Polaronic slowing of fermionic impurities in lattice Bose-Fermi mixtures

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We generalize the application of small polaron theory to ultracold gases [M. Bruderer, A. Klein, S. R. Clark, and D. Jaksch, New J. Phys. **10**, 033015 (2008)] to the case of Bose-Fermi mixtures, where both components are loaded into an optical lattice. In a suitable range of parameters, the mixture can be described within a Bogoliubov approach in the presence of fermionic (dynamic) impurities; an effective description in terms of polarons applies. In the dilute limit of the slow-impurity regime, the hopping of fermionic particles is exponentially renormalized due to polaron formation, regardless of the sign of the Bose-Fermi interaction. This should lead to clear experimental signatures of polaronic effects, once the regime of interest is reached. The validity of our approach is analyzed in the light of currently available experiments. We provide results for the hopping renormalization factor for different values of temperature, density, and Bose-Fermi interaction for three-dimensional ^{87}Rb-^{40}K mixtures in an optical lattice.

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I. INTRODUCTION

Polaron physics and, more generally, electron-phonon interactions are one of the most influential areas of modern condensed-matter physics and are believed to play a major role in the physics of high-T_c superconductors [1,2] and strongly correlated materials.

Ultracold gases, on the other hand, allow for the investigation of open issues in condensed matter using clean and highly tunable systems (see, for example, [3–5]). In the context of polaron physics, the so-called spin-polaron, that is, a single-spin-down impurity immersed in a Fermi sea of spin-up particles, has been realized as the extreme limit of imbalanced Fermi mixtures whenever $N_\uparrow/N_\downarrow \gg 1$ and a remarkable agreement between theory [6,7] and experiments [8,9] has been achieved. The original polaron problem [10] deals, however, with fermionic particles (electrons) interacting with lattice vibrations (phonons), which obey the bosonic statistics, and is therefore somehow closer to the physics of Bose-Fermi mixtures.

Bose-Fermi mixtures have been widely investigated during the past few years, both theoretically [11–13] and experimentally [14–16]. The main focus, however, has been on the effect of the fermionic component of the mixture on the coherence properties of the bosonic condensate and on the superfluid–to–Mott-insulator transition. In addition, theoretical efforts were devoted to investigation of the emergence of supersolid and other exotic phases [12,13].

In a strongly imbalanced mixture of $N_{\rm B}$ bosons and $N_{\rm F}$ spinless fermions with $N_{\rm F}/N_{\rm B} \ll 1$, the dilute fermionic particles act as dynamic impurities in the bosonic condensate. On the other hand, if one focuses on the fermionic component, the experimental setup closely resembles the polaronic problem in condensed matter, since fermionic atoms interact with phononic excitations of the condensate. Again, the main advantage of ultracold gases is that both the relative densities of the components and their mutual interactions can be tuned much more easily and to a larger extent than the corresponding condensed-matter case. The extreme imbalanced limit allows one, for example, to neglect the interactions between different polarons and address the *single-polaron* regime with relative simplicity.

A remarkable achievement in this direction has been, for example, the recent experiment performed by the Bloch group [16], where a lattice Bose-Fermi mixture of ^{87}Rb-^{40}K was studied, exploiting an interspecies Fano-Feshbach resonance to tune the Bose-Fermi scattering length $a_{\rm BF}$ and varying the relative densities $N_{\rm F}/N_{\rm B}$ of the species. This allowed investigation of the effect of the interspecies interaction and of the population imbalance between bosons and fermions on the transition from superfluid to Mott insulator in a very controlled way.

A theoretical description of one-dimensional Bose-Fermi mixtures in terms of a Luttinger liquid of polarons has been proposed in [17], while the problem of polaron formation for a single impurity immersed in a three-dimensional (3D) homogeneous condensate has been studied in [18] and more recently in [19]. Other works addressed the emergence of polarons in the context of cold atoms in optical lattices [20,21]. They considered bosonic impurities loaded in an optical lattice with the whole system immersed in a large condensate of a different bosonic species. Only the impurities were affected by the lattice, allowing for an arbitrary slowing down of the impurities without perturbing the condensate (see Sec. III for further details). This scenario could, in principle, be realized in experiments using a species-selective optical lattice. However, this kind of setup, to our knowledge, has not yet been applied to Bose-Fermi mixtures, although several experimental schemes have been proposed [22] and species-selective lattices have already been successfully applied to Bose-Bose mixtures [23,24]. In current experiments on Bose-Fermi mixtures in optical lattices (see, for example, Ref. [16]), *both* species are affected (though to a different extent) by the same optical lattice. In the latter case, the tunneling properties of both species are intrinsically connected to each other, and the properties of the Bogoliubov modes of the condensate and their coupling to the fermionic particles are modified by the lattice.

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For these reasons, in this work we generalize the theory developed in Ref. [21] to the case where both the fermions and the bosons move in the same optical lattice. Despite the presence of the lattice, we show that, in a suitable parameter regime, the bosonic condensate still sustains phononlike excitations and the general framework developed for the homogeneous case in Ref. [21] still applies. We find that fermionic particles are exponentially slowed down by the interaction with the Bogoliubov modes of the condensate, due to polaron formation. We also discuss the relevance of our approach to current experiments on Bose-Fermi mixtures, analyzing the assumptions we made in order to derive our theory. For the specific case of a ^{87}Rb-^{40}K mixture, we provide results for the polaronic hopping renormalization of a single fermionic impurity in several experimental setups, that is, for different values of the bosonic density, lattice depth, Bose-Fermi scattering length, and temperature. This effect can actually be measured by looking at the expansion of the fermionic component of the mixture in a lattice when the trapping potential is suddenly removed and $N_F/N_B \ll 1$ [25].

The layout of the paper is as follows: In the next section we explain how, under suitable conditions, a Bose-Fermi mixture can be effectively described in terms of polarons, and we derive an expression for the fermionic hopping renormalization due to polaronic effects. In Sec. III we analyze our assumptions within a generic experimental setup for Bose-Fermi mixtures in optical lattices. Results for the fermionic hopping renormalization in a ^{87}Rb-^{40}K mixture are provided in Sec. IV. Conclusions are drawn in Sec. V.

II. THEORY

A. Gross-Pitaevskii theory for static impurities

The derivation of this section closely follows the one in Ref. [21], generalizing it to the case where single-hyperfine states of a bosonic and fermionic species are loaded together into an optical lattice generated by counterpropagating laser beams of wavelength λ and frequency ω_L. For far-off-resonant laser beams, the atoms experience a potential $V_{B/F} = V^0_{B/F}\sum_{i=1}^{D}\sin^2(\pi x_i/l)$ with $V^0_{B/F} = s_{B/F}E_r^{B/F}$, where $E_r^{B/F} = \frac{4\pi^2}{2m_{B/F}\lambda^2}$ ($\hbar = 1$) is the bosonic (fermionic) recoil energy, $s_{B/F}$ denotes the dimensionless lattice depth for bosons and fermions in the respective recoil energy, and $l = \lambda/2$ is the lattice spacing, which we use as a unit length. We choose the *fermionic* recoil energy E_r^F as the energy unit throughout the paper.

The effect of the trapping potential is neglected, and we postpone a thorough discussion about the correctness of our assumptions to the next section. The system under investigation is assumed to be described by a single-band Bose-Fermi–Hubbard model, with the Hamiltonian

$$\hat{H} = \hat{H}_B + \hat{H}_F + \hat{H}_{BF}, \tag{1}$$

where

$$\hat{H}_B = -J_B\sum_{\langle i,j\rangle}(\hat{b}_i^\dagger\hat{b}_j + \text{H.c.}) - \mu_B\hat{N}_B + \frac{U_{BB}}{2}\sum_i \hat{n}_i^B(\hat{n}_i^B - 1), \tag{2}$$

$$\hat{H}_F = -J_F\sum_{\langle i,j\rangle}(\hat{c}_i^\dagger\hat{c}_j + \text{H.c.}) - \mu_F\hat{N}_F, \tag{3}$$

$$\hat{H}_{BF} = U_{BF}\sum_i \hat{b}_i^\dagger\hat{b}_i\hat{c}_i^\dagger\hat{c}_i. \tag{4}$$

