Polaronic mass renormalization of impurities in Bose-Einstein condensates: Correlated Gaussian-wave-function approach

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We propose a class of variational Gaussian wave functions to describe Fröhlich polarons at finite momenta. Our wave functions give polaron energies that are in excellent agreement with the existing Monte Carlo results for a broad range of interactions. We calculate the effective mass of polarons and find smooth crossover between weak- and intermediate-coupling strength. Effective masses that we obtain are considerably larger than those predicted by the mean-field method. A prediction based on our variational wave functions is a special pattern of correlations between host atoms that can be measured in time-of-flight experiments.

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I. INTRODUCTION

Renormalization of particle masses due to their interaction with the environment is a ubiquitous phenomenon in physics. In the standard model of high-energy physics elementary particles acquire a mass through interaction with the Higgs field [1]. In solid-state systems heavy fermion materials exhibit renormalization of electron masses of up to two orders of magnitude due to interaction of electrons with localized spins [2]. Complete localization of quantum degrees of freedom caused by interaction with the environment has been discussed in spin-bath models [3,4] and quantum Josephson junctions [5–7].

Surprisingly one of the first systems in which strong mass renormalization due to particle-bath interaction has been predicted, the so-called Fröhlich polaron model introduced by Landau in 1933 [8,9], remains a subject of considerable debate. This model describes interaction of a quantum particle with a bosonic bath, such as an electron interacting with phonons in a crystal (see Refs. [10–12] for reviews). While the limiting cases of weak and strong coupling can be analyzed using controlled perturbative expansions (see Refs. [13,14] for weak-coupling analysis and Refs. [9,15] for strong-coupling expansion), the intermediate-coupling regime remains poorly understood with the effective mass of the polaron being the most contentious issue [16]. For example, considerable disagreement between different approximations for the effective mass of Fröhlich-Bogoliubov polarons has been reported in the literature (see Fig. 1). Perturbative expansion for small interaction strength suggest a divergence of the effective mass beyond a certain interaction strength, indicating localization of the impurity particle [17]. Variational method based on the Feynman path-integral approach exhibits a sharp crossover in the effective mass [18,19]. By contrast mean-field approach to the problem shows only a gradual evolution of the effective mass [20].

Recent experimental progress in the field of ultracold atoms brought new interest in the study of impurity problems. Feshbach resonances made it possible to realize both Fermi [21–24] and Bose polarons [25–31] with tunable interactions between impurity and host atoms and the rich toolbox of atomic physics has been used to study their properties including the effective mass [21,24,32].

In this paper we show that an analytical class of wave functions based on the correlated Gaussian ansatz can describe Fröhlich polarons at finite momentum for a wide range of parameters (see Refs. [35–37] for earlier works). Fröhlich type Hamiltonians can be used to describe several different families of physical systems including electrons interacting with lattice phonons in polar [8,9,35–40], organic [41], and piezoelectic [42–44] semiconductors, magnetic polarons in strongly correlated electron systems [45,46], ^{3}He atoms in superfluid ^{4}He [47], and impurity atoms in Bose-Einstein condensates in the weak-coupling limit [18–20,33,34,48–59]. In this paper we focus on the Fröhlich-Bogoliubov polarons which can be realized with ultracold atoms. However, our method can be easily adapted to other systems and generalized to dynamics.

The essence of our approach is an extension of the earlier mean-field variational wave function (after performing Lee-Low-Pines transformation on the Hamiltonian; see [60] and discussion below) to Gaussian wave functions that include entanglement between different phonon modes. The explicit form of these wave functions is given in Eq. (6) and from now on we will refer to them as correlated Gaussian wave functions (CGW) [61]. We demonstrate that CGWs show excellent agreement with the Monte Carlo (MC) results for the ground-state energy of the Fröhlich-Bogoliubov polaron at zero momentum: from weak to intermediate coupling (see Fig. 2).

The key ingredient of our new class of wave functions is the appearance of additional correlations for the host atoms introduced through their interaction with mobile impurities. We show how they can be observed with ultracold atoms in time-of-flight experiments. Although we study such correla-

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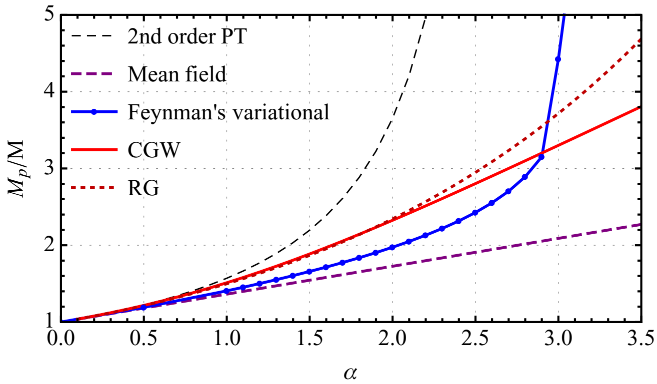

FIG. 1. Polaron effective mass computed using different approaches as a function of the dimensionless interaction parameter α defined by Eq. (2). Our result (CGWs) is compared with Feynman's variational method [18], mean-field [20], and renormalization-group approach (RG) [33]. For the comparison with Refs. [18,34] we fix the mass imbalance to be $M/m_B = 0.23$ (^{6}Li/^{23}Na).

tions using the Fröhlich Hamiltonian, we expect them to be present even in more sophisticated models describing impurity atoms in a BEC. Their observation would be an important test of the variational wave function introduced in this paper even beyond the Fröhlich model.

Compared to the mean-field solution the number of variational parameters in our approach increases only by a factor of three, which keeps the number of self-consistent equations reasonably small. In the context of Fröhlich-Bogoliubov polaron MC method has only been used to calculate polaron binding energies at zero momentum, which makes it impossible to obtain the effective mass (for other types of polarons, however, effective mass analysis based on MC calculations has been done; see e.g. [39,40].) CGW analysis at finite polaron momentum does not introduce additional complications which allows us to calculate the effective mass of polarons.

