Polaron Interactions and Bipolarons in One-Dimensional Bose Gases in the Strong Coupling Regime

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Bose polarons, quasiparticles composed of mobile impurities surrounded by cold Bose gas, can experience strong interactions mediated by the many-body environment and form bipolaron bound states. Here we present a detailed study of heavy polarons in a one-dimensional Bose gas by formulating a nonperturbative theory and complementing it with exact numerical simulations. We develop an analytic approach for weak boson-boson interactions and arbitrarily strong impurity-boson couplings. Our approach is based on a mean-field theory that accounts for deformations of the superfluid by the impurities and in this way minimizes quantum fluctuations. The mean-field equations are solved exactly in the Born-Oppenheimer approximation, leading to an analytic expression for the interaction potential of heavy polarons, which is found to be in excellent agreement with quantum Monte Carlo (QMC) results. In the strong coupling limit, the potential substantially deviates from the exponential form valid for weak coupling and has a linear shape at short distances. Taking into account the leading-order Born-Huang corrections, we calculate bipolaron binding energies for impurity-boson mass ratios as low as 3 and find excellent agreement with QMC results.

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Introduction.—Interactions between quantum particles mediated by a many-body environment play an important role in condensed-matter physics. Examples range from the Ruderman-Kittel-Kasuya-Yodsia interaction of spins in a Fermi liquid [1–3] to Cooper pairing of electrons in a solid induced by lattice vibrations [4]. The mechanism that causes such interactions can also substantially modify the properties of individual impurities by forming quasiparticles. A paradigmatic example is the polaron [5,6] resulting from the electron-phonon coupling, also responsible for Cooper pairing. In the strong coupling limit, impurity interaction and quasiparticle formation are strongly intertwined. Bipolarons are suspected to be essential for high-temperature superconductivity [7–9]. They are important for the electric conductivity of polymers [10–14] or organic magnetoresistance [15]. Their understanding is one of the key questions of many-body physics.

In recent years, neutral atoms immersed in degenerate quantum gases have become versatile experimental platforms for accessing polaron physics in novel regimes and with an unprecedented degree of control [16–31]. Length and energy scales are very different from solids and can be resolved and manipulated much more easily. Most importantly, polarons can be studied out of equilibrium with the prospect of engineering their properties beyond what is possible in equilibrium. One-dimensional (1D) gases are of particular relevance as they show pronounced quantum effects and powerful tools are available for their theoretical description. It is possible to tune the impurity-bath interaction all the way through weak to strong coupling, e.g., by employing Feshbach and confinement-induced resonances [32]. Contrary to higher dimensions, the system remains stable even for infinite coupling since three-body losses are greatly suppressed. Polaron interactions have so far mostly been studied in regimes where the mediated interaction between them is weak. A perturbative treatment yields an exponential (1D) or Yukawa (3D) potential between two impurities with the characteristic length scale set by the healing length ξ [33–36]. A universal low-energy theory of mobile impurities in one dimension has been developed in Ref. [37], restricted to particle separations much larger than ξ where the interaction is weak. A unified treatment for all distances, but for immobile impurities and small impurity-boson couplings has been given in Refs. [38,39]. While quantum Monte Carlo (QMC) methods have been used to obtain polaron properties in a nonperturbative manner [40–45] and there are numerical mean-field studies in trapped systems extending into the nonperturbative regime [46], analytic approaches have been restricted to weak polaron-polaron couplings or noninteracting host gases [47–49]. The first attempt at strong polaron coupling in interacting gases has been made only recently by using a scattering-matrix expansion [50]. The authors predict a deviation from the 3D Yukawa potential in agreement with QMC simulations, but with some notable quantitative differences.

Here we develop an analytic theory of polaron interactions in 1D Bose gases for arbitrary strength of the

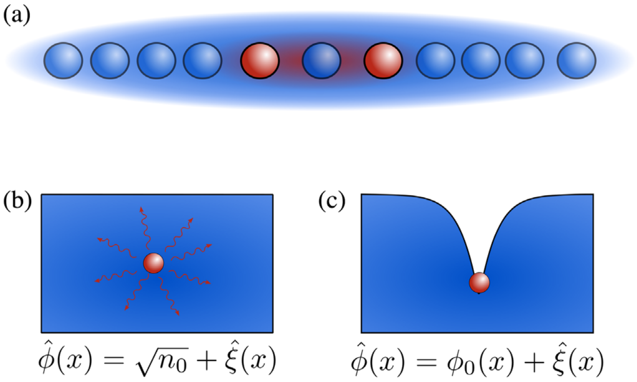

FIG. 1. (a) Sketch of a bipolaron composed of two impurities in a 1D Bose gas. (b) In the commonly used extended Fröhlich model, a large number of phonons are created around the impurity and phonon-phonon interactions need to be taken into account. (c) In a description based on a deformed condensate, this can be avoided.