The fermions do not interact (directly) with each other. However, as we will see later, they can still interact via boson-mediated interactions, a situation which is very similar to the BCS model for standard superconductivity, where phonons mediate the attractive interactions between the electrons. We first consider the case $J_F = 0$, where the fermions act as a set of static impurities on the bosonic system and their position is specified by the (discrete) distribution function f_i. We assume that the bosonic system in the presence of impurities can be treated within Bogoliubov theory, meaning that we consider the solution of the Gross-Pitaevskii (GP) equation in the presence of impurities and quantize the oscillations around the classical deformed ground state. If the fermionic impurities were absent ($f_i = 0\ \forall i$ or equivalently $U_{BF} = 0$), then for the unperturbed system of bosons we can write the following GP equation by approximating the bosonic field operators with c numbers $\hat{b}_i \approx \psi_i^0$ and $\hat{b}_i^\dagger \approx (\psi_i^0)^*$ [26,27]:

$$-J_B\sum_{j\in nn_i}\psi_j^0 + U_{BB}|\psi_i^0|^2\psi_i^0 = \mu_B\psi_i^0, \tag{5}$$

where the sum in the first term runs over the nearest neighbors of the lattice site i. In the case of a uniform system (in the lattice), this equation is trivially solved by $\psi_i^0 = \sqrt{n_0}$ and $\mu_B = U_{BB}n_0 - zJ_B$, where z is the coordination number of the lattice and n_0 is the density of particles per lattice site in the fully condensed state described by the classical GP theory (no quantum depletion of the condensate). In the presence of static fermionic impurities ($J_F = 0$), the previous result has to be modified because the condensate macroscopic wave function is distorted by the impurities. If this distortion is sufficiently small then we can expand the classical field around the unperturbed solution, that is, $\hat{b}_i \approx \psi_i^0 + \delta_i$, and keep only the leading nonzero terms in the fluctuation δ_i. This approximation is valid if $\frac{|\delta_i|}{\psi_i^0} \ll 1$ and in this case the GP Hamiltonian has the form $H_{GP} = H_0 + H_\delta + H_{lin}$, where

$$H_0 = -J_B\sum_{\langle i,j\rangle}\left[(\psi_i^0)^*\psi_j^0 + \text{H.c.}\right] - \mu_B\sum_i|\psi_i^0|^2 + \frac{U_{BB}}{2}\sum_i|\psi_i^0|^4 + U_{BF}\sum_i|\psi_i^0|^2 f_i, \tag{6}$$

$$H_\delta = -J_B\sum_{\langle i,j\rangle}[\delta_i^*\delta_j + \text{H.c.}] - \mu_B\sum_i|\delta_i|^2 + 2U_{BB}\sum_i|\delta_i|^2|\psi_i^0|^2 + \frac{U_{BB}}{2}\sum_i\left(\delta_i^*|\psi_i^0|^2\delta_i^* + \delta_i|\psi_i^0|^2\delta_i\right), \tag{7}$$

$$H_{lin} = U_{BF}\sum_i\left[\psi_i^0\delta_i^* + (\psi_i^0)^*\delta_i\right]f_i, \tag{8}$$

where f_i is the impurity distribution. The linear term in the fluctuation δ_i in H_δ is identically zero because we choose ψ_i^0 as the solution of the unperturbed GP equation.

By imposing the first derivative of this expression with respect to δ_i^* to vanish, and using the conditions $\psi_i^0 = \sqrt{n_0}$ and $-\mu_B + U_{BB}n_0 = zJ$, we obtain the following GP equation for the fluctuation field δ:

$$-J_B \sum_{j\in nn_i} \delta_j + zJ_B\delta_i + 2U_{BB}n_0\delta_i + U_{BF}\sqrt{n_0} f_i = 0. \quad (9)$$

This equation can be recast in the following form:

$$\frac{\sum_{j\in nn_i}(\delta_j - \delta_i)}{l^2} - \left(\frac{2}{\xi}\right)^2 \delta_i = \frac{U_{BF}\sqrt{n_0}}{J_B l^2} f_i, \quad (10)$$

where we introduce the healing length of the condensate:

$$\xi = \sqrt{\frac{2J_B}{U_{BB}n_0}}\, l. \quad (11)$$

Therefore the GP equation for the fluctuation field δ_i has the form of a discrete modified Helmholtz equation where the impurity distribution acts as a source term. For a weakly interacting condensate, the healing length ξ is larger than the lattice spacing l and we can consider the continuum limit of Eq. (10), applying the same considerations discussed in [21]. The healing length ξ fixes the typical scale for the variation in space of the fluctuation field δ_i due to the impurities. This means that the perturbation induced in the condensate by the impurities decays exponentially in space with the healing length ξ, and the condition $\frac{|\delta_i|}{\psi_i^0} \ll 1$ (small perturbation of the condensate due to the impurities) implies ($U_{BB} > 0$)

$$\alpha = \frac{|U_{BF}|}{U_{BB}} \frac{1}{n_0 \xi^D} = \frac{|U_{BF}|(U_{BB}n_0)^{(D/2)-1}}{(2J_B)^{D/2}} \ll 1, \quad (12)$$

where D is the dimension of the system under consideration. Using the solution of Eq. (10), the GP Hamiltonian provides the classical value of the ground-state energy as a function of the impurity distribution f_i; that is, $E = E^{cl}(f_i)$.

B. Bogoliubov corrections

In the previous subsection, we considered how the classical condensate is distorted in the presence of static impurities without including any quantum effects. We now consider the Bogoliubov excitations on top of the classical theory, decomposing the bosonic quantum operators in a classical and a quantum part; that is, $\hat{b}_i = \psi_i + \hat{\theta}_i$, where $\psi_i = \psi_i^0 + \delta_i$ is the solution of the GP equation previously described. If we insert this expression into the Hamiltonian and retain only the terms up to the second order in the fluctuation fields, we find that all the linear terms in the fluctuation fields (classical and quantum) disappear since we have chosen the classical part as the solution of the GP equation in the presence of impurities. Therefore the Hamiltonian of the system has the form $\hat{H} = \hat{H}_\theta + E^{cl}(f_i)$, where

$$\hat{H}_\theta = -J_B \sum_{\langle i,j\rangle} (\hat{\theta}_i^\dagger \hat{\theta}_j + \text{H.c.}) - \mu_B \sum_i \hat{\theta}_i^\dagger \hat{\theta}_i + 2U_{BB} \sum_i \hat{\theta}_i^\dagger \hat{\theta}_i |\psi_i^0|^2 + \frac{U_{BB}}{2} \sum_i [\hat{\theta}_i^\dagger (\psi_i^0)^2 \hat{\theta}_i^\dagger + \hat{\theta}_i (\psi_i^0)^2 \hat{\theta}_i]. \quad (13)$$

As evident from this expression, the quantum part of the Hamiltonian is independent of the impurity distribution and only depends on the unperturbed classical ground state through ψ_i^0. The quadratic Hamiltonian $\hat{H}_\theta$ can be diagonalized using a Bogoliubov transformation (see [28,29] for a general treatment) and we can re-express $\hat{H}_\theta$ in terms of the Bogoliubov modes of the condensate.

This can be done by introducing the following transformation which express the original bosonic fluctuation operators $\hat{\theta}$ in term of new bosonic operators $\hat{\beta}$ and $\hat{\beta}^\dagger$; that is,

$$\hat{\theta}_i = \sum_{\mathbf{k}\in FBZ}{}' u_{\mathbf{k},i}\hat{\beta}_{\mathbf{k}} + v_{\mathbf{k},i}^* \hat{\beta}_{\mathbf{k}}^\dagger, \quad (14)$$

where the sum runs over the quasimomenta $\mathbf{k}$ of the lattice within the first Brillouin zone (FBZ) and $\mathbf{k} = 0$ (the condensate) is excluded from the sum. To make $\hat{H}_\theta$ quadratic the coefficients $u_{\mathbf{k},i}$ and $v_{\mathbf{k},i}$ have the form

$$u_{\mathbf{k},i} = \frac{1}{\sqrt{N_s}} e^{i\mathbf{k}\cdot\mathbf{R}_i} u_{\mathbf{k}}, \quad v_{\mathbf{k},i} = \frac{1}{\sqrt{N_s}} e^{i\mathbf{k}\cdot\mathbf{R}_i} v_{\mathbf{k}}, \quad (15)$$

$$u_{\mathbf{k}} = \sqrt{\frac{\epsilon_{\mathbf{k}}^* + U_{BB}n_0}{\hbar\omega_{\mathbf{k}}} + 1}, \quad v_{\mathbf{k}} = \sqrt{\frac{\epsilon_{\mathbf{k}}^* + U_{BB}n_0}{\hbar\omega_{\mathbf{k}}} - 1}, \quad (16)$$

where $\epsilon_{\mathbf{k}}^* = \epsilon_{\mathbf{k}} + zJ_B = 2J_B \sum_{i=1}^{D} [1 - \cos(k_i l)] \geqslant 0$ is the (shifted) single-particle spectrum in the tight-binding approximation, $\hbar\omega_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^*(\epsilon_{\mathbf{k}}^* + 2U_{BB}n_0)}$ is the energy of the Bogoliubov mode [26,27], and N_s is the number of lattice sites. The major difference in these expressions with respect to the continuum case treated in [21] is that the FBZ provides a natural cutoff for the single-particle energy and therefore also for the energy of the Bogoliubov modes. In Fig. 1 we sketched for comparison the shifted single-particle spectrum $\epsilon_{\mathbf{k}}^*$ and the energy spectrum $\hbar\omega_{\mathbf{k}}$ of the Bogoliubov modes.