The Fröhlich-Bogoliubov model provides a description of impurity atoms in Bose-Einstein condensates in the limit when

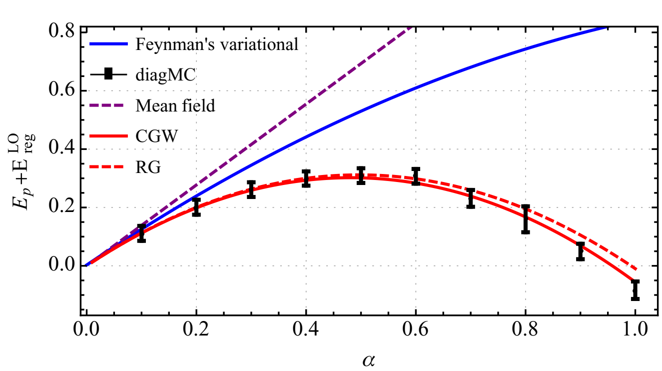

FIG. 2. Ground-state energy of the Fröhlich-Bogoliubov model $E_p + E_{\rm reg}^{\rm LO}$ for zero-momentum impurity ($P = 0$) predicted by different theoretical approaches as a function of the dimensionless coupling constant α. Our result (CGWs) is compared with MC calculations [34], Feynman's variational method [18], mean field [20], and RG [33]. For the comparison with Refs. [18,34] we fix the mass imbalance to be $M/m_B = 0.23$ (^{6}Li/^{23}Na) and the UV cutoff $\Lambda = 2 \times 10^3 \xi^{-1}$.

the condensate density depletion caused by the impurity is smaller than the density of the condensate itself. Conditions on the applicability of this model for describing impurity-boson systems are discussed below. We find that the intermediate-coupling regime of Fröhlich-Bogoliubov polarons should be accessible in existing experimental setups, e.g., with ^{41}K or ^{133}Cs atoms in ^{87}Rb BEC, both of which have interspecies Feshbach resonances that can be used to tune the impurity-boson interaction. Physics of the impurities interacting with BEC shows wide range of physical phenomena, such as a formation of the molecular and Efimov bound states [59]. Our approach can be extended to capture these phenomena.

II. FRÖHLICH-BOGOLIUBOV MODEL

We use the Bogoliubov model to describe BEC of the host atoms and limit ourselves to small deviations of the BEC density from the homogeneous case. In this case interaction of the impurity with phonons of the BEC can be described using the Fröhlich Hamiltonian [18,48,62]

$$\hat{\mathcal{H}} = g_{IB} n_0 + \frac{\hat{\vec{p}}^2}{2M} + \sum_k V_k (\hat{b}_k + \hat{b}^\dagger_{-k}) e^{i\vec{k}\hat{\vec{r}}} + \sum_k \omega_k \hat{b}^\dagger_k \hat{b}_k. \tag{1}$$

Here $\hat{\vec{p}}$ and $\hat{\vec{r}}$ are momentum and position operators of the impurity atom with mass M, $\hat{b}^\dagger_k$ is the annihilation operator of the Bogoliubov phonon excitation with momentum $\vec{k}$, $\omega_k = ck\sqrt{1 + (\xi k)^2/2}$ is the Bogoliubov mode dispersion, with c being the sound velocity and ξ the coherence length of the condensate. The impurity-phonon interaction strength is given by $V_k = g_{\rm IB}\sqrt{n_0 \mathcal{V}^{-1}\xi k}(2 + (\xi k)^2)^{-1/4}$, where n_0 is the BEC density, $g_{\rm IB}$ denotes the interaction strength between the impurity atom and host atoms with mass m, and $\mathcal{V}$ is the volume of the system. From now on we will set $\mathcal{V} = 1$ in the rest of the paper. In the first-order Born approximation this interaction strength can be related to the impurity-BEC atom scattering length via $g_{\rm IB} = 2\pi a_{\rm IB}(m^{-1} + M^{-1})$; this allows one to regularize the leading order UV divergence of the ground-state energy [18]. We describe the strength of this interaction using a dimensionless parameter

$$\alpha = 8\pi n_0 a_{IB}^2 \xi. \tag{2}$$

Applicability of the Fröhlich-Bogoliubov Hamiltonian relies on the condition that the condensate density depletion caused by the impurity is smaller than the density of the condensate itself. This allows us to restrict ourselves to linear terms in Bogoliubov operators in the Fröhlich Hamiltonian (1) and gives rise to the condition $|g_{IB}| \ll 4c\xi^2$ [63]. We find that for ^{41}K impurities in ^{87}Rb BEC [25,32] and ^{133}Cs impurities in ^{87}Rb BEC [30,64] this condition can be satisfied even for the intermediate couplings α, if the condensate density is sufficiently small. Both setups have interspecies Feshbach resonances that can be used to tune the impurity-boson interaction. They correspond to the cases of moderately light impurities with $M/m_B = 0.46$ for ^{41}K/^{87}Rb and $M/m_B = 1.53$ for ^{133}Cs/^{87}Rb.

To utilize translational symmetry of the Fröhlich Hamiltonian (1) we apply the Lee-Low-Pines (LLP) transformation

[14] $\hat{U}_{\rm LLP} = e^{i\hat{S}}$, $\hat{S} = \hat{\vec{r}}\sum_k \vec{k}\hat{b}_k^\dagger \hat{b}_k$. The transformed Hamiltonian $\hat{\mathcal{H}}_{\rm LLP} = \hat{U}_{\rm LLP}\hat{\mathcal{H}}\hat{U}_{\rm LLP}^\dagger$ is

$$\hat{\mathcal{H}}_{LLP} = g_{IB}n_0 + \frac{1}{2M}\left(\vec{P} - \sum_k \vec{k}\hat{b}_k^\dagger \hat{b}_k\right)^2 + \sum_k \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_k V_k(\hat{b}_k + \hat{b}_{-k}^\dagger). \quad (3)$$

Here $\vec{P}$ is a conserved total momentum of the system which can be treated as a c-number. Equation (3) no longer has degrees of freedom corresponding to the impurity: they were integrated out using conservation of the total momentum. This generated an interaction term between phonon modes which is proportional to $1/M$. The appearance of the phonon-phonon interaction can be understood as exchange of momentum between phonons via the impurity.