impurity-boson coupling, see Fig. 1(a) for a sketch. A common description of the Bose-polaron takes into account a coupling of the impurity only to Bogoliubov phonons [36,51], see Fig. 1(b). This extended Fröhlich model is, however, not adequate for strong coupling, $g_{\mathrm{IB}} \gg g$, even if the boson-boson interaction itself is weak, since the impurity generates a high-density cloud of phonons around it and phonon-phonon interactions can no longer be neglected. Here we use a different approach that accounts for deformation of the superfluid by the impurities, see Fig. 1(c) [43,52,53]. As shown in Ref. [53] and elucidated in the Supplemental Material [54], this approach minimizes quantum fluctuations and leads to highly accurate predictions for single-polaron properties already on the mean-field level, precise enough to differentiate finite-size effects. Employing this approach, we develop a mean-field theory of bipolarons assuming a weakly interacting condensate and moderately heavy impurities and verify the semi-analytic predictions with QMC results.

Model.—We consider two impurities of equal mass M in a 1D gas of bosons of mass $m < M$. We assume contact impurity-boson interactions with coupling strength g_{IB} which can be repulsive, $g_{\mathrm{IB}} > 0$, or attractive, $g_{\mathrm{IB}} < 0$. We disregard a direct interaction between the impurities. Introducing center-of-mass (c.m.) and relative impurity coordinates $\hat{R}, \hat{r}$ and momenta $\hat{P}, \hat{p}$, the Hamiltonian reads ($\hbar = 1$)

$$\hat{H} = \frac{\hat{P}^2 + 4\hat{p}^2}{4M} + \int dx\, \hat{\Phi}^\dagger(x)\left\{\frac{-1}{2m}\partial_x^2 + \frac{g}{2}\hat{\Phi}^\dagger(x)\hat{\Phi}(x) - \mu + g_{\mathrm{IB}}\left[\delta\left(x - \hat{R} - \frac{\hat{r}}{2}\right) + \delta\left(x - \hat{R} + \frac{\hat{r}}{2}\right)\right]\right\}\hat{\Phi}(x). \tag{1}$$

Here μ is the chemical potential of the gas, which in mean-field approximation is $\mu = gn_0$, with n_0 being the linear density far away from both impurities. In the thermodynamic limit, n_0 converges to the mean density $n = N/L$. The interaction between the bosons of strength g is assumed to be weak so that a Bogoliubov approximation applies; i.e., the healing length $\xi = 1/\sqrt{2m\mu}$ [56] is large compared to the mean interparticle distance $1/n$. This regime is characterized by a small Lieb-Liniger parameter $\gamma = mg/n$ [57]. The dependence of the c.m. coordinate can be eliminated using a Lee-Low-Pines (LLP) transformation [58] $\hat{U} = \exp(-i\hat{R}\hat{P}_B)$, where $\hat{P}_B = -i\int dx\, \hat{\Phi}^\dagger(x)\partial_x\hat{\Phi}(x)$ is the total momentum of the Bose gas,

$$\hat{H}_{\mathrm{LLP}} = \frac{:(P - \hat{P}_B)^2: + 4\hat{p}^2}{4M} + \int dx\, \hat{\Phi}^\dagger(x)\left\{\frac{-1}{2m_r}\partial_x^2 - \mu + \frac{g}{2}\hat{\Phi}^\dagger\hat{\Phi} + g_{\mathrm{IB}}\left[\delta\left(x - \frac{\hat{r}}{2}\right) + \delta\left(x + \frac{\hat{r}}{2}\right)\right]\right\}\hat{\Phi}(x), \tag{2}$$

where $::$ denotes normal ordering, i.e., interchanging all creation operators to the left and annihilation to the right, and $m_r = 2Mm/(2M + m)$ is the reduced mass. $\hat{P}$, which previously was the c.m. momentum of the two impurities, is in the new frame the total momentum of the system. It is a constant of motion that can be replaced by a c-number P, and we set $P = 0$. Note that the LLP transformation is needed for any $M < \infty$, even if one considers an impurity at rest.

