Polaron physics in optical lattices

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(Received 6 March 2007; published 13 July 2007)

We investigate the effects of a nearly uniform Bose-Einstein condensate (BEC) on the properties of im-
mersed trapped impurity atoms. Using a weak-coupling expansion in the BEC-impurity interaction strength,
we derive a model describing polarons, i.e., impurities dressed by a coherent state of Bogoliubov phonons, and
apply it to ultracold bosonic atoms in an optical lattice. We show that, with increasing BEC temperature, the
transport properties of the impurities change from coherent to diffusive. Furthermore, stable polaron clusters
are formed via a phonon-mediated off-site attraction.

DOI: 10.1103/PhysRevA.76.011605

The lack of lattice phonons is a distinguishing feature of
optical lattices, i.e., conservative optical potentials formed by
counterpropagating laser beams, and contributes to the excel-

lent coherence properties of atoms trapped in them [1]. However,
some of the most interesting phenomena in condensed
matter physics involve phonons, and thus it is also desirable
to introduce them in a controlled way into optical lattices.
Recently, it has been shown that immersing an optical lattice
into a Bose-Einstein condensate (BEC) leads to interband
phonons, which can be used to load and cool atoms to ex-
tremely low temperatures [2].

Furthermore, polarons aggregate on adjacent lattice sites into
stable clusters, which are not prone to loss from inelastic
collisions. Since these phenomena are relevant to the physics
of conduction in solids, introducing phonons into an optical
lattice system may lead to a better understanding of high-
temperature superconductivity [3,5] and charge transport in
organic molecules [6]. Additionally, this setup may allow the
investigation of the dynamics of classically indistinguishable
particles [7].

Experimental progress in trapping and cooling atoms has
recently made a large class of interacting many-body quan-
tum systems [8] accessible. For instance, the formation of
repulsively bound atom pairs on a single site has been demon-

strated [9], and strongly correlated mixtures of degenerate
quantum gases have been realized [10]. In such Bose-Fermi
mixtures, rich phase diagrams, including charge and spin
density wave phases [11,12], pairing of fermions with bosons
[13], and a supersolid phase [14], can be expected. Here we
instead consider one atomic species, denoted as the impuri-
ties, confined to a trapping potential, for example an optical
lattice, immersed in a nearly uniform BEC, shown in Fig. 1.

Based on a weak-coupling expansion in the BEC-impurity
interaction strength, we derive a model in terms of polarons,
which are composed of impurity atoms dressed by a coherent
state of Bogoliubov phonons [3,4]. The model also includes
attractive impurity-impurity interactions mediated by the
phonons [15,16]. An essential requirement for our model is
that neither interactions with impurities nor the trapping poten-
tial confining the impurities impairs the ability of the sur-
rounding gas to sustain phononlike excitations. The first con-
dition limits the number of impurity atoms [10], whereas the
latter requirement can be met by using a species-specific opti-
cal lattice potential [17]. Moreover, unlike in the case of
self-localized impurities [18], we assume that the one-

FIG. 1. (Color online) A quantum degenerate gas confined to an
optical lattice is immersed in a much larger BEC. For increasing
BEC temperature $T$, a crossover from coherent to diffusive hopping,
characterized by $J$ and $E_p$, respectively, can be observed. The
phonon-induced interaction potential $V_{ij}$ leads to the formation of
off-site polaron clusters, separated by a gap $E_p$ from the continuum
of unbound states.
A common approach to find the elementary excitations of the BEC in the presence of impurities is to solve the Gross-Pitaevskii equation (GPE) [19] for the full system, i.e., for $\kappa \neq 0$, and to subsequently quantize small oscillations around the classical ground state. To obtain a quantum description of the impurity dynamics, we instead solve the GPE without taking $H_0$ into account, and express the BEC deformations around the impurities as coherent states of Bogoliubov phonons. Specifically, we write $\hat{\phi}(r) = \phi_0(r) + \delta \hat{\phi}(r)$, with $\phi_0(r) = \phi_0^0(r)$ the solution of the GPE for $\kappa = 0$. Provided that the impurity-boson coupling is sufficiently weak, i.e., $|\kappa|/gn_0(r) \ll 1$, with $\xi(r) = \hbar/\sqrt{m_\phi gn_0(r)}$ the healing length, $n_0(r) = \phi_0^0(r)$, and $D$ the number of spatial dimensions, we expect that the deviation of $\hat{\phi}(r)$ from $\phi_0(r)$ is of order $\kappa$, i.e., $\langle \delta \hat{\phi}(r) \rangle \approx \kappa$, where $\langle \cdot \rangle$ stands for the expectation value. We insert $\phi_0(r) + \delta \hat{\phi}(r)$ into the Hamiltonian $H_0 + H_1$, keep terms up to second order in $\kappa$, and obtain the linear term $\kappa \int dr \chi(r) \hat{\chi}(r) \phi_0^0(r)[\delta \hat{\phi}(r) + \delta \hat{\phi}(r)]$, in addition to the standard constant and quadratic terms in $\delta \hat{\phi}(r)$ and $\delta \hat{\phi}(r)$, since $\phi_0(r)$ is no longer the ground state of the system.