III. MEAN-FIELD SOLUTION

To motivate the mean-field solution we first discuss the limit of infinitely heavy impurity, $M \to \infty$. In this case interactions between phonon modes in Eq. (3) vanish and the Hamiltonian can be transformed to the canonical form using the displacement transformation $\hat{D}(\{\beta_k^0\}) = \exp\left(\sum_k \beta_k^0 \hat{b}_k^\dagger - \text{H.c.}\right)$ with $\beta_k^0 = -V_k/\omega_k$. Then the ground state is given by a coherent state $\hat{D}(\{\beta_k^0\})|0\rangle$, where $|0\rangle$ is the phonon vacuum. Note the key feature of this solution: it factorizes into a product of wave functions for different k modes. Now we can generalize this result to the interacting case at finite M. The mean-field approach to polarons assumes a similar structure of the polaron wave function even in the interacting case of finite impurity mass [65]. In this method a product of coherent states for different phonon modes is taken as a variational ansatz

$$|MF\rangle = \hat{D}(\{\beta_k\})|0\rangle \quad (4)$$

and coefficients β_k are determined from minimizing the energy $\langle\hat{\mathcal{H}}_{LLP}\rangle_{\rm MF}$. Straightforward calculation [20] gives $\beta_k = -V_k/\Omega_k$, where the renormalized dispersion Ω_k is given by

$$\Omega_k = \omega_k + \frac{k^2}{2M} - \frac{\vec{k}}{M}(\vec{P} - \vec{P}_{\rm ph}). \quad (5)$$

The parameter $\vec{P}_{\rm ph}$ describes the part of the total polaron momentum which is carried by the phonon cloud, and in the mean-field approximation reads $\vec{P}_{\rm ph} = \sum_q \vec{q}|\beta_q|^2$. A major limitation of the mean-field state is that it does not include correlations between different phonon modes since the wave function factorizes into a product of wave functions for individual k's. Different modes affect each other only through the self-consistency condition on β_k.

IV. CORRELATED GAUSSIAN WAVE-FUNCTION SOLUTION

To account for correlations between different phonon modes in the polaron problem we introduce a Gaussian wave function

$$|\text{CGW}\rangle = \hat{\text{D}}(\{\beta\})\hat{\text{S}}(\{\text{Q}\})|0\rangle, \quad (6)$$

where $\hat{S}(\{Q\}) = \exp(\frac{1}{2}\sum_{k,k'} Q_{kk'}\hat{b}_k^\dagger \hat{b}_{k'}^\dagger - \text{H.c.})$. Variational wave function of this type have been suggested before [35–37] but full optimization of the wave functions with respect to both β and Q was considered computationally impossible. For example, in Ref. [35] energy was minimized with respect to the boson displacement part $\{\beta_k\}$ and the Gaussian part was used to diagonalize Hamiltonian, where terms of the order higher than two were truncated. One of the key results of this paper is development of an approach finding the optimal values of β and Q, which makes variational functions (6) a powerful tool for studying many-body systems of interacting bosons.

A convenient way of understanding this ansatz is to interpret it as a generalized Bogoliubov transformation with

$$\hat{S}^\dagger(\{Q\})\hat{D}^\dagger(\{\beta\})\hat{b}_k\hat{D}(\{\beta\})\hat{S}(\{Q\}) = \beta_k + \sum_{k'}[\cosh Q]_{kk'}\hat{b}_{k'} + \sum_{k'}[\sinh Q]_{kk'}\hat{b}_{k'}^\dagger. \quad (7)$$

A new feature of wave function (6) is that expectation values of boson creation and annihilation operators no longer factorize. We have $\langle\hat{b}_k\rangle = \beta_k$, $\langle\hat{b}\cdot\hat{b}\rangle = \beta_k\cdot\beta_{k'} + (\cosh Q\,\sinh Q)_{kk'}$, and $\langle\hat{b}^\dagger\cdot\hat{b}\rangle = \beta_k\cdot\beta_{k'} + (\sinh^2 Q)_{kk'}$. All higher-order expectation values of b_k and $b_k^\dagger$ operators can be computed using Wick's theorem. Variational parameters $Q_{kk'}$ and β_k should be determined by minimizing the energy.

Explicit expression for the expectation value of $\hat{\mathcal{H}}_{LLP}$ in state (6) is given in the Appendix. In the regime of interest for cold atoms systems, where the Bogoliubov-Fröhlich Hamiltonian describes impurity atoms in a BEC, it is sufficient to expand the hyperbolic functions in (7) up to second order in matrices $Q_{kk'}$. We find that the ground-state energy as a function of the variational parameters, $E_p = \langle\hat{\mathcal{H}}_{LLP}\rangle_{\rm CGW} - g_{IB}n_0$, has the following form:

$$E_p = \frac{\vec{P}^2 - \vec{P}_{\rm ph}^2}{2M} + \sum_k\left(2V_k\beta_k + \Omega_k\left(\beta_k^2 + \sum_{k'}Q_{kk'}^2\right)\right) \times \sum_{kk'}\frac{\vec{k}\vec{k}'}{M}Q_{kk'}^2 + \sum_{kk'}\frac{\vec{k}\vec{k}'}{M}\beta_k\beta_{k'}\left(Q_{kk'} + \sum_q Q_{kq}Q_{qk'}\right). \quad (8)$$