Bipolaron of heavy impurities.—Different from the single-polaron case, the LLP transformation does not remove the impurity coordinates entirely. To this end, we apply a Born-Oppenheimer (BO) approximation, valid for $M \gg m$, where the kinetic energy of the relative motion is neglected and one can replace $\hat{r}$ by a c-number r. This turns $\hat{H}_{\mathrm{LLP}}$ into a pure boson Hamiltonian.

In the following, we determine the ground state of (2) for a weakly interacting gas, which amounts to assume small quantum fluctuations $\hat{\xi}(x)$ on top of the mean-field solution $\phi_0(x)$ of Eq. (2), $\hat{\phi}(x) = \phi_0(x) + \hat{\xi}(x)$. Note that this differs from the common approach, where a small-fluctuation expansion is applied in the absence of the impurities first. In contrast, we take the backaction of the impurity into account already at the mean-field level. As shown in Ref. [53], this (i) leads to modified Bogoliubov phonons, coinciding with the standard ones only in the longwavelength limit $k\xi \gg 1$, and (ii) minimizes their generation by the impurity, see Fig. 1. The smallness of quantum fluctuations allows us to ignore them altogether when considering the mediated impurity-impurity interaction at distances of the order of a few rescaled healing lengths, $\bar{\xi} = \sqrt{m/m_r}\xi$. Only at large separations do quantum fluctuations become relevant. They are responsible for weak Casimir-type interactions scaling as $1/r^3$ [37–39] for finite g_{IB} and $1/r^2$ or $1/r$ if either one or both of the static impurities have infinitely strong coupling [59,60]. We will not consider these contributions here, but show *a posteriori* that the corrections are small on absolute scale.

The mean-field solutions of (2) can be obtained analytically in the BO limit, see Supplemental Material [54]. In particular, one finds for the interaction potential between two impurities

$$V(r) = g n_0^2 r\left(\frac{1}{2} - \frac{4+2\nu}{3(\nu+1)^2}\right) + \frac{4}{3}\frac{g n_0^2 \bar{\xi}}{\sqrt{1+\nu}}\Bigg\{\sqrt{2\nu+2} + 2E(\mathrm{am}(u,\nu),\nu) - \frac{\sqrt{\tilde{\nu}^3}}{1+\nu}\mathrm{cd}(u,\nu)^{\pm 3}[1+\sqrt{\tilde{\nu}}\mathrm{sn}(u,\nu)] - \sqrt{\tilde{\nu}}\mathrm{cd}(u,\nu)^{\pm 1}\left[\frac{3}{2} + \frac{1+\nu+\tilde{\nu}}{1+\nu}\sqrt{\tilde{\nu}}\mathrm{sn}(u,\nu)\right]\Bigg\}, \tag{3}$$

where $u = r/(2\bar{\xi}\sqrt{1+\nu})$ is a normalized distance, and the upper (lower) sign stays for repulsive (attractive) impurity-boson interaction, $E(x,\nu)$ is the incomplete elliptic integral of the second kind, $\mathrm{cd}(x,\nu)$ and $\mathrm{sn}(x,\nu)$ are Jacobi elliptic functions, and $\mathrm{am}(x,\nu)$ is the amplitude of these functions [61]. The dimensionless parameter $\nu = \nu(r,\eta)$ with $|\nu| < 1$ is given implicitly by

$$2\frac{|\eta|}{n_0\bar{\xi}}\frac{\sqrt{\tilde{\nu}(\nu+1)}}{(1-\nu)}\mathrm{cn}\,(u,\nu)\,\mathrm{dn}\,(u,\nu) = [1+\sqrt{\tilde{\nu}}\mathrm{sn}(u,\nu)]^2,$$

involving the Jacobi elliptic sn, cn, and dn functions and $\eta = g_{\mathrm{IB}}/g$. Here $\tilde{\nu} = \nu$ for $\eta > 0$ and $\tilde{\nu} = 1$ for $\eta < 0$. In general, this equation has several solutions; however, the physically relevant one is that with the largest ν.

Figure 2 shows examples of the effective interaction potential $V(r)$, having a finite range defined by $\bar{\xi}$. The strong coupling regime is reached when $\eta \gtrsim n_0\bar{\xi} = 1/\sqrt{2(m_r/m)\gamma}$ [53]. In this case, the impurity causes a sizable deformation of the Bose gas and $V(r)$ deviates substantially from the perturbative exponential behavior at short distances predicted in Ref. [39]. The logarithmic scale in Fig. 2(b) emphasizes the exponential long-range behavior of our result, $V(r) \sim \exp(-\sqrt{2}r/\bar{\xi})$ (see Supplemental Material [54]), which is sufficient for experimentally relevant energy scales, while the Casimir term $\sim 1/r^3$ [37,38] affects only the already small tails of the potential.