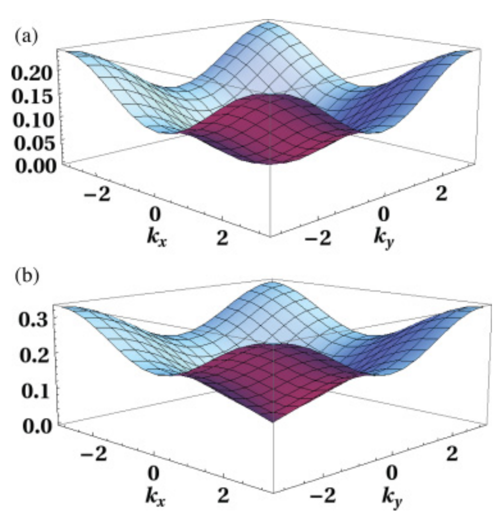

FIG. 1. (Color online) (a) Shifted single-particle dispersion $\epsilon_{\mathbf{k}}^*$ and (b) Bogoliubov spectrum $\hbar\omega_{\mathbf{k}}$ in the $k_z = 0$ plane for D = 3 and $J_B = 0.029, U_{BB} = 0.11, U_{BF} = 0.065$, and $n_0 = 1$. Energies are expressed in units of the fermionic recoil energy E_r^F and momenta in units of l^{-1}, where l is the lattice spacing.

Once expressed in terms of the Bogoliubov operators, the Hamiltonian of the system is diagonal and assumes the form

$$\hat{H}^{\text{stat}} = E^{\text{cl}}(f_i) + \Delta E^q + \hat{H}_\beta \quad \hat{H}_\beta = \sum_{\mathbf{k}\in\text{FBZ}}{}' \hbar\omega_{\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}}\hat{\beta}_{\mathbf{k}}, \tag{17}$$

where ΔE^q is the quantum correction to the classical ground-state energy due to the zero-point motion of Bogoliubov modes.

As already noticed in [21], since the Bogoliubov Hamiltonian (13) does not depend on the impurities distribution, this means that the Bogoliubov spectrum is unaffected by the position of the impurities and we have the same oscillation frequencies that we would have in the absence of the impurities. The equilibrium position of these condensate oscillations is, however, shifted by the presence of impurities. Since the Bogoliubov spectrum does not depend on the impurity positions, we can also switch the order of the steps in the preceding derivation and calculate the Bogoliubov theory around the unperturbed ground state (no impurities), which is given by the assumption $\hat{b}_i = \psi_i^0 + \hat{\theta}_i$ and keeping only terms up to second order in the fluctuation fields $\hat{\theta}_i$. In this case, we obtain the same expression as before for the Bogoliubov part while the classical part is no longer the solution of the GP equation in the presence of impurities. The Hamiltonian operator now has the form $\hat{H} = E_{\psi^0} + \hat{H}_\theta + \hat{H}_{\text{lin}}$, where

$$H_{\text{lin}} = U_{\text{BF}}\sqrt{n_0}\sum_i f_i[\hat{\theta}_i^\dagger + \hat{\theta}_i] \tag{18}$$

and E_{ψ^0} is a c number. Using the Bogoliubov transformation (14), we get in terms of the Bogoliubov modes

$$\hat{H} = E_{\psi^0} + \hat{H}_\theta + \hat{H}_{\text{lin}}, \tag{19}$$

$$H_\theta = \sum_{\mathbf{k}\in\text{FBZ}}{}' \hbar\omega_{\mathbf{k}}\beta^\dagger_{\mathbf{k}}\beta_{\mathbf{k}}, \tag{20}$$

$$H_{\text{lin}} = \sum_i \sum_{\mathbf{k}\in\text{FBZ}}{}' \hbar\omega_{\mathbf{k}}[M_{i,\mathbf{k}}\beta_{\mathbf{k}} + M^*_{i,\mathbf{k}}\beta^\dagger_{\mathbf{k}}]f_i, \tag{21}$$

where

$$M_{i,\mathbf{k}} = \frac{U_{\text{BF}}\sqrt{n_0}}{\hbar\omega_{\mathbf{k}}}(u_{\mathbf{k},i} + v_{\mathbf{k},i}) = M_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{R}_i} \tag{22}$$

and

$$M_{\mathbf{k}} = U_{\text{BF}}\sqrt{\frac{n_0\epsilon^*_{\mathbf{k}}}{N_s(\hbar\omega_{\mathbf{k}})^3}}. \tag{23}$$

In this case, the new bosonic operators annihilate Bogoliubov excitations around the unperturbed ground state and therefore do not annihilate the real vacuum defined previously, which is distorted by the impurities. This leaves us with a generalized Holstein model with phonons coupled to the fermionic density [30,31]. The main difference with respect to the original Holstein model is that here we have a *continuum* of phonons instead of a single-phononic mode. The high-energy-phonon contribution in this expression is cut off due to the FBZ, while in the continuum case [21] the physical cutoff is provided by the inverse of the typical localization length of the impurities in the Wannier states, which appears explicitly in the matrix elements M (see Sec. II D). For static impurities, this Hamiltonian can be diagonalized by introducing a unitary Lang-Firsov [32] transformation, which shifts the equilibrium position of the condensate around the places where the impurities are localized:

$$\hat{U} = \exp\left[\sum_j \sum_{\mathbf{k}\in\text{FBZ}}{}' (M^*_{j,\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}} - M_{j,\mathbf{k}}\hat{\beta}_{\mathbf{k}})\right] f_j. \tag{24}$$

This makes the Hamiltonian diagonal in the bosonic operators recovering Eq. (17).

C. Slowly moving impurities

If J_{F} is not zero, that is, if the impurities can move through the lattice, then the problem is not fully solved using (24). However, the Lang-Firsov transformation provides physical insight on how to proceed. Indeed, introducing now the fermionic operators $\hat{c}_i$ and $\hat{c}_i^\dagger$, we can repeat the steps by simply replacing the density distribution f_i with the density operator $\hat{n}_i = \hat{c}_i^\dagger\hat{c}_i$ everywhere. The Lang-Firsov transformation now acts simultaneously on fermionic and bosonic degrees of freedom:

$$\hat{U} = \exp\left[\sum_j \sum_{\mathbf{k}\in\text{FBZ}}{}' (M^*_{j,\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}} - M_{j,\mathbf{k}}\hat{\beta}_{\mathbf{k}})\right] \hat{n}_j. \tag{25}$$

Using the Baker-Campbell-Hausdorff formula it is possible to show that $\hat{U}\hat{\beta}^\dagger_{\mathbf{k}}\hat{U}^\dagger = \hat{\beta}^\dagger_{\mathbf{k}} - \sum_j M_{j,\mathbf{k}}\hat{n}_j$, $\hat{U}\hat{n}_j\hat{U}^\dagger = \hat{n}_j$, and $\hat{U}\hat{c}^\dagger_j\hat{U}^\dagger = \hat{c}^\dagger_j\hat{X}^\dagger_j$, where the operator $\hat{X}^\dagger_j$ creates a coherent cloud of Bogoliubov modes around the position j, that is,

$$\hat{X}^\dagger_j = \exp\left[\sum_{\mathbf{k}\in\text{FBZ}}{}' (M^*_{j,\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}} - M_{j,\mathbf{k}}\hat{\beta}_{\mathbf{k}})\right]. \tag{26}$$

The Lang-Firsov-transformed Hamiltonian now has the form

$$\hat{H}_{\text{LF}} = -J_{\text{F}}\sum_{\langle i,j\rangle}(\hat{X}_i\hat{c}_i)^\dagger(\hat{X}_j\hat{c}_j) - \tilde{\mu}\hat{N}_{\text{F}} - \frac{1}{2}\sum_{i\neq j}V_{i,j}\hat{n}_i\hat{n}_j + \sum_{\mathbf{k}\in\text{FBZ}}{}' \hbar\omega_{\mathbf{k}}\hat{\beta}^\dagger_{\mathbf{k}}\hat{\beta}_{\mathbf{k}} + E. \tag{27}$$

As already pointed out, the presence of Bogoliubov modes induces (off-site) interactions between the impurities. The interaction potential has the form

$$V_{i,j} = 2\sum_{\mathbf{k}\in\text{FBZ}}{}' \hbar\omega_{\mathbf{k}}|M_{\mathbf{k}}|^2\cos\left[\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)\right]. \tag{28}$$

Therefore, even though spin-polarized fermionic impurities do not interact directly with each other, their coupling to the Bogoliubov modes of the condensate creates an effective interaction between them. As shown in Fig. 2, the interaction is always attractive ($V_{i,j} > 0$) regardless of the sign of the Bose-Fermi interaction and decays very quickly with the distance between the impurities. Moreover, during its motion, the impurity drags a Bogoliubov cloud, and this affects its kinetic energy, as evident from the first term in Eq. (27). If the impurities are not moving ($J_{\text{F}} = 0$), their energies are lowered by an amount of energy that represents the potential energy

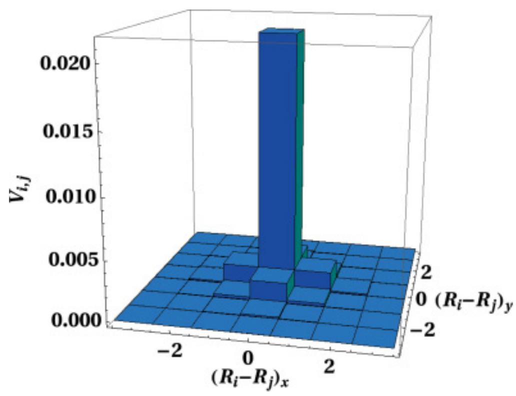

FIG. 2. (Color online) Effective interaction potential $V_{i,j}$ between the impurities for $(\mathbf{R}_i-\mathbf{R}_j)_z=0$ and D = 3 ($J_\mathrm{B}=0.029, U_\mathrm{BB}=0.11, U_\mathrm{BF}=0.065$, and $n_0=1$). The central peak for $i=j$ is proportional to the polaron shift ($V_{i,i}=2E_p$). Energies are expressed in units of E_r^F and lengths in units of l.

gain due to the interaction with the Bogoliubov cloud. This characteristic energy scale for static impurities is the polaron shift E_p, where

$$E_p=\sum_{\mathbf{k}\in\mathrm{FBZ}}{}' \hbar\omega_\mathbf{k}|M_\mathbf{k}|^2=U_\mathrm{BF}^2\frac{1}{N_s}\sum_{\mathbf{k}\in\mathrm{FBZ}}{}'\frac{n_0\epsilon_\mathbf{k}^*}{(\hbar\omega_\mathbf{k})^2} \quad (29)$$

and $\tilde{\mu}=\mu_\mathrm{F}+E_p$ in Eq. (27).