In this approximation the momentum of phonon cloud is defined as $\vec{P}_{\rm ph} = \sum_k \vec{k}\beta_k^2 + \sum_{kk'}\vec{k}(Q_{kk'})^2$, where $Q_{kk'}^2$ is the square of the matrix element. Minimizing the expression with respect to $Q_{kk'}$ we obtain equations

$$\left(\Omega_k + \frac{\vec{k}\vec{k}'}{M} + \Omega_{k'}\right)Q_{kk'} + \frac{\vec{k}\vec{k}'}{M}\beta_k\beta_{k'} + \sum_q \frac{\vec{q}}{M}\beta_q\left(\vec{k}'\beta_{k'}Q_{kq} + \vec{k}\beta_k Q_{qk'}\right) = 0, \quad (9)$$

where Ω_k is still given by Eq. (5). At first sight this integral equation on the matrix $Q_{kk'}$ appears quite challenging. Fortunately, it can be reduced to a much simpler vector equation by introducing $\vec{F}_k = -\beta_k^{-1}\sum_q \beta_q Q_{kq}\vec{q}$. Then Eq. (9) is equivalent to

$$\vec{F}_k = \frac{1}{M}\sum_{k'}\frac{\beta_{k'}^2\vec{k}'}{\Omega_k + \frac{\vec{k}\vec{k}'}{2M} + \Omega_{k'}}(\vec{k}\vec{k}' - \vec{F}_k\vec{k}' - \vec{k}\vec{F}_{k'}). \quad (10)$$

Minimization of (8) with respect to β_k gives

$$V_k + \beta_k \Omega_k - \frac{\vec{k}}{M} \sum_q \frac{\beta_q}{M} Q_{qk}(\vec{F}_q - \vec{q}) = 0. \tag{11}$$

Equations (10) and (11) can now be solved numerically. Details of the derivation of these equations can be found in Appendix 1 and 2.

To benchmark the approach we compare the ground-state energy of the Fröhlich-Bogoliubov Hamiltonian E_p for the mass imbalance $M/m_B = 0.23$ (^{6}Li/^{23}Na) with other known theoretical results in Fig. 2 for the weak and intermediate couplings (the comparison in strong-coupling limit is provided in Appendix 3). To make such comparison quantitative we regularize the leading-order UV divergence of the polaron energy by adding $E_{\text{reg}}^{\text{LO}} = 4a_{\text{IB}}^2 n_0(1 + m/M)\Lambda$ [18,20], where Λ is the UV cutoff. The remaining energy $E_p + E_{\text{reg}}^{\text{LO}}$ has a subleading UV divergence, $\sim \log \Lambda$. This divergence is present in most approaches accounting for quantum fluctuations, CGW, RG, and diagMC (see discussion in [33]). Our approach shows excellent agreement with the MC approach and drastically improves the mean-field solution.

Effective mass of the polaron can be obtained by taking the second derivative of the polaron energy with respect to the total momentum. In practice this is not the most convenient way of computing it because the polaron energy for the Fröhlich Hamiltonian (1) has UV divergencies (detailed discussion is presented in Ref. [33]). One can however circumvent dealing with UV divergences for the calculations of the polaron mass if we use the following argument: When analyzing the variational wave function (6) we can calculate momentum of the polaron carried by the impurity $\vec{P}_{\text{imp}} = \vec{P} - \vec{P}_{\text{ph}}$. The velocity of the impurity, P_{imp}/M, should coincide with the velocity of the polaron, P/M_p. Thus we find

$$\frac{M}{M_p} = 1 - \frac{P_{\text{ph}}}{P}. \tag{12}$$

For the comparison with other theoretical results we show the polaron mass for the mass imbalance $M/m_B = 0.23$ in Fig. 1. In contrast with Feynman's variational approach the polaron mass calculated with CGWs shows smooth crossover from the regime of weak to intermediate coupling.

Figure 3 shows our predictions for the effective mass of Bogoliubov-Frölich polarons for the mass imbalance $M/m_B = 0.46$ (^{41}K/^{87}Rb) and $M/m_B = 1.53$ (^{133}Cs/^{87}Rb) as a function of the impurity-boson interaction strength α. The particle mass renormalization is stronger for lighter impurities.

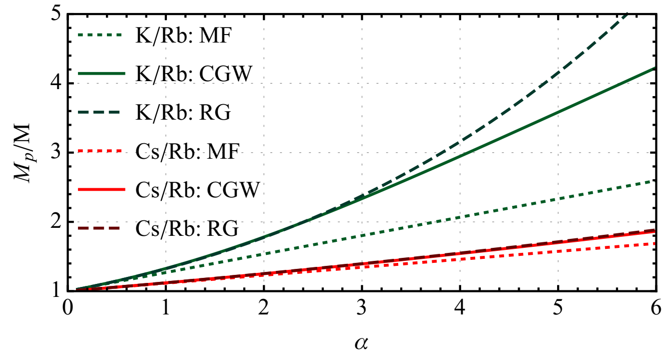

FIG. 3. Polaron mass for the mass imbalance $M/m_B = 0.46$ (^{41}K/^{87}Rb) and $M/m_B = 1.53$ (^{133}Cs/^{87}Rb) in units of bare impurity mass M. Increase of the interaction strength α between impurity atom and BEC enhances quantum fluctuations and results in stronger renormalization of M_{p}.

Note that we will focus on the additional correlations among host atoms caused by the impurity and will not include correlations present in the BEC itself. The latter are expected only for $\pm k$ atoms, as described by the Bogoliubov wave function [69]. Figure 4 presents results of correlations described by Eq. (13) for experimental systems with the mass imbalance $M/m_B = 0.46$ (^{41}K/^{87}Rb) and $M/m_B = 1.53$ (^{133}Cs/^{87}Rb).