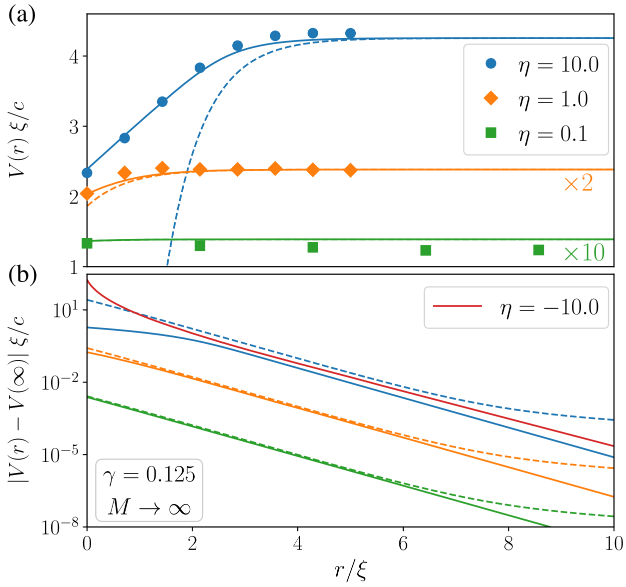

FIG. 2. Effective impurity-impurity interaction as function of distance in units of $\bar{\xi} = \xi$ for different interactions $\eta = g_{\mathrm{IB}}/g$ and $M \to \infty$, where $c = \sqrt{g n_0/m}$ is the speed of sound. Solid lines represent semianalytical approximation Eq. (3), circles are QMC results (error bars smaller than circle size), and dashed lines give perturbative predictions from [38], including Casimir-type contribution. (a) Comparison of effective potential $V(r)$ for repulsive impurity-boson interaction. The perturbative results were shifted to match our predictions at infinite distance. (b) Interaction potential on a semilog scale. Exponential decay for weak impurity-boson couplings, $\eta \lesssim 1$, is seen as straight lines. The Casimir effect (absent in the mean-field description) results in the slower $1/r^3$ decay at $r \gtrsim 6\xi$.

In the limit $\eta \to \infty$, one finds the simple explicit form

$$V(r)|_{\eta\to\infty} = \frac{4}{3}\sqrt{2}g n_0^2\bar{\xi} + \frac{1}{2}g n_0^2 r \quad \text{for } r \le \pi\bar{\xi}, \tag{4}$$

where the potential is linear, corresponding to a constant attractive force acting between the impurities. This is because for strong repulsion the Bose gas is completely expelled in between the impurities, as long as $r \lesssim \pi\bar{\xi}$ and the attractive force results only from the pressure of the Bose gas outside of the pair. This is further illustrated in the Supplemental Material [54].

In the BO limit of massive impurities, the effective interaction potential can be accurately obtained in QMC simulations. In Fig. 2 we compare our analytic predictions for repulsive impurity-boson coupling, $\eta > 0$, with QMC data and find excellent agreement within a few-percent margin. Unless stated otherwise, we used $N = 100$ bosons in the QMC simulations. While lowest-order perturbative theory predicts the same interaction strength in repulsive ($\eta > 0$) and attractive cases ($\eta < 0$), nonperturbative approaches show that $V(r)$ is substantially stronger for attraction [see Fig. 2(b)]. This can be qualitatively understood, as the maximal density defect produced is limited in the repulsive case by full depletion, while it is unlimited in the attractive case. This makes numerical calculations in the attractive case more challenging.

Bipolaron of finite impurity mass.—The BO approximation applies to infinitely heavy impurities and becomes increasingly inaccurate for light impurities. The leading-order modification is the Born-Huang diagonal correction, $V(r) \to V(r) + W(r)$ [62,63]