Whenever this energy scale is much larger than the hopping parameter of the impurities, that is,

$$\zeta=\frac{J_\mathrm{F}}{E_p}\ll 1, \quad (30)$$

we expect that the impurity and its surrounding cloud will tunnel together like a composite object, that is, they form a *polaron*. The expressions (19)–(21) and their Lang-Firsov-transformed version (27) are, in practice, valid even beyond the condition (30) (slow-impurity regime), while the results we derive in the next subsection assume that impurities are slow in the sense specified by Eq. (30). In this sense, this treatment is analogous to the antiadiabatic limit (fast phonons) of the small-polaron theory introduced by Holstein [30,31], where the impurities move much more slowly than the time taken by the coherent cloud to rearrange itself. Here we point out that in expression (30), the bare fermionic hopping J_F is not compared with the bare bosonic hopping J_B but with E_p, which explicitly depends also on the Bose-Bose interaction and the bosonic density. This is because in Bose-Fermi mixtures the *excitations* of the bosonic condensate and not the original bosonic particles play the role analogous to that of phonons in the standard polaronic problem.

D. Single fermionic impurity in the strong-coupling small-polaron regime

We consider now the case of a single fermionic impurity immersed in a much larger Bose-Einstein condensate (BEC). In real experiments, this *single-polaron* regime is realized whenever $N_\mathrm{B}\gg N_\mathrm{F}$ such that $(n_\mathrm{F})^{-1/D}\gg\xi/l$, where $n_\mathrm{F}=N_\mathrm{F}/N_s$ is the number of fermions per lattice site. This implies that the average interparticle distance is much larger than the healing length of the BEC, so that also interactions induced by the Bogoliubov modes can be neglected. For a single impurity, the Lang-Firsov Hamiltonian becomes

$$H_{1-\mathrm{imp}}=\sum_{\mathbf{k}\in\mathrm{FBZ}}{}'\hbar\omega_\mathbf{k}\beta_\mathbf{k}^\dagger\beta_\mathbf{k}-J_\mathrm{F}\sum_{\langle i,j\rangle}(\hat{X}_i\hat{c}_i)^\dagger(\hat{X}_j\hat{c}_j)+E_0, \quad (31)$$

where E_0 is a c number. For $J_\mathrm{F}=0$, the fermionic and bosonic parts are completely disconnected and the impurity can sit everywhere in the lattice with the same energy. If J_F is nonzero but $\zeta=\frac{J_\mathrm{F}}{E_p}\ll 1$, the polaron is the appropriate quasiparticle and the hopping term can be treated as a small perturbation. We focus now on the regime of temperature $k_\mathrm{B}T\ll E_p$, where incoherent phononic scattering is highly suppressed [21]. The degeneracy of the Wannier states can be removed by introducing Bloch waves labeled by $\mathbf{k}'$ for the impurity and considering

$$\Delta E(\mathbf{k}',\{N_\mathbf{k}\})=\langle\mathbf{k}',\{N_\mathbf{k}\}|-J_\mathrm{F}\sum_{\langle i,j\rangle}(\hat{X}_i\hat{c}_i)^\dagger(\hat{X}_j\hat{c}_j)|\mathbf{k}',\{N_\mathbf{k}\}\rangle, \quad (32)$$

where $\{N_\mathbf{k}\}$ indicates the configuration of Bogoliubov modes. This matrix element can be calculated using standard techniques for phonons [10]. If we assume thermally distributed phonons, the bare hopping of the impurity J_F is exponentially renormalized to $J_\mathrm{F}^r=J_\mathrm{F}e^{-S}$ and the renormalization factor S is given by

$$S=\sum_{\mathbf{k}\in\mathrm{FBZ}}{}'|M_{0,\mathbf{k}}|^2[1-\cos(\mathbf{k}\cdot\mathbf{a})](2N_\mathbf{k}+1), \quad (33)$$

where $N_\mathbf{k}=\frac{1}{e^{\hbar\omega_\mathbf{k}/k_\mathrm{B}T}-1}$. Inserting expression (22) of the matrix elements M, one obtains $S(T,U_\mathrm{BF})=U_\mathrm{BF}^2 f(T)$, where

$$f(T)=\frac{1}{N_s}\sum_{\mathbf{k}\in\mathrm{FBZ}}\frac{n_0\epsilon_\mathbf{k}^*}{(\hbar\omega_\mathbf{k})^3}[1-\cos(\mathbf{k}\cdot\mathbf{a})]\,[2N_\mathbf{k}(T)+1]. \quad (34)$$

In practice, within this approach, the renormalization factor S is proportional to the square of the Bose-Fermi interaction U_BF, while the factor f only depends on the condensate properties. As evident from this expression, S does not depend on the sign of the Bose-Fermi interaction. This results in a Gaussian dependence of the renormalized hopping on the Bose-Fermi interaction; that is, $J_\mathrm{F}^r=J_\mathrm{F}e^{-U_\mathrm{BF}^2 f}$. The prefactor f, together with its dependency on the temperature T and on other parameters like $U_\mathrm{BB}, J_\mathrm{B}$, and n_0, can then be calculated independently and results are presented in Sec. IV for the ^{87}Rb-^{40}K case.

All the results presented in this section are expressed in terms of the parameter n_0, the density of particles in the condensate. However, a fixed value of n_0 corresponds to different values of the bosonic density n_B, whenever one changes the temperature T or the Hamiltonian parameters $U_\mathrm{BB}, J_\mathrm{B}$. In order to compare data with experiments, the results have to be expressed in terms of the bosonic density n_B, and $n_0(T)_{|n_\mathrm{B}}$ has to be calculated self-consistently, as explained in the next section. This point is crucial for the understanding of the temperature dependence of the S factor. For example,

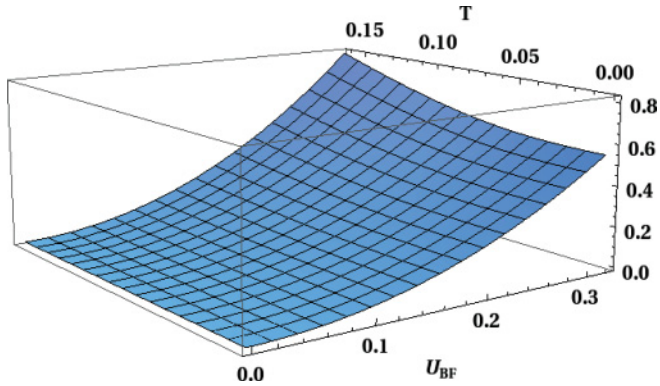

FIG. 3. (Color online) Sketch of the renormalization factor S as a function of Bose-Fermi coupling U_{BF} and temperature T ($k_{\mathrm{B}} = 1$) for fixed n_0. Energies are expressed in units of E_r^{F}.

for fixed values of n_0, S increases with temperature due to the increasing number of excited phonons, and therefore one would expect that the minimal slowing of the impurities occurs at $T = 0$, where only the zero- point motion of the Bogoliubov modes contributes. At the same time, however, n_0 decreases with T for fixed bosonic density n_{B} and the overall temperature dependence is determined by the competition between thermal depletion of the condensate and thermal excitation of the Bogoliubov modes. The energy spectrum of the Bogoliubov modes $\hbar\omega_{\mathbf{k}}$ acquires a temperature dependence through $n_0(T)_{|n_{\mathrm{B}}}$, which is missing in the standard condensed-matter case, where an increasing temperature only increases the phononic population and therefore the S factor [31]. This results in a major difference between the condensed-matter and present cases and also suggests the existence of a richer temperature dependence of polaronic effects in the Bose-Fermi mixtures realization. Indeed, it is possible that different mixtures (or even the same mixture for a different parameter range) show different slopes in $S(T)$ or even a nonmonotonic behavior. A sketch of the dependence of the renormalization factor S on T and U_{BF} for fixed n_0 is shown in Fig. 3. This would be the relevant case whenever the depletion can be neglected in the range of parameters under investigation and $n_0 \approx n_{\mathrm{B}}$. As shown in Sec. IV, this is not the case for the ^{87}Rb-^{40}K setup we considered. In any case, it is worth noting that also at $T = 0$ there is a sizable contribution to the S factor from all the Bogoliubov modes with quasimomenta within the FBZ.