We obtain asymptotic values of these correlations in several regimes. In the long-wavelength limit phonon modes decouple and $g^{(2)}$ approaches unity. For high momenta occupation numbers of atoms n_k decrease but $g^{(2)}(k,k')$ saturates at values that depend on the angle θ between $\vec{k}$ and $\vec{k}'$: $g^{(2)}(k = \infty, k' = \infty)(1 + \sqrt{2}m_B/M)^{-1}$ and $g^{(2)}(k = \infty, k' = -\infty) = (1 + \sqrt{2}m_B/M)$. This indicates antibunching of bosons for

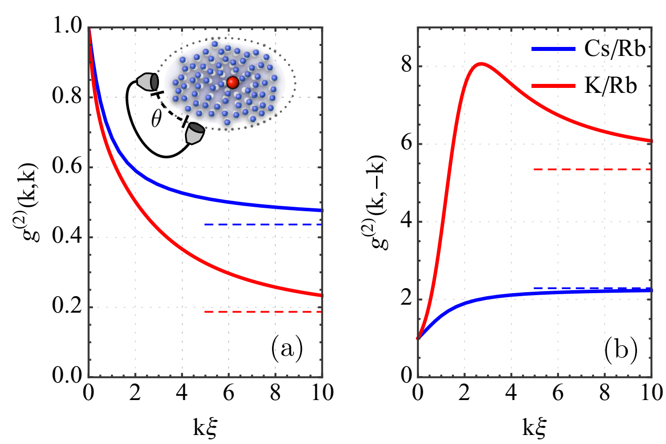

FIG. 4. Inset in the panel (a) shows the typical experimental setup for measuring noise correlation functions $g^{(2)}(k,k')$ [see Eq. (13)]. TOF measurement should be performed with two detectors placed at relative angle θ between two directions of measurement. Panels (a) and (b) show noise correlations for (a) $\theta = 0$ and (b) $\theta = \pi$ for the mass imbalance $M/m_B = 0.46$ (^{41}K/^{87}Rb) and $M/m_B = 1.53$ (^{133}Cs/^{87}Rb) at $\alpha = 4$. In the case $\theta = 0$ BEC atoms show antibunching. In the case of $\theta = \pi$ we find atom bunching. For the ^{41}K/^{87}Rb mixture this bunching has a peak at $k/\xi = 3$. Large momentum asymptotics can be computed analytically and are shown with dashed lines.

V. EXPERIMENTAL SIGNATURES OF CORRELATIONS

The main new features of the CGW (6) compared to the mean-field wave function (4) are correlations between different phonon modes. Such correlations will also be present for atoms of the host BEC itself and can be measured using noise correlation analysis in the time-of-flight experiments (TOF) [66,67]. The quantity that can be extracted from TOF images is the second-order correlation function [68]

$$g^{(2)}(k,k') \approx \frac{\langle \hat{b}_k^\dagger \hat{b}_{k'}^\dagger \hat{b}_k \hat{b}_{k'} \rangle}{\langle \hat{b}_k^\dagger \hat{b}_k \rangle \langle \hat{b}_{k'}^\dagger \hat{b}_{k'} \rangle}. \tag{13}$$

small θ and bunching for $\theta = \pi$. These results are consistent with our intuition that an impurity colliding with one of the BEC atoms and giving it momentum $\vec{k}$ is more likely to scatter the next BEC atom in the opposite direction. Correlations induced between host atoms are stronger for light impurities. One of the intriguing features in Fig. 4(b) is a peak in the correlation function at stronger coupling $\alpha = 4$ and $k\xi \approx 2$.

We point out that while our analysis considered only a single impurity, experiments are performed at finite impurity concentration. Assuming that impurities are sufficiently dilute and their polarization clouds do not overlap, we can neglect interaction between polarons. Then changes in the occupation number of host bosons at finite k due to several impurities will be proportional to the number of impurities. In the case of the mass imbalance $M/m_B = 0.46$ (^{41}K/^{87}Rb), interaction strength $\alpha = 4$, and impurity concentration 5%, we estimate the number of atoms excited from the condensate to finite momentum states by scattering on impurity atoms to be 3%. This sets the magnitude of the signal of correlations.

Before concluding this paper we point out that wave functions (6) are commonly used in quantum optics [70–74]. However, theoretical analysis so far focused either on time-dependent quadratic Hamiltonians, nonlinear Hamiltonians with only few modes, for which direct optimization is possible, or many-body multimode Hamiltonians that have translational symmetry, which allowed factorization of the many-body wave functions into separate contribution from $(k, -k)$ pairs (translational invariance allows only $\langle b_k^\dagger b_{-k}\rangle$ and $\langle b_k^\dagger b_k\rangle$ expectation values). We expect that the approach developed in this paper can become a useful tool for analyzing quantum optical systems with many modes, strong nonlinearities, and no translational symmetry, such as Rydbergs systems, circuit QED, coupled nonlinear resonators, and plasmonic systems.

VI. SUMMARY AND OUTLOOK

We proposed a class of variational Gaussian wave functions for Fröhlich-Bogoliubov polarons that gives excellent agreement with Monte Carlo results for the ground-state energy in a wide range of parameters. We find a smooth crossover of the effective polaron mass as the interaction strength changes from from weak to intermediate coupling. Our wave function predicts a specific pattern of correlations between host atoms that can be measured in TOF experiments. We suggest that our predictions can be checked in such systems as ^{41}K or ^{133}Cs impurities in ^{87}Rb BEC for intermediate-coupling constant α, while the Fröhlich-Bogoliubov polaron description remains appropriate. We point out that Gaussian wave functions can be used to describe not only equilibrium states (ground states at finite momentum) but also dynamics. Thus our formalism can be extended to compute spectral functions of polarons and study response of polarons to external fields.

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APPENDIX: VARIATIONAL GAUSSIAN APPROACH

Gaussian wave functions take into account entanglement between different phonon modes, which are absent in mean-field theories. As a consequence pairwise averages, e.g., $\langle b_k b_{k'}\rangle$, have a nonzero irreducible part. Because of the Gaussian statistics all higher-order correlators as $\langle b_k^\dagger b_{k'}^\dagger b_k b_{k'}\rangle$ can be reduced to simple two-point expressions using Wick's theorem. In particular the average of Fröhlich Hamiltonian over arbitrary Gaussian trial state $\langle\hat{\mathcal{H}}_{LLP}\rangle$ becomes