$$W(r) = \frac{1}{M} \int dx\, |\partial_r \phi_0(x)|^2, \tag{5}$$

where $\phi_0(x)$ is the mean-field wave function in the presence of two impurities at (fixed) distance r. $W(r)$ accounts for the dependence of the background-gas wave function on the impurity coordinates when calculating the impurity kinetic energy. Including this term, the approach is correct up to terms of order $(m/M)^{3/2}$. Since the derivative of $\phi_0(x)$ with respect to r is analytically complicated, we do not give an explicit expression for $W(r)$. In Fig. 3(a) we plot the total potential for $\eta = 40$ and different characteristic mass ratios. Note that the finite impurity mass enters here in two ways, through the reduced healing length $\bar{\xi}$ and by the Born-Huang term $W(r)$. A prominent feature is the emergence of a local maximum at distance $r_{\max} \simeq \pi\bar{\xi}$ when $W(r)$ is included. As discussed in the Supplemental Material [54] this maximum appears only for strong impurity-boson coupling, i.e., if $\eta \gtrsim n_0\bar{\xi}$. Since for large values of r, $W(r)$ decays faster than $V(r)$, the total potential remains attractive at large distances.

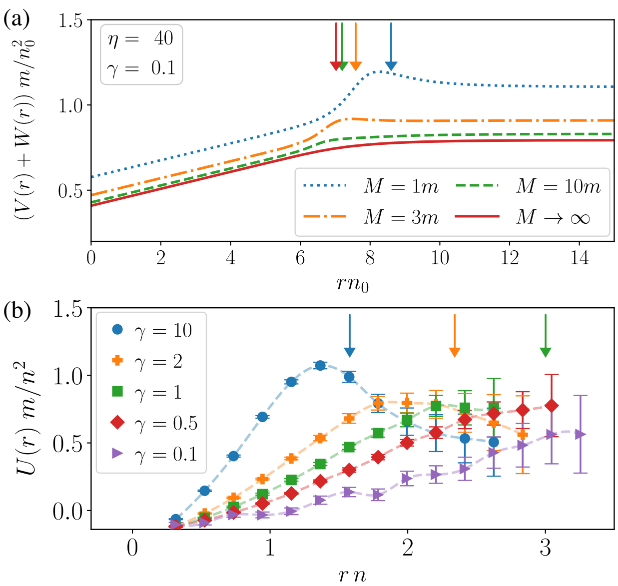

FIG. 3. Interaction potential for mobile impurities. (a) Mean-field potential including Born-Huang correction for different mass ratios. (b) Total interaction potential $U(r)$ from QMC simulations for the mass ratio $M = 3m$, but $\eta \to \infty$ and different Lieb-Liniger parameters. Arrows point to analytical predictions of maxima $r_{\max} = \pi\bar{\xi} = \pi/\sqrt{2m_r\mu}$, where we used the equation of state for μ from Bethe ansatz [64].

While for an infinite impurity mass, the interaction potential can be obtained directly in QMC simulations from the ground-state energy, its estimation is more delicate for finite values of M and involves the impurity-impurity correlation function, $g_{ii}(x)$. Here the degrees of freedom of the gas are integrated out and $\sqrt{g_{ii}(x)}$ is interpreted as a wave function of the effective two-impurity Schrödinger equation. The effective potential is proportional to $[\sqrt{g_{ii}(x)}]''/\sqrt{g_{ii}(x)}$, for details see Supplemental Material [54]. The large statistical noise arising from division by $\sqrt{g_{ii}(x)}$ does not allow one to unambiguously identify a local potential maximum in a weakly interacting gas, $\gamma \ll 1$. The maximum conjectured by the analytic theory is, however, clearly seen in the regime of strong interactions, $\gamma \gtrsim 1$, and although being outside the range of validity, its position is reasonably well predicted, see arrows in Fig. 3(b). Note that, in the limit of a Tonks-Girardeau gas [65], $\gamma \to \infty$, the maxima coincide with the first maximum of Friedel oscillations [66] at $n_0 r = 1$ and in a super-Tonks-Girardeau gas would correspond to quasi-crystal lattice spacing. The attractive polaron interactions can lead to bound bipolaron states. In one dimension, at least one two-body bound state exists if the Fourier transform of the interaction potential at zero momentum is negative. We calculated the bipolaron energy of the lowest bound states for repulsive and attractive impurity-boson couplings with and without the Born-Huang corrections and compared the results to QMC simulations. While an attractive contact interaction only allows for a single bound state, here several ones are possible due to the finite extension of the effective potential. Note, however, that the first excited state of two bosonic impurities, mappable to the ground state of two fermions, becomes bound only above a critical interaction strength η_c. In Fig. 4 we plot the energies of the ground and first excited states of the bipolaron as a function of $\eta = g_{\mathrm{IB}}/g$ for a Bose gas with Lieb-Liniger parameter $\gamma = 0.125$ for repulsive and attractive interactions. Since the effective interaction potential is unbounded in the attractive case, much larger bipolaron energies are obtained for $\eta \to -\infty$. Once the Born-Huang corrections are included, an excellent quantitative agreement is found for mass ratios as small as $M/m = 3$. As shown in the Supplemental Material [54], the predictions become less precise if the boson-boson interaction is increased, but even for $\gamma = 1$, the discrepancy is below the few-percent level for $\eta \le 1$ and saturates below 15% for $\eta \to \infty$. The bipolaron energies are in the same order as typical single-polaron energies and in the strongly repulsive regime $g_{\mathrm{IB}} \gg g n_0 \bar{\xi}$ they are comparable to the energy of a dark soliton $E \sim \hbar n_0 c$. For the experimental data of