Whenever the condensate is unaffected by the lattice, for example, in the case considered in [21], the Bogoliubov modes are labeled like plane waves and the sum runs over all the possible momenta $\mathbf{q}$. In the lattice the FBZ provides a natural cutoff to the high-energy phonons' contribution, while the analogous role of the physical cutoff in the continuum case is played by an additional exponential decay of the matrix elements M for large momenta. Indeed, the matrix elements M in the continuum case [21] are given by

$$M_{j,\mathbf{q}} \propto \sqrt{\frac{n_0\epsilon_{\mathbf{q}}}{(\hbar\omega_{\mathbf{q}})^3}}\, f_j(\mathbf{q}), \qquad (35)$$

where $\epsilon_{\mathbf{q}}$ is the free-particle dispersion, $\hbar\omega_{\mathbf{q}}$ is the energy of the Bogoliubov modes in the continuum [21],

$$f_j(\mathbf{q}) = \int d\mathbf{r}|\chi_j(\mathbf{r})|^2 \exp{(i\mathbf{q}\cdot\mathbf{r})}, \qquad (36)$$

and $\chi_j(\mathbf{r})$ is the Wannier wave function of the impurity localized at site j. Therefore, M is proportional to the Fourier transform with respect to the momentum $-\mathbf{q}$ of the density profile of the impurity in a Wannier state. Using a Gaussian approximation of the Wannier wave function, Eq. (36) reduces to

$$f_j(\mathbf{q}) \approx \left[\exp\left(-\frac{q^2\sigma^2}{4}\right)\right]^{\mathrm{D}} \exp{(i\mathbf{q}\cdot\mathbf{r})}, \qquad (37)$$

where σ is the width of the Gaussian wave function. Therefore the modulus of the matrix element M decays exponentially for $q \gg q_c = 1/\sigma$. In a deep lattice, typically $\sigma \ll l$ and the cutoff is much larger than the Brillouin zone. Therefore, the continuum theory cannot be used to quantitatively address the lattice case, not even by introducing an effective mass m_e to take the lattice into account. On the other hand, a situation in which the bosonic condensate is unaffected by the lattice would be more favorable to realize the *slow-impurity* regime described previously, since the impurity can be slowed down arbitrarily without affecting the bosonic kinetic energy. In current experiments on Bose-Fermi mixtures in a lattice, this is not the case, as explained in the next section, and the hopping parameters J_{F} and J_{B} are related to each other.

III. LIMITS OF VALIDITY OF THE THEORY

In this section, we analyze the assumptions we made in deriving our approach within a generic experimental setup for Bose-Fermi mixtures in optical lattices.

Since bosons and fermions are loaded into a single optical lattice of frequency ω_L, both species experience the same laser intensity I and $V^0_{\mathrm{B/F}} = \alpha_{\mathrm{B/F}}(\omega_L)I$, where $\alpha(\omega_L)$ is the atomic dynamic polarizability at the laser frequency. We define the dimensionless parameter

$$\gamma = \frac{s_{\mathrm{B}}}{s_{\mathrm{F}}} = \frac{\alpha_{\mathrm{B}}(\omega_L)m_{\mathrm{B}}}{\alpha_{\mathrm{F}}(\omega_L)m_{\mathrm{F}}}, \qquad (38)$$

which rules the ratio between the lattice depth experienced by bosons and fermions and therefore between their kinetic energies. For fixed atomic species, γ can be varied by changing the wavelength of the optical lattice.

In the presence of an interspecies Fano-Feshbach resonance, the Bose-Fermi scattering length a_{BF} can be tuned by a magnetic field B, while the Bose-Bose scattering length a_{B} can be considered in practice as constant in the same range of B. As already discussed previously, polarized fermions do not interact directly with each other.

In a real experiment, the atomic gas is confined in a trapping potential, which is not included in our approach. In the 3D case and for sufficiently shallow trapping potentials, our results can still be considered locally in a local-density-approximation (LDA) framework. The situation is very different in the two-dimensional case (2D). In this case, the trap radically modifies the properties of the system, providing a cutoff to the long-wavelength Goldstone modes, which would destroy the condensate at any finite temperature in the homogeneous case. Therefore, even though formally our approach to the homogeneous setup in the 2D case is well defined at $T = 0$, the Bogoliubov treatment of the bosonic component immediately breaks down at any finite temperature in that case, and therefore we cannot directly apply our findings to a 2D setup.

In practice (quasi-) 2D systems are obtained by strongly increasing the optical lattice in one direction (for example, in the z direction) such that the motion in this direction is frozen and only the zero-point motion has to be considered [33]. Under this condition, it is possible to distinguish between two regimes. Whenever $a_B \ll \sigma_z$, where σ_z is the typical width of the on-site wave function in the direction of the tight confinement, then the scattering process is still essentially 3D even if the motion is essentially two-dimensional. In this case, the 3D scattering length can be safely used and the local interaction U increases with the confinement in the z direction since the overlap between the local wave functions is increased. For the case $a_B \leqslant \sigma_z$, a more refined treatment is required [34]. In this case, strong modifications of the interaction both in modulus and sign can occur in the system. The main feature of interest for the present paper is that the confinement can actually be used to further tune the interaction between the bosons in order to access different regimes in Bose-Fermi mixtures. Even though the existence of a real condensate has been predicted for the case of trapped (quasi-) two-dimensional setups [35,36] at low temperature, the application of the Bogoliubov approach necessarily needs the trapping potential to be explicitly included in the treatment. Since in this case a full numerical solution of the corresponding Bogoliubov theory is required, we postpone the analysis of this interesting case to the future despite its intrinsic interest. On the other hand, we expect the general conclusions of the paper to still be valid as well in a 2D setup. For the reasons given previously, the approach is developed in the general case, when possible, but only results for the 3D case are shown.

A. Single-band Bose-Fermi–Hubbard model

Our first assumption is that the Bose-Fermi mixture under investigation is described using the single-band Bose-Fermi–Hubbard model (1). This requires that (i) higher band contributions, (ii) nonlocal interaction terms, and (iii) next-nearest-neighbor hopping terms are negligible in the parameter range under investigation. The first condition is particularly crucial for the bosonic component where the local density can take arbitrarily large values. For deep-enough optical lattices, a Gaussian approximation can be used to estimate on-site parameters for our model. In this approximation $W_j(\mathbf{x}) = \prod_{i=1}^{D} W_j^G(x_i)$, where $W_j^G(x_i)$ is a Gaussian wave function in one dimension ($x_i = x, y, z$ for $D = 3$) localized around the site j of the optical lattice; that is,

$$W_j^G(x_i) = (\pi\sigma^2)^{-1/4} \exp\left[-(x_i - R_j)^2/(2\sigma^2)\right], \quad (39)$$

where $\sigma_{B/F} = \sqrt{\hbar/m_{B/F}\omega_{B/F}}$ and $\hbar\omega_{B/F} = 2E_r^{B/F}\sqrt{s_{B/F}}$. In the same approximation,

$$U_{BB} = \frac{4\pi a_B}{m_B}\left(\frac{\pi^2 s_B}{4}\right)^{D/4}, \quad (40)$$

$$U_{BF} = \frac{2\pi a_{BF}}{m_r}\left(\frac{\pi}{s_B^{-1/2} + s_F^{-1/2}}\right)^{D/2}, \quad (41)$$

where we have set ($E_r^F = \hbar = l = 1$) and $m_r = 1/(m_B^{-1} + m_F^{-1})$, and a δ-like pseudopotential has been used to model the interaction between particles. The Gaussian approximation provides a very poor estimate of the hopping parameter, which can be expressed in a simple way for deep-enough lattices (large s) using the asymptotic solution of the Mathieu equation [37]:

$$J_B/E_r^B = \frac{4 s_B^{3/4}}{\sqrt{\pi}} \exp\left[-2\sqrt{s_B}\right], \quad (42)$$

and analogously for the fermionic component. In practice, however, this formula applies with reasonable accuracy only for $s \geqslant 10$, while for smaller s values the hopping term is overestimated and a direct numerical evaluation of the hopping parameter is required. Consistency with the model (1) requires [11]

$$a_{BF}, a_B \ll \sigma_{B/F} \ll l \quad \text{and} \quad \frac{U_{BB}}{2} n_B(n_B - 1) \ll \hbar\omega_B. \quad (43)$$

These conditions are reasonably well satisfied in practice if the on-site density of bosons n_B is not too large. For increasing lattice depth s, the hopping parameter J decreases exponentially, while the interaction term is slightly increased because of the increasing on-site overlap of the Wannier orbitals. It is important to point out that since both species move in the same optical lattice, the following relation applies for large s_F and fixed γ:

$$\frac{J_F}{J_B} = \frac{m_B}{m_F}\gamma^{-(3/4)} \exp\left[(2\sqrt{s_F})^{(\sqrt{\gamma}-1)}\right], \quad (44)$$

and therefore the ratio J_F/J_B is not constant for fixed γ but still depends on the lattice depth s_F.