In order to diagonalize the quadratic terms in $\delta \hat{\phi}(r)$ and $\delta \hat{\phi}(r)$, we use the expansion $\delta \hat{\phi}(r) = \sum_\mu \mu_\mu(r) \hat{b}_\mu - \nu_\mu(r) \hat{b}_\mu^\dagger$, where $\mu_\mu(r)$ and $\nu_\mu(r)$ are the solutions of the Bogoliubov–de Gennes equations [19] for $\kappa = 0$, and $\hat{b}_\mu^\dagger$ are the bosonic Bogoliubov annihilation (creation) operators, labeled by the quantum numbers $\mu$. We assume that the mode functions $\eta_\mu(r)$ are localized on a length scale much smaller than is set by $V_{\text{ext}}(r)$, and that $\int dr \eta_\mu(r)^2 \eta_\mu(r)^2 = 0$ for $\nu \neq \tau$, i.e., the probability densities $\eta_\mu(r)^2$ for different mode functions deviate appreciably from zero only within mutually exclusive spatial regions. In this case, $\int dr \phi_0^0(r)[\mu_\mu(r) - \nu_\mu(r)] \eta_\mu(r) \eta_\mu(r)^* = 0$ and $\int dr n_0^\mu(r) \eta_\mu(r) \eta_\mu(r)^* = 0$ hold for $\nu \neq \tau$, and hence the non-diagonal impurity-phonon coupling is negligible. The total Hamiltonian can thus be rewritten in the form of a Hubbard-Holstein model [20] $\hat{H} = \hat{H}_0 + \sum_\nu V_\nu \omega_\nu (M_\nu \hat{b}_\nu + M_\nu^* \hat{b}_\nu^\dagger) \hat{n}_\nu + \sum_\nu \Xi_\nu \hat{b}_\nu^\dagger + \sum_\nu \Xi_\nu \hat{b}_\nu$, with $\omega_\nu$ the energies of the Bogoliubov excitations, the number operator $\hat{n}_\nu = \hat{b}_\nu^\dagger \hat{b}_\nu$, the dimensionless matrix elements $M_\nu = (\kappa/\hbar \omega_\nu) \int dr \phi_0^0(r) \times [\mu_\mu(r) - \nu_\mu(r)] \eta_\mu(r)^2$, and the mean field shift $\Xi_\nu = \kappa \int dr n_0^\mu(r) \eta_\mu(r)^2$. We obtain an effective Hamiltonian $\hat{H}_\text{eff}$ including corrections to $\phi_0^0(r)$ of order $\kappa$ by applying the unitary Lang-Firsov transformation $[3,4]$ $\hat{H}_\text{eff} = \hat{U} \hat{H} \hat{U}^\dagger$, with $\hat{U} = \exp[\sum_\nu \omega_\nu (M_\nu^* \hat{b}_\nu + M_\nu^* \hat{b}_\nu^\dagger) \hat{n}_\nu]$, which yields $\hat{H}_\text{eff} = \hat{H}_0 + \sum_\nu \left( \epsilon_\nu - \epsilon_\nu^\prime \right) \hat{n}_\nu - \sum_\nu \epsilon_\nu \hat{b}_\nu^\dagger \hat{b}_\nu - \frac{1}{2} \sum_{\nu \neq \tau} V_\nu \hat{n}_\nu \hat{n}_\tau + \sum_\mu \hbar \omega_\mu \hat{b}_\mu^\dagger \hat{b}_\mu$.