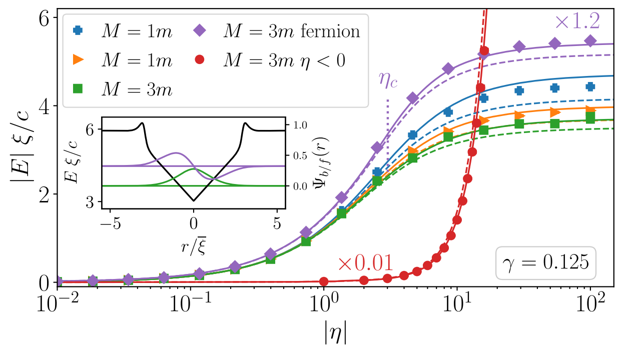

FIG. 4. Comparison of ground- and first excited-state energies of bipolarons with QMC results (dots) for different mass ratios m/M and weak-to-moderate boson-boson coupling $\gamma = 0.125$. Dashed lines correspond to BO potential $V(r)$; solid lines include Born-Huang correction $V(r) + W(r)$. The red curves correspond to attractive impurity-boson interaction (scaled by 0.01) and all others to repulsive. The purple line is the ground-state energy for fermionic impurities (i.e., first excited bipolaron state, scaled by 1.2), where the vertical line marks the interaction strength $\eta_c \simeq 3$, above which the two fermions form a bound state, calculated from the mean-field potential. The inset ($\eta = 30$; $M = 3m$) illustrates the corresponding impurity wave functions in green (purple) for bosonic (fermionic) impurities, as well as $V(r) + W(r)$ (black).

Ref. [26], where $n_0 \approx 7\mu\mathrm{m}^{-1}$ and $c \approx 3.4$ mm/s, the latter corresponds to temperatures of $T = E/k_B \approx 240$ nK.

Conclusions.—We presented a detailed study of bipolarons and polaron-polaron interactions in ground-state 1D Bose gases. We have developed a semianalytical theory applicable for weakly interacting bosons and valid for arbitrarily strong impurity-boson interactions. As opposed to solid-state systems, where impurities couple only to collective excitations, the high compressibility of the Bose gas makes it necessary to take into account the action of the impurity to the quasicondensate. This was done by expanding the quantum field of the bosons around a deformed quasicondensate [53]. In this way the density of phonons created by the impurities remains small also for strong impurity-boson couplings and phonon-phonon interactions can be disregarded. We derived the short-range potential from analytic mean-field solutions in BO approximation and found excellent agreement with QMC simulations. In the limit of strong impurity-boson interactions, $g_{\mathrm{IB}}/g \gg 1/\sqrt{2(m_r/m)\gamma}$, the potential deviates substantially from the perturbative exponential form and attains a linear short-range dependence. When lowest-order corrections to the BO result are included, the potential becomes nonmonotonic and attains a local maximum at a distance of $\pi\bar{\xi}$. As the interactions in the gas are made stronger, the height of the peak is increased and its position moves toward the first maximum of the Friedel oscillations. Comparison with QMC simulations shows that the analytic model provides a precise prediction for bipolaron energies for bosonic and fermionic impurities. Thus, the mean-field description beyond the Froehlich model constitutes an excellent basis for the analysis of nonequilibrium and many-body properties of Bose polarons. Going away from equilibrium, e.g., by applying periodic drive or similar Floquet techniques, will open new avenues to modify interactions of impurities mediated by a many-body environment with applications to fields such as high-T_c superconductivity and others. For this it is important to have tractable theoretical tools at hand. The application of our approach to the nonequilibrium physics of interacting polarons will be the subject of future work.

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Note added.—Recently, we became aware of a recent related work on bipolarons in the limiting case of infinite impurity masses, using a different approach [67]. The conclusions are in agreement with ours in this limit.

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