$$\begin{aligned}\langle\hat{\mathcal{H}}_{LLP}\rangle &= \frac{P^2}{2M} + \frac{1}{\sqrt{V}}\sum_k V_k(\langle\hat{b}_k^\dagger\rangle + \langle\hat{b}_k\rangle) + \sum_k\left(\omega_k + \frac{k^2}{2M} - \frac{\vec{P}\vec{k}}{M} + \frac{\vec{k}}{2M}\sum_{k'}\vec{k}'\langle\hat{b}_{k'}^\dagger\hat{b}_{k'}\rangle\right)\langle\hat{b}_k^\dagger\hat{b}_k\rangle\\ &+ \frac{1}{2M}\sum_{kk'}\vec{k}\vec{k}'\big(\langle\hat{b}_k^\dagger\rangle\langle\hat{b}_{k'}^\dagger\rangle\langle\hat{b}_k\hat{b}_{k'}\rangle_c + \langle\hat{b}_k^\dagger\hat{b}_{k'}^\dagger\rangle_c\langle\hat{b}_k\rangle\langle\hat{b}_{k'}\rangle + \langle\hat{b}_k^\dagger\rangle\langle\hat{b}_{k'}\rangle\langle\hat{b}_{k'}^\dagger\hat{b}_k\rangle_c + \langle\hat{b}_k^\dagger\hat{b}_{k'}\rangle_c\langle\hat{b}_{k'}^\dagger\rangle\langle\hat{b}_k\rangle\big)\\ &+ \frac{1}{2M}\sum_{kk'}\vec{k}\vec{k}'\big(\langle\hat{b}_k^\dagger\hat{b}_{k'}^\dagger\rangle_c\langle\hat{b}_k\hat{b}_{k'}\rangle_c + \langle\hat{b}_k^\dagger\hat{b}_{k'}\rangle_c\langle\hat{b}_{k'}^\dagger\hat{b}_k\rangle_c\big),\end{aligned} \tag{A1}$$

where we defined the irreducible connected correlations as $\langle\hat{A}\hat{B}\rangle_c = \langle\hat{A}\hat{B}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle$.

Our variational CGW given by Eq. (6) give the most general Gaussian wave functions. For the ground-state (equilibrium) problem under consideration it is sufficient to consider real vector β and real symmetric matrix Q, up to an overall phase, which provide minimum to the energy in Eq. (A1).

The unitary transformations $\hat{D}(\{\beta\})\hat{S}(\{Q\})$ can be understood either as a transformation of the bosonic vacuum wave function into a correlated Gaussian state $|0\rangle \to |\mathrm{CGW}\rangle$, or as

Bogoliubov rotations of the creation (annihilation) operators. To evaluate $\langle\hat{\mathcal{H}}_{LLP}\rangle$ in Eq. (3) with the CGWs, we find it most convenient to perform a Bogoliubov basis transformation,

$$\begin{aligned}\hat{\mathcal{B}}_k &\equiv \hat{S}^\dagger(\{Q\})\hat{D}^\dagger(\{\beta\})\hat{b}_k\hat{D}(\{\beta\})\hat{S}(\{Q\})\\ &= \beta_k + \sum_{k'}[\cosh Q]_{kk'}\hat{b}_{k'} + \sum_{k'}[\sinh Q]_{kk'}\hat{b}^\dagger_{k'},\end{aligned} \tag{A2}$$

and calculate the vacuum expectation value in the new basis, e.g., $\langle\hat{\mathcal{H}}_{LLP}(\hat{b}^\dagger_k,\hat{b}_k)\rangle = \langle 0|\hat{\mathcal{H}}_{LLP}(\hat{\mathcal{B}}^\dagger_k,\hat{\mathcal{B}}_k)|0\rangle$. Here, and in what follows, functions of the matrix Q (e.g., $\cosh Q$) should be understood as being defined through their Taylor expansion. Using the relation (A2), we can now calculate the irreducible two-point functions required to evaluate the variational energy,

$$\begin{aligned}\langle\hat{b}_k\rangle &= \beta_k,\\ \langle\hat{b}_k\hat{b}^\dagger_{k'}\rangle_c &= \tfrac{1}{2}[\cosh 2Q]_{kk'},\\ \langle\hat{b}_k\hat{b}_{k'}\rangle_c &= \tfrac{1}{2}[\sinh 2Q]_{kk'}.\end{aligned} \tag{A3}$$

In order to derive self-consistency equations for β and Q, we minimize the variational energy (A1) with the expectation values given by Eq. (A3). In addition, to obtain tractable equations, we consider only terms up to second order in Q in the energy $\langle\hat{\mathcal{H}}_{\rm LLP}\rangle$. Physically, this corresponds to the assumption that phonon-phonon correlations are small, albeit nonvanishing. Note that this truncation cannot be justified on the grounds that matrix elements $Q_{kk'}$ are of the order of inverse volume $1/\mathcal{V}$. Summations implied in matrix multiplication $[Q^2]_{kk'} = \sum_p Q_{kp}Q_{pk'} = \mathcal{V}\int_p Q_{kp}Q_{pk'}$ show that higher-order terms have the same scaling in powers of $1/\mathcal{V}$. However, analysis shows that even for intermediate interaction strength the matrix norm $\|Q\|$ is numerically small justifying the expansion. Thus we obtain the truncated variational energy given by Eq. (8). To find the minimum of (8) we vary the last expression with respect to β and Q, and derive the self-consistency equations.

1. Equations for $Q_{kk'}$

Minimization of E_p (8) with respect to Q gives

$$\begin{aligned}&\left(\Omega_k + \frac{\vec{k}\vec{k}'}{M} + \Omega_{k'}\right)Q_{kk'} + \frac{\vec{k}\vec{k}'}{M}\beta_k\beta_{k'}\\ &\quad + \sum_q \frac{\vec{q}}{M}\beta_q\left(\vec{k}'\beta_{k'}Q_{kq} + \vec{k}\beta_k Q_{qk'}\right) = 0,\end{aligned} \tag{A4}$$

where the dispersion relation reads

$$\Omega_k = \omega_k + \frac{k^2}{2M} - \frac{\vec{P}\vec{k}}{M} + \frac{\vec{k}}{M}\sum_{k'}\vec{k}'\beta^2_{k'}. \tag{A5}$$

It is similar to the mean-field expression [see Eq. (3)], except that the coherent amplitude β_k is now determined by a different self-consistent procedure.