B. Bogoliubov approach

Our approach is based on the possibility of describing the bosonic component of the mixture in the presence of static or slowly moving impurities within Bogoliubov approach. This requires in general that neither quantum nor thermal fluctuations are strong enough to substantially deplete the condensate; that is, the condensate fraction

$$\phi = N_0/N_B \leqslant 1 \quad (45)$$

needs to be close to 1.

The parameter α introduced in Eq. (12) quantifies the effect of the impurities on the condensate wave function, such that if $\alpha \ll 1$ we can expand the GP equation around the unperturbed solution in the absence of impurities. It is worth mentioning that α is markedly dependent on the dimension of the system since $\alpha_{3D} = \frac{|U_{BF}|(U_{BB}n_0)^{1/2}}{(2J_B)^{3/2}}$, while $\alpha_{2D} = \frac{|U_{BF}|}{2J_B}$; that is, α is independent of the Bose-Bose interaction U_{BB} and the condensate density n_0 in $D = 2$. The condition $\alpha \ll 1$ provides a constraint to the maximum value of the Bose-Fermi interaction where our theory can still be safely applied. Indeed, we have

$$\begin{cases} |U_{\mathrm{BF}}^{\max}| = 2J_{\mathrm{B}} & \text{in} \quad \mathrm{D}=2 \\ |U_{\mathrm{BF}}^{\max}| = \frac{(2J_{\mathrm{B}})^{3/2}}{(U_{\mathrm{BB}}n_0)^{1/2}} & \text{in} \quad \mathrm{D}=3 \end{cases}. \tag{46}$$

Strictly speaking, however, the condition $\alpha > 1$ does not imply that the bosonic condensate can no longer be described within the Bogoliubov approach, but only that the distortion of the condensate wave function due to the impurities is sizable and a full solution of the GP equation in the presence of impurities is required.

In this sense, we would expect that for $|U| > U_{\mathrm{BF}}^{\max}$ our theory still *qualitatively* applies, being, however, no longer quantitatively accurate, if the condensate fraction ϕ of the mixture is close enough to 1. Whenever ϕ is instead much smaller than 1, the Bogoliubov modes are no longer the appropriate quasiparticles to describe the bosonic system and an alternative treatment is needed.

As discussed in Sec. II, the Bogoliubov spectrum in our approach does not depend on the impurity distribution and therefore the properties of the Bogoliubov modes can be estimated by applying the Bogoliubov approach for the pure system. The condensate density n_0 is in general unknown and has to be calculated self-consistently within Bogoliubov theory for a given density n_{B} and temperature T. This requires adding one more equation to our approach; that is, the number equation of Bogoliubov theory in the condensed phase [26]:

$$n_{\mathrm{B}} = n_0 + \frac{1}{N_s}\sum_{\mathbf{k}\in\mathrm{FBZ}}{}' \left(\frac{\epsilon_{\mathbf{k}}^* + U_{\mathrm{BB}}n_0}{\hbar\omega_{\mathbf{k}}} N_{\mathbf{k}}(T) + \frac{\epsilon_{\mathbf{k}}^* + U_{\mathrm{BB}}n_0 - \hbar\omega_{\mathbf{k}}}{2\hbar\omega_{\mathbf{k}}} \right), \tag{47}$$

which we solve numerically. As already discussed, strictly in the homogeneous two-dimensional case, the Hohenberg-Mermin-Wagner theorem predicts that thermal fluctuations destroy the condensate for arbitrarily low temperatures and Eq. (47) cannot be used for finite T in $\mathrm{D}=2$.

C. ζ parameter

For $\alpha \ll 1$ and $\phi \approx 1$, the condensate in the presence of static impurities can be safely described within the Bogoliubov approach presented in Sec. II. Moreover, within these approximations the Hamiltonian description given in Eq. (27) also applies to the case of mobile impurities. However, in order to obtain a simple expression for the renormalization factor S in the single-impurity case, we had to assume that the fermionic hopping J_{F} is much smaller than the polaron shift E_p ($\zeta \ll 1$), where E_p has to be calculated from the theory. According to the definition given in Eq. (29), the polaron shift is given by $E_p = U_{\mathrm{BF}}^2 g$, where

$$g = \frac{1}{N_s}\sum_{\mathbf{k}\in\mathrm{FBZ}} \frac{n_0\epsilon_{\mathbf{k}}^*}{(\hbar\omega_{\mathbf{k}})^2}, \tag{48}$$

and only depends on the properties of the bosonic component. Therefore, since the polaron shift increases with the modulus of the Bose-Fermi interaction U_{BF}, the condition $\zeta \ll 1$ limits the minimum value of the Bose-Fermi interaction for which the formalism can be applied to $|U_{\mathrm{BF}}| \gg |U_{\mathrm{BF}}^{\min}| = \sqrt{J_{\mathrm{F}}/g}$.

Motivated by the large number of parameters present in the theory, we summarize the range of parameters where our approach can be applied by introducing the ratio

$$R = \left|\frac{U_{\mathrm{BF}}^{\max}}{U_{\mathrm{BF}}^{\min}}\right| = \left|\frac{a_{\mathrm{BF}}^{\max}}{a_{\mathrm{BF}}^{\min}}\right|, \tag{49}$$

such that for $R > 1$ there is a window of parameters where our approximations can be simultaneously satisfied. Intuitively, the condition $\zeta \ll 1$ requires that the fermionic impurities move much more slowly than the typical time taken by the phononic cloud to rearrange itself. Therefore, in general small values of the fermionic hopping J_{F} and γ are more favorable to our approach, meaning that mixtures where the bosons move faster than the fermions would be in general a better choice to reach the regime under investigation, even though the energy scales involved also crucially depend on the interaction U_{BB} and on the density n_{B} of the condensate.

IV. HOPPING RENORMALIZATION IN A THREE-DIMENSIONAL ^{87}Rb-^{40}K MIXTURE

To be more concrete in this section, we refer to the most commonly studied Bose-Fermi mixture, that is, a ^{87}Rb-^{40}K mixture loaded into an optical lattice in an experimental setup similar to the one used in Ref. [16]. For ^{87}Rb-^{40}K close to the interspecies Feshbach resonance, the bosonic scattering length is $a_{\mathrm{B}} \approx 100a_0 = 5.3$ nm, where a_0 is the Bohr radius. Increasing values of the Bose-Bose scattering length are generally unfavorable to our approach, since this increases both α and ζ [Eqs. (12) and (30)] and decreases the condensate fraction ϕ [Eq. (45)] if the other parameters stay unchanged. We found that smaller values of the Bose-Bose scattering length substantially enlarge the range of parameters where our approach is quantitatively valid. This suggests that different mixtures with smaller a_{B}, like the ^{6}Li-^{23}Na mixture theoretically studied in [19] ($a_{\mathrm{B}} \approx 53a_0 = 2.8$ nm for ^{23}Na [38]), could be even better candidates to realize the regime under investigation, if loaded into optical lattices. Since, however, experimental data about lattice Bose-Fermi mixtures involving those species are not yet available to the best of our knowledge, we decided in this work to focus on the ^{87}Rb-^{40}K mixture and postpone the analysis of other mixtures to future publications.

As explained in the previous section, we only present results for the case $\mathrm{D}=3$, and we first focus on the $T=0$ case. Due to the large value of the Bose-Bose scattering length, we have to restrict our analysis to rather small values of the parameter γ; that is, $\gamma = 1/3, 1/2$, where the bosons are substantially faster than the fermions [39]. Results are summarized in Fig. 4. As evident in Figs. 4(a) and 4(b) for both setups, the condensate fraction ϕ is relatively large and for $\gamma = 1/3$ is always above 90%. Small values of the lattice depth are in general favorable to the consistence of Bogoliubov approach since for a given a_{B} the bosonic system is less correlated. However, s_{F} cannot be reduced at will in order to stay in a parameter regime where the Hamiltonian in Eq. (1) applies. For $\gamma = 1/2$, the quantum depletion of the condensate is much larger and only for the lowest lattice depth under investigation ($s_{\mathrm{F}} = 10$–12) is the

