameter of the bath, which corresponds to the effective 2D coupling strength $\tilde{g}_B = \frac{4\pi}{\ln(1/na_B^2)} = 0.136$ close to the experimental conditions of Ref. [59].

B. Trial wave functions

We describe the trial wave functions implemented in the QMC simulations. In general, the trial wave function is written as a pair product of Jastrow functions for both boson-boson and boson-impurity correlations [see Eq. (8)], featuring appropriate short and long-range asymptotic behaviors.

The short-range part of both the boson-boson and boson-impurity Jastrow function is taken from the zero-energy solution of the two-body scattering problem $-\frac{k^2}{2m} \nabla^2 \psi(r) + V(r) \psi(r) = 0$, where $V(r)$ is the corresponding interaction potential and $m_r$ is the reduced mass. Notice that the impurity is considered to have the same mass as the bath particles yielding in both cases $2m_r = m$.

The long-range part of the boson-impurity term is taken instead from hydrodynamic theory. As it was shown by Reatto and Chester in Ref. [61], if phonons are the lowest-energy excitations present in the system, the long-range behavior of the many-body wave function can be factorized as a pair-product of Jastrow functions. In 2D the resulting Jastrow term is expected to behave as $\exp(-\text{const}/r)$.

The long-range behavior of the boson-impurity term is constructed using perturbation theory. It can be shown [62] that a stationary impurity of infinite mass induces the following perturbation, $\delta \psi_k$, to the wave function of the bath in momentum space,

\[
\delta \psi_k = -\frac{\tilde{g} \phi_0}{\hbar^2 c^2 + 2m c^2},
\]

where $c = \sqrt{\frac{\hbar m}{m}}$ is the speed of sound in the bath and $\phi_0$ is the wave function of the unperturbed condensate. In coordinate space, the perturbation decays exponentially with the characteristic length given by $\xi = \hbar/(\sqrt{2}mc)$ in 3D and 1D, while in 2D it involves the modified Bessel function of the second kind

\[
\delta \psi(r) \propto \frac{mg \phi_0}{\hbar^2} K_0 \left( \frac{\sqrt{2}r}{\xi} \right).
\]

The above expression can be expanded with logarithmic accuracy at large distances as

\[
\delta \psi(r) \propto \frac{mg \phi_0}{\hbar^2} \exp \left\{ -\frac{\sqrt{2}r}{\xi} + O \left( \frac{\ln \xi}{r} \right) \right\}.
\]

1. Boson-boson trial wave function

The interaction between bosons in the bath is modelled by a repulsive soft-disk potential: $V_B(r) = V_0 \Theta(R_0 - r)$, where $V_0 > 0$. The range of the interaction potential is chosen to be small compared to the mean interparticle distance, $nR_0^2 = 0.01$. The height $V_0$ is adjusted in order to get the desired value of the scattering length $a_B$, in particular it is tuned such as to get $na_B^2 = 10^{-40}$.
The Jastrow term for boson-boson correlations is chosen of the following form,

\[ f_B(r) = \begin{cases} 
  I_0(k_0r) & r < R_0 \\
  A \ln \left( \frac{r}{a_B} \right) & R_0 \leq r < R \\
  B \exp \left( -\frac{C}{r} + \frac{D}{r^2} \right) & R \leq r < L/2 
\end{cases} \]  

(S4)

Here, \( I_0 \) is the modified Bessel function of the first kind, \( k_0 = \sqrt{\frac{mV_0}{\hbar^2}} \) and \( A = \frac{I_0(k_0R_0)}{\ln(R_0/a_B)} \) to ensure continuity of \( f_B(r) \) at \( r = R_0 \). Furthermore, the coefficients \( B, C \) and \( D \) are chosen such that \( f_B \) and its first derivative \( f'_B \) are continuous functions at the matching point \( R \) and \( f'_B(r = L/2) = 0 \), complying with the periodic boundary conditions. The position \( R \) of the matching point is a parameter optimized by minimizing the energy in a variational calculation. As stated, the short-range part corresponds to the two-body scattering solution at zero energy and the leading long-range part reproduces the phononic tail [61]. One should also notice that the scattering length \( a_B \) is the position of the node in the scattering solution at zero energy.

2. Impurity-boson trial wave function: Attractive branch

The interaction potential between the impurity and bath particle is modelled by a zero-range pseudo-potential, which is imposed as an appropriate boundary condition on the wave function at short distances. The pseudo-potential supports a bound state of energy \( E_b = -\frac{4}{\exp(2\gamma)} \frac{\hbar^2}{ma^2} = -\frac{\hbar^2 k^2}{m} \), where \( k = 2/(e^\gamma a) \) is the characteristic momentum in terms of scattering length \( a \).

In the attractive branch the Jastrow term is constructed from the two-body bound-state solution matched to an exponential decay at large distances [see Eq. (S3)],

\[ f_I(r) = \begin{cases} 
  AK_0(kr), & r < \rho_1 \\
  B + \exp(-Cr) + \exp(-C(L - r)), & \rho_1 \leq r < L/2 
\end{cases} \]  

(S5)

Here, the parameters \( A \) and \( B \) are chosen such that \( f_I(r) \) and its first derivative are continuous at \( r = \rho_1 \). The parameter \( C \) and the matching point \( \rho_1 \) are instead additional parameters used to minimize the variational energy. Notice that, by construction, \( f'_I(r = L/2) = 0 \).

3. Impurity-boson trial wave function: Repulsive branch

In the repulsive branch scattering states of the pseudo-potential are used at short distances. The Jastrow correlation term is chosen by matching this two-body scattering solution to the same exponential decay as in Eq. (S5),

\[ f_I(r) = \begin{cases} 
  A \ln \left( \frac{r}{a} \right), & \rho \leq \rho_1 \\
  B + \exp(-Cr) + \exp(-C(L - r)), & \rho_1 \leq r < L/2 
\end{cases} \]  

(S6)

The parameters \( A, B, C \) and \( \rho_1 \) entering Eq. (S6) are chosen similarly to Eq. (S5).

Note that the Jastrow term (S6) has a node when \( r = a \) and the corresponding two-body wave function is orthogonal to the bound state. This choice of trial many-body wave function describes an excited state of the polaron which is expected to be metastable when the mean interparticle distance is much larger than \( a \), i.e. \( \ln(k_F a) \ll 1 \). In the opposite limit when the relevant distances are much smaller than \( a \), the attractive (S5) and repulsive (S6) Jastrow terms become similar, in fact \( K_0(kr) \approx \ln(r/a) \) if \( r \ll a \). This means that, at the variational level, the upper repulsive branch constructed from the Jastrow term (S6) connects smoothly with the lower attractive branch (S5) for \( \ln(k_F a) \gg 1 \).