To cast Eq. (9) into a more tractable form, we now define the following auxiliary quantities, $\eta_{k,k'}$ and $D_{k,k'}$ [75] by the following formulas:

$$\eta_{k,k'} = -MQ_{kk'}\frac{D_{k,k'}}{\beta_k\beta_{k'}},$$

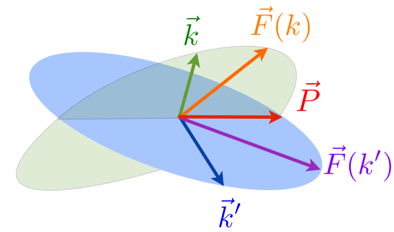

FIG. 5. Schematic of the respect direction of vectors: total momentum $\vec{P}$, momentum of given mode $\vec{k}$, and vector $\vec{F}(k)$. Vectors $\vec{P}$ and $\vec{k}$ define a plane $(\vec{P},\vec{k})$ and vector $\vec{F}(k)$ is in this plane.

$$D_{k,k'} = \Omega_k + \frac{kk'}{M} + \Omega_{k'}. \tag{A6}$$

We express $Q_{kk'}$ via $\eta_{kk'}$ and substitute it into Eq. (9):

$$\eta_{k,k'} = kk' - \sum_q \frac{\beta_q^2}{M}\left(\frac{\eta_{k,q}qk'}{D_{k,q}} + \frac{kq\eta_{q,k'}}{D_{q,k'}}\right). \tag{A7}$$

Let us now introduce the vector

$$\vec{F}_k = \sum_q \frac{\beta_q^2}{MD_{k,q}}\eta_{k,q}\vec{q}, \tag{A8}$$

so that Eq. (9) takes a particularly simple form

$$\eta_{k,k'} = \vec{k}\vec{k}' - \vec{F}_k\vec{k}' - \vec{k}\vec{F}_{k'}. \tag{A9}$$

We introduce the tensorial quantities $\boldsymbol{A}$

$$\boldsymbol{A}^{(0)}_k = \sum_{k'}\frac{\beta^2_{k'}}{MD_{k,k'}}\vec{k}'\otimes\vec{k}', \tag{A10}$$

$$\boldsymbol{A}^{(1)}_k = \sum_{k'}\frac{\beta^2_{k'}}{MD_{k,k'}}\vec{F}_{k'}\otimes\vec{k}', \tag{A11}$$

$$\boldsymbol{A}^{(2)}_k = \sum_{k'}\frac{\beta^2_{k'}}{MD_{k,k'}}\vec{F}_{k'}\otimes\vec{F}_{k'}, \tag{A12}$$

where the outer product of two vectors is $\vec{k}\otimes\vec{k}'$.

Then a multiplication of Eq. (A7) by $\frac{\beta^2_{k'}}{MD_{k,k'}}\vec{k}'$ and subsequent summation over k' gives the self-consistency equation for the vector $\vec{F}_k$

$$\vec{F}_k = (\vec{k} - \vec{F}_k)\boldsymbol{A}^{(0)}_k - \vec{k}\boldsymbol{A}^{(1)}_k. \tag{A13}$$

This equation is solved numerically together with the equation for β, which will be derived in the next subsection.

Let us first discuss the geometrical properties of the vector $\vec{F}_k$. In the case of $P = 0$ vector $\vec{F}_k$ is collinear to $\vec{k}$ as there are no other vector quantities in the formalism. Formally this corresponds to $\vec{F}_k = R_k\vec{k}$, with the proportionality coefficient R_k. In the general case $P \neq 0$, $\vec{F}_k$ belongs to the plane of the vectors $\vec{P}$ and $\vec{k}$, and $\boldsymbol{R}_k$ is a tensor that describes a combination of rotation in this plane and rescaling (see Fig. 5 for illustration).

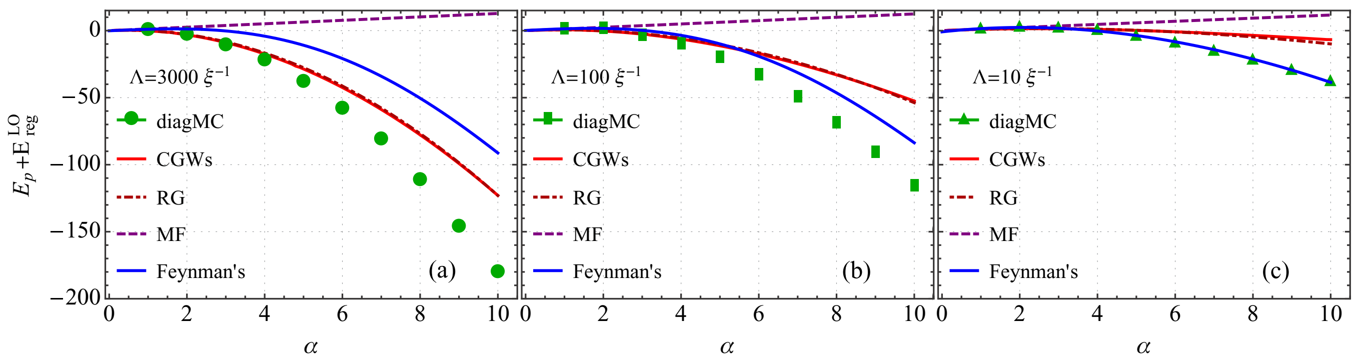

FIG. 6. Polaron energy $E_p + E_g^{\rm O}$ for static ^{6}Li impurity ($P = 0$) in ^{23}Na BEC predicted by different theoretical approaches as a function of the dimensionless coupling constant α in the strong-coupling regime for different values of cutoff parameter: (a) $\Lambda = 3000\ \xi^{-1}$, (b) $\Lambda = 100\ \xi^{-1}$, and (c) $\Lambda = 10\ \xi^{-1}$. Our result (CGWs) is compared with MC calculations [34], Feynman's variational method [18], mean field [20], and renormalization group [33].