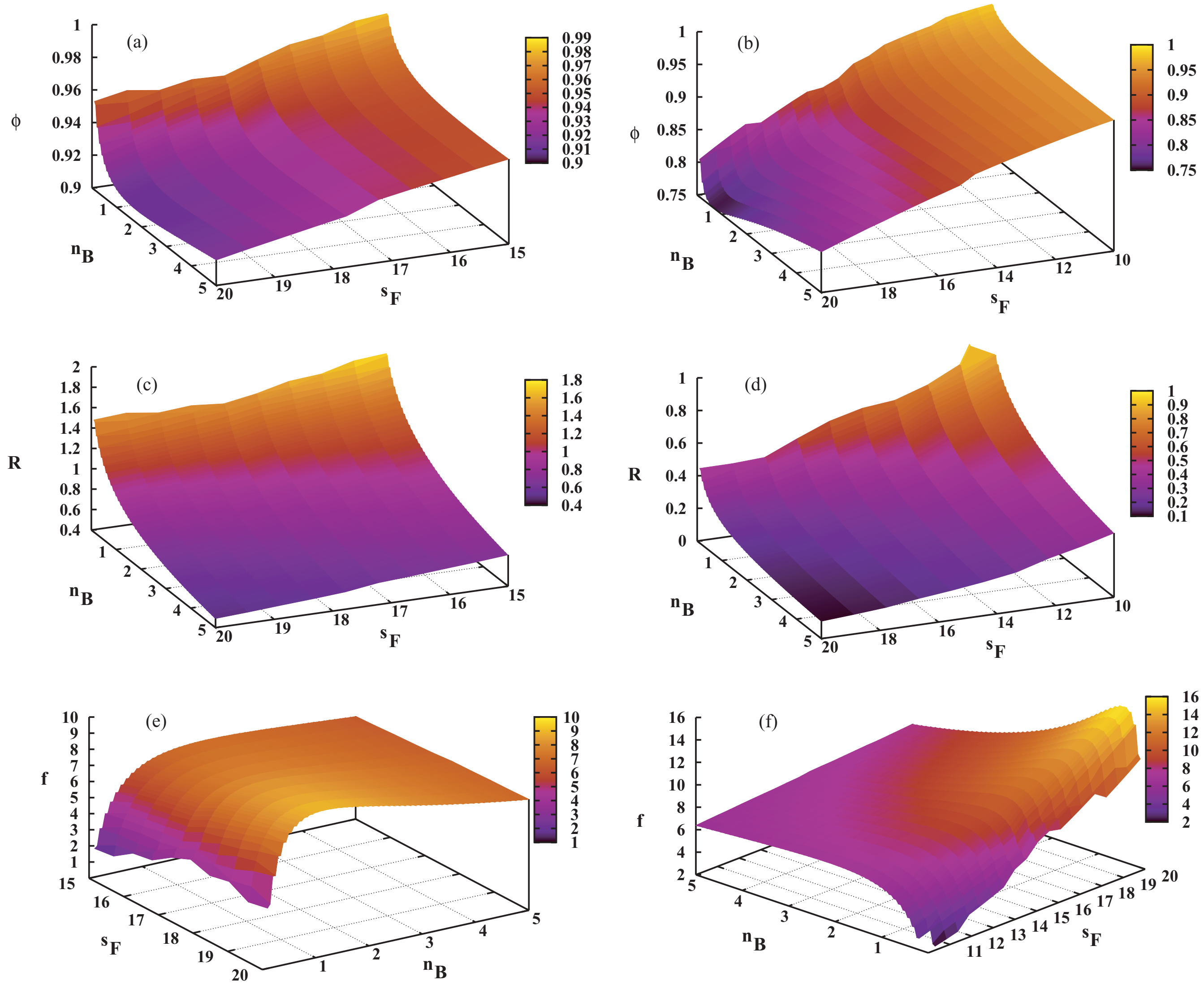

FIG. 4. (Color online) (a,b) Condensate fraction ϕ, (c,d) R parameter, and (e,f) f factor, defined in Eqs. (45), (49), and (34), respectively, for two 3D ^{87}Rb-^{40}K setups with (a,c,e) $\gamma = 1/3$ and (b,d,f) $\gamma = 1/2$ as a function of the bosonic density $n_{\rm B}$ and of the lattice depth $s_{\rm F}$ at $T = 0$. The term f is expressed in units of $(E_r^{\rm F})^{-2}$. The minimum value of the lattice depth $s_{\rm F}$ is chosen such that $s_{\rm B} \geqslant 5$ in both cases.

condensate fraction above 0.9. Considering the parameter R defined in Eq. (49) in Figs. 4(c) and 4(d), it is evident that only for $\gamma = 1/3$ there is a sizable window of parameters where our approach is quantitatively valid, that is, $R > 1$. We realized, however, that the strongest limitations arise from the condition $\alpha \ll 1$, which constrains the maximum value of the Bose-Fermi interaction, rather than $\zeta \ll 1$. As discussed in the previous section, whenever $\alpha \ll 1$ is violated but the Bogoliubov approach is still expected to apply, we expect our results to be qualitatively valid and therefore show the results for $\gamma = 1/2$ in the plot for comparison. Low bosonic densities and shallow lattices are favorable to the theory. Indeed, by reducing the lattice depth $s_{\rm F}$, the range of densities where the theory applies is substantially increased.

In Figs. 4(e) and 4(f), we plotted results for the parameter $f[n_0(n_{\rm B}),s_{\rm F}]_{|T=0}$ defined in Eq. (34), recalling that the renormalized hopping $J_{\rm F}^r$ is related to f by the simple relation $J_{\rm F}^r = J_{\rm F} e^{-U_{\rm BF}^2 f}$. Both setups show a similar behavior of the f parameter, though the numerical values are quite different for different setups and the data for $\gamma = 1/2$ are only shown for comparison since $R < 1$ in that case. For fixed (and small) values of the lattice depth $s_{\rm F}$, f increases quite rapidly with the density $n_{\rm B}$ and then saturates. For larger values of $s_{\rm F}$ instead, f shows a maximum at intermediate densities and then slightly decreases. However, the decrease at large $n_{\rm B}$ and $s_{\rm F}$ and the nonmonotonic behavior could also result from a loss of accuracy in our approach, since in that region of parameters $R < 1$ in both setups.

For finite temperature, we concentrate on a specific set of parameters; that is, we choose $\gamma = 1/3, s_{\rm F} = 15$ $(s_{\rm B} = 5)$, and low-density $n_{\rm B} = 0.1$, which is the regime where our approach quantitatively applies in a larger parameter range. In a real experiment where the hopping renormalization is measured by observing the cloud expansion, the initial configuration of the gas would be inhomogeneous due to the confining potential. This would mean that, once the trapping potential is

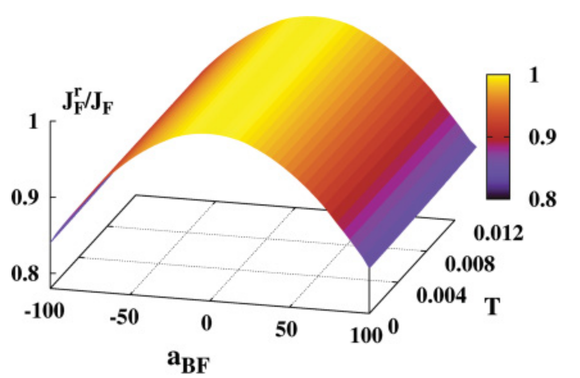

FIG. 5. (Color online) Hopping renormalization J_F^r/J_F for $n_B = 0.1, \gamma = 1/3$, and $s_F = 15$ as a function of the Bose-Fermi scattering length expressed in units of Bohr radii a_0 and of the temperature T expressed in units of fermionic recoil energy E_r^F.

removed, different parts of the fermionic cloud would expand in the lattice with a different renormalized hopping J_F^r due to local value of the bosonic density n_B. We found that the renormalization factor S in general increases with increasing density n_B, which would imply that the edge of the cloud, where n_B is smaller, will expand faster. The results shown in Fig. 5 for the hopping renormalization J_F^r/J_F as a function of the temperature T and of the Bose-Fermi scattering length a_{BF} are representative of the experimental situation at the edge of an expanding cloud and provide an upper bound for the renormalized hopping. The temperature range is chosen such that $T < T^{max} = E_p(U_{BF}^{max})$, where E_p is the polaron shift, and $\phi > 0.9$. We expect our estimate to be quantitatively more accurate for $40a_0 > |a_{BF}| > 60a_0$.

As evident from Fig. 5, for fixed temperature the hopping renormalization as a function of a_{BF} takes in our approach a Gaussian shape and the renormalized hopping decreases with the modulus of the Bose-Fermi scattering length, such that $J_F^r/J_F \approx 0.95$ for $|a_{BF}| \approx 50a_0$ at the border of the bosonic cloud ($n_B = 0.1$). A much larger renormalization effect is expected for larger densities.

The effect of the temperature is very small in the range of parameters investigated and it is hardy visible in Fig. 5. We found that for fixed a_{BF} the renormalization factor S slightly *decreases* (J_F^r/J_F increases) with increasing temperature, due to the dominant effect of the thermal depletion of the condensate. This trend is opposite to the one naively expected (see Fig. 3) and also in contrast with the condensed-matter case, where S increases with T [31]. It is may be worth mentioning that for higher densities (not shown) we found a nonmonotonic behavior in $J_F^r/J_F(T)$, due to the increasing relevance of the thermal population of Bogoliubov modes at larger T. Since, however, large densities are generally unfavorable to our approach, this effect could result as well from a loss of accuracy.