2. Equations for β_k

Variation of the expression (8) with respect to β gives

$$V_k + \beta_k\left(\omega_k + \frac{k^2}{2M} - \frac{\vec{k}}{M}(\vec{P} - \vec{P}_{\rm ph})\right) + \frac{\beta_k\vec{k}}{M}\sum_q \frac{\beta_q^2}{MD_{k,q}}\eta_{q,k}(\vec{F}(q) - \vec{q}) = 0, \qquad \text{(A14)}$$

where we substituted Q with the corresponding expressions (A6) in terms of $\eta_{k,k'}$ after the variation. The total momentum carried by the phonons is $\vec{P}_{\rm ph} = \sum_{kk'}\vec{k}(\beta_k^2\delta_{kk'} + Q_{kk'}^2)$. The last term on the left-hand side of Eq. (A14) can be interpreted as a renormalizition of the phonon dispersion relation Ω_k. Let us rewrite the expressions so that this statement is more clear. We use Eqs. (A7) and (A13), and also recall the geometrical properties of vector $\vec{F}_k$ discussed above: $\vec{F}_k = \boldsymbol{R}_k\vec{k}$. We rewrite the expression (A14) as follows:

$$V_k + \beta_k\left(\omega_k + \frac{k^2}{2M} - \frac{\vec{k}}{M}(\vec{P} - \vec{P}_{\rm ph}) + \vec{k}\frac{1}{M}\left(\left(\boldsymbol{A}_k^{(1)} - \boldsymbol{A}_k^{(0)}\right)(\boldsymbol{I} - \boldsymbol{R}_k) - \boldsymbol{A}_k^{(2)}\right)\vec{k}\right) = 0. \quad \text{(A15)}$$

Thus the equation for β_k can be written in a compact form

$$\beta_k = -\frac{V_k}{\omega(k) + \frac{\vec{k}\boldsymbol{\mathcal{M}}^{-1}(k)\vec{k}}{2} + \frac{\vec{k}}{M}(\vec{P} - \vec{P}_B)}. \qquad \text{(A16)}$$

Here the effective impurity mass

$$M\boldsymbol{\mathcal{M}}^{-1}(k) = \boldsymbol{I} - 2\left(\left(\boldsymbol{A}_k^{(1)} - \boldsymbol{A}_k^{(0)}\right)(\boldsymbol{I} - \boldsymbol{R}_k) - \boldsymbol{A}_k^{(2)}\right) \quad \text{(A17)}$$

is a tensor quantity which is nondiagonal for $P \neq 0$.

3. Observables

Equations (A13) and (A16) for β_k and $\vec{F}_k$ form a self-consistent set for β_k and $\vec{F}_k$ which we solve iteratively. After obtaining β_k and $\vec{F}_k$ all observables can be calculated using Wick's theorem. In particular, the ground-state energy of the Fröhlich-Bogoliubov Hamiltonian reads E_p

$$E_p = \langle\hat{\mathcal{H}}_{\rm LLP}\rangle - g_{IB}n_0 = \frac{\vec{P}^2}{2M} - \frac{\vec{P}_{\rm h}^2}{2M} + \sum_k V_k\beta_k - \sum_k \beta_k^2\frac{\vec{F}_k^2}{2M} + \sum_k \beta_k^2\frac{k_\mu\left(M^{-1}\delta_{\mu\nu} - \mathcal{M}_{\mu\nu}^{-1}(k)\right)k_\nu}{2}. \qquad \text{(A18)}$$

The energy E_p by itself is UV divergent. This divergence appears at the mean-field level and comes from the term $\sum_k V_k\beta_k$. Indeed one can check that in UV limit $\beta_k \propto k^{-2}$ and V_k tends to a constant value. Therefore, in $d > 2$ this gives rise to a power-law divergency of the polaron energy $\sum_k V_k\beta_k \propto \Lambda^{d-2}$, where Λ is a sharp UV momentum cutoff. This divergence is resolved by the standard regularization procedure [18,20,54], expressing g_{IB} in terms of the scattering length a_{IB} and the cutoff Λ. When quantum fluctuations are taken into account an additional logarithmic divergence with Λ appears as we discuss in detail in [33]. The presence of this logarithmic behavior makes a direct comparison with the experimental data involved. Thus our results for polaron energy are only used to benchmark the approach by comparing to other known theoretical results.

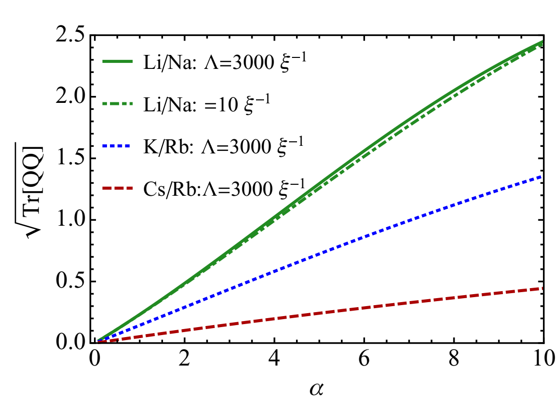

FIG. 7. Measure of the correlation strength, $\sqrt{{\rm Tr}[QQ]}$, as a function of the dimensionless coupling constant α for systems with various mass imbalance: $M/m_B = 0.23$ (Li/Na), $M/m_B = 0.47$ (K/Rb), and $M/m_B = 1.53$ (Cs/Rb).

The ground-state energy of the Fröhlich Hamiltonian with the regularized leading-order divergence $E_p + E_g^{LO}$ is shown in Fig. 2 and in Fig. 6. The results obtained by the CGWs approach is in good agreement with the diagMC up to $\alpha = 4$ for any value of the UV cutoff parameter. In the strong-coupling limit there is a discrepancy between the numerically exact solution and the results obtained by the CGWs, which is due to the perturbative expansion of the energy as a function of the squeezing parameter Q. To supplement this statement with concrete numbers we calculate the matrix norm of the squeezing parameter $\sqrt{\mathrm{Tr}[QQ]}$, shown in Fig. 7. The perturbative expansion is no longer valid when the matrix norm is of the order of unity, $\sqrt{\mathrm{Tr}[QQ]} \approx 1$. Note that the squeezing parameter is smaller for heavier impurities, since the nonlinear term in the Hamiltonian (A1) is proportional to the inverse mass of the impurity M^{-1}.

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