V. CONCLUSIONS

In this work, we described the emergence of polaronic effects in Bose-Fermi mixtures in optical lattices. Our approach is closely related to Ref. [21] and is based on using the Bogoliubov approach to describe the bosonic component of the mixture, considering first static and then slowly moving fermionic impurities. The main difference from the case addressed in Ref. [21] is that in our case both species are substantially affected by the same optical lattice, as in currently available experimental setups. We showed that the effect of the optical lattice on the bosonic condensate does not radically change the main conclusions for the homogeneous case [40]. However, the range of experimental parameters where the approach applies is substantially modified whenever fermions and bosons move through the same optical lattice, since their hopping parameters J_F and J_B are related to each other.

For static impurities weakly coupled to the condensate ($\alpha \ll 1$), we have shown that an approximate treatment of the GP equation for the condensate wave function is possible and the Bogoliubov spectrum does not depend on the distribution of the fermionic impurities. However, we expect the Bogoliubov treatment of the condensate in the presence of impurities to still be valid for larger α values, provided the condensate fraction ϕ is large. Consequently, our results are expected to be qualitatively valid even beyond the regime $\alpha \ll 1$. We postpone a more quantitative treatment of the the regime with larger α and $\phi = O(1)$, which would require a fully self-consistent GP + Bogoliubov approach, to a future work.

We derived an analytical expression for the hopping renormalization of a single impurity in the regime $\zeta \ll 1$ (slow impurity). This effect can be measured in experiments involving strongly imbalanced ($N_F/N_B \ll 1$) Bose-Fermi mixtures in an optical lattice, by observing the expansion of the fermionic cloud in the lattice when the trapping potential is suddenly removed [25]. Within our approach, the fermionic hopping in this regime is *exponentially* renormalized due to polaron formation; that is, $J_F^r = J_F e^{-S}$. In the relevant parameter range, the renormalization factor S is found to be proportional to the square of the Bose-Fermi interaction. Therefore, we expect for J_F^r a Gaussian dependence on the Bose-Fermi interaction U_{BF} (or equivalently a_{BF}) and no dependence on the sign of U_{BF} (a_{BF}). This would lead to very strong experimental signatures of polaron physics once the considered regime is reached.

The temperature dependence of the renormalization factor S results from a competition between the thermal depletion of the condensate, which induces a temperature dependence on the Bogoliubov spectrum $\hbar\omega_{\mathbf{k}}$ through the condensate density $n_0(T)_{|n_B}$, and the thermal population of phononic modes. This dependence of the phononic spectrum on the temperature is missing in the standard condensed-matter case, where the renormalization factor S always increases with T.

In order to provide a better connection with experiments, we discussed the relevant parameter regime for a 3D ^{87}Rb-^{40}K mixture in an optical lattice. Due to the large value of the bosonic scattering length a_B, we have considered setups where $J_F \ll J_B$ and with low bosonic densities. We found a sizable renormalization effect already for $n_B = 0.1$. For a fixed value of the Bose-Fermi scattering length a_{BF}, the temperature dependence of the renormalized hopping is found to be opposite to the one naively expected. The renormalization factor S slightly *decreases* for increasing T, being dominated by the thermal depletion of the condensate rather than by the increasing phononic population. This represents a major difference with the standard condensed-matter case.

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[1] A. Lanzara *et al.*, Nature (London) **412**, 510 (2001).
[2] J. T. Devreese and A. S. Alexandrov, Rep. Prog. Phys. **72**, 066501 (2009).
[3] R. Jördens, N. Strohmaier, K. Gunter, H. Moritz, and T. Esslinger, Nature (London) **455**, 204 (2008).
[4] U. Schneider, L. Hackermüller, S. Will, Th. Best, I. Bloch, T. A. Costi, R. W. Helmes, D. Rasch, and A. Rosch, Science **322**, 1520 (2008).
[5] G.-B. Jo, Y. R. Lee, J. H. Choi, C. A. Christensen, T. H. Kim, J. H. Thywissen, D. E. Pritchard, and W. Ketterle, Science **325**, 1521 (2009).
[6] N. V. Prokof'ev and B. V. Svistunov, Phys. Rev. B **77**, 020408 (2008).
[7] C. Mora and F. Chevy, Phys. Rev. A **80**, 033607 (2009).
[8] A. Schirotzek, C. H. Wu, A. Sommer, and M. W. Zwierlein, Phys. Rev. Lett. **102**, 230402 (2009).
[9] S. Nascimbene, N. Navon, K. J. Jiang, L. Tarruell, M. Teichmann, J. McKeever, F. Chevy, and C. Salomon, Phys. Rev. Lett. **103**, 170402 (2009).
[10] G. D. Mahan, *Many-Particle Physics*, 3rd ed. (Kluver Academic/ Plenum, New York, 2000), Chap. 7.
[11] A. Albus, F. Illuminati, and J. Eisert, Phys. Rev. A **68**, 023606 (2003).
[12] I. Titvinidze, M. Snoek, and W. Hofstetter, Phys. Rev. Lett. **100**, 100401 (2008).
[13] I. Titvinidze, M. Snoek, and W. Hofstetter, Phys. Rev. B **79**, 144506 (2009).
[14] K. Günter, T. Stöferle, H. Moritz, M. Köhl, and T. Esslinger, Phys. Rev. Lett. **96**, 180402 (2006).
[15] S. Ospelkaus, C. Ospelkaus, O. Wille, M. Succo, P. Ernst, K. Sengstock, and K. Bongs, Phys. Rev. Lett. **96**, 180403 (2006).
[16] Th. Best, S. Will, U. Schneider, L. Hackermüller, D. van Oosten, I. Bloch, and D.-S. Lühmann, Phys. Rev. Lett. **102**, 030408 (2009).
[17] L. Mathey, D.-W. Wang, W. Hofstetter, M. D. Lukin, and E. Demler, Phys. Rev. Lett. **93**, 120404 (2004).
[18] F. M. Cucchietti and E. Timmermans, Phys. Rev. Lett. **96**, 210401 (2006).
[19] J. Tempere, W. Casteels, M. K. Oberthaler, S. Knoop, E. Timmermans, and J. T. Devreese, Phys. Rev. B **80**, 184504 (2009).
[20] M. Bruderer, A. Klein, S. R. Clark, and D. Jaksch, Phys. Rev. A **76**, 011605 (2007).
[21] M. Bruderer, A. Klein, S. R. Clark, and D. Jaksch, New J. Phys. **10**, 033015 (2008).
[22] L. J. LeBlanc and J. H. Thywissen, Phys. Rev. A **75**, 053612 (2007).
[23] J. Catani, G. Barontini, G. Lamporesi, F. Rabatti, G. Thalhammer, F. Minardi, S. Stringari, and M. Inguscio, Phys. Rev. Lett. **103**, 140401 (2009).
[24] G. Lamporesi, J. Catani, G. Barontini, Y. Nishida, M. Inguscio, and F. Minardi, Phys. Rev. Lett. **104**, 153202 (2010).
[25] S. Will and I. Bloch (private communication).
[26] D. van Oosten, P. van der Straten, and H. T. C. Stoof, Phys. Rev. A **63**, 053601 (2001).
[27] K. Burnett, M. Edwards, C. W. Clark, and M. Shotter, J. Phys. B **35**, 1671 (2002).
[28] A. L. Fetter, Ann. Phys. **70**, 67 (1972).
[29] K. Huang and H.-F. Meng, Phys. Rev. Lett. **69**, 644 (1992).
[30] T. Holstein, Ann. Phys. **8**, 325 (1959).
[31] T. Holstein, Ann. Phys. **8**, 343 (1959).
[32] I. J. Lang and Y. A. Firsov, Zh. Eksp. Teor. Fiz. **43**, 1843 (1962).
[33] Z. Hadzibabic, P. Krüger, M. Cheneau, S. P. Rath, and J. Dalibard, New J. Phys. **10**, 045006 (2008).
[34] D. S. Petrov and G. V. Shlyapnikov, Phys. Rev. A **64**, 012706 (2001).
[35] D. S. Petrov, M. Holzmann, and G. V. Shlyapnikov, Phys. Rev. Lett. **84**, 2551 (2000).
[36] C. Gies, B. P. van Zyl, S. A. Morgan, and D. A. W. Hutchinson, Phys. Rev. A **69**, 023616 (2004).
[37] W. Zwerger, J. Opt. B: Quantum Semiclass. Opt. **5**, S9 (2003).
[38] C. Samuelis, E. Tiesinga, T. Laue, M. Elbs, H. Knockel, and E. Tiemann, Phys. Rev. A **63**, 012710 (2000).
[39] The condition $\gamma = 1/3, 1/2$ can be realized by choosing $\lambda \approx 764$ nm, 762 nm, respectively. These values of the lattice wavelength are, however, rather close to the atomic resonances, where a substantial heating effect from photon scattering is expected. This could make the experimental observation more difficult on long time scales.
[40] During the completion of this work, we became aware that similar expressions for the matrix elements M in Eq. (22) have been very recently derived independently in M. Bruderer, T. H. Johnson, S. R. Clark, D. Jaksch, A. Posazhennikova, and W. Belzig, e-print arXiv:1007.3828, for mixtures of fermions and bosons in different optical lattices where tilting of the lattice for fermions was considered.