The transformed impurity Hamiltonian $\hat{U} \hat{H}_0 \hat{U}^\dagger$ is obtained using the relation $\hat{U} \hat{a}_\nu^\dagger \hat{U}^\dagger = \hat{a}_\nu^\dagger \hat{X}_\nu^\dagger$, where $\hat{X}_\nu^\dagger = \exp[\sum_\mu (M_\nu^* \hat{b}_\mu + -M_\nu \hat{b}_\mu^\dagger)]$ is a Glauber displacement operator that creates a coherent phonon cloud, i.e., a BEC deformation, around the impurity. In the limit where the BEC adjusts instantaneously to the impurity configuration, polarons created by $\hat{a}_\nu^\dagger \hat{X}_\nu^\dagger$ are the appropriate quasiparticles, and $\hat{H}_\text{eff}$ describes a non retarded interaction with the potential $V_\nu = \sum_\mu \omega_\mu (M_\nu \hat{b}_\mu + M_\nu^* \hat{b}_\mu^\dagger) \hat{n}_\mu$, the polaronic level shift $E_\nu = \sum_\mu \hbar \omega_\mu |M_{\nu \mu}|^2$ is equal to the characteristic potential energy of an impurity in the deformed BEC.

We now turn to the specific case of bosons loaded into an optical lattice immersed in a homogeneous BEC [2]. In the tight-binding approximation, the impurity dynamics is well described by the Bose-Hubbard model $\hat{H}_J = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + (U/2) \sum_{i,j} \hat{n}_i (\hat{n}_i - 1) + \mu \sum_{i,j} \hat{n}_i$, where $\mu$ describes the energy offset, $U$ the on-site interaction strength, and $J$ the hopping matrix element between adjacent sites [8,21]. The modes of the lattice atoms are Wannier functions $\eta_i(r)$ of the lowest Bloch band localized at site $j$, and $\langle i,j \rangle$ denotes the sum over nearest neighbors. Noting that $\langle \hat{U}, \hat{n}_j \rangle = 0$, we find

$$\hat{U} \hat{H}_J \hat{U}^\dagger = -J \sum_{\langle i,j \rangle} (\hat{X}_i \hat{a}_i^\dagger \hat{X}_j + \frac{1}{2} U \sum_{j} \hat{n}_j (\hat{n}_j - 1) + \mu \sum_{j} \hat{n}_j,$$

with the corresponding matrix elements $M_{\nu \mu} = \kappa \langle \eta_i \eta_j \rangle f_{\nu \mu}(q)$, where $q$ is the phonon momentum, $v_F = (\hbar q^2/2m_\phi)^{1/2}$ the free particle energy, $\hbar \omega_\nu = \sqrt{\epsilon(q) + 2gn_0}$ the Bogoliubov dispersion relation, and $f_{\nu \mu}(q) = \Omega^{-1/2} \int dr \eta_\mu(r) \eta_\mu(r)^* \exp(iq \cdot r)$, with $\Omega$ the quantization volume. We note that, for $|q| \ll 1/\xi$, we have $M_{\nu \mu} \approx f_{\nu \mu}(q)/\sqrt{|q|}$, whereas, for $|q| \gg 1/\xi$, one obtains $M_{\nu \mu} \approx f_{\nu \mu}(q)/q^2$.

The Hamiltonian $\hat{H}_\text{eff}$ describes the dynamics of hopping polarons according to an extended Hubbard model [8], provided that $c \gg aJ/\hbar$, with $c \sim \sqrt{gn_0} m_\phi$ the phonon velocity and $a$ the lattice spacing. We gain qualitative insight into the dependence of $V_{ij}$ and the constant polaronic level shift $E_\nu = E_p$ on the system parameters by considering a one-dimensional quasi-BEC in the thermodynamic limit. We assume a sufficiently deep lattice to approximate the Wannier functions by Gaussians of width $\sigma \ll \xi$, and find $V_{ij} = (\sigma^2/\xi^2) e^{-2|j-i|\sigma^2/\xi^2}$ and $E_p = \sigma^2/2 \xi^2$. We note that the interaction between impurities is always attractive. More importantly, for realistic experimental parameters, $\xi \sim a$, and hence the off-site parameters $V_{ij,\neq i}$ are non-negligible. This interaction potential is a direct consequence of the local deformation of the BEC around each impurity, as shown in Fig. 1. For a set of static impurities at positions $x_j = aj$, the overall deformation of the BEC density to order $\kappa$ is given by $n(x) = n_0 + \sum_\mu \omega_\mu (\hat{b}_\mu^\dagger \hat{b}_\mu$, where $n_0 = \int dx n(x)$, and $\omega_\mu = gn_0$ for $\nu = 0$. We therefore consider coherent hopping of polarons at small BEC temperatures $k_B T \ll E_p$, where incoherent phonon scattering is highly suppressed. Provided that $\xi = J/E_p \ll 1$, we can apply the so-called strong-coupling theory [5], and treat the hopping term in Eq. (2) as a perturbation. Including terms of first order in $\xi$, we obtain the impurity Hamiltonian $\hat{H}_J = -J \sum_{\langle i,j \rangle} \hat{X}_i \hat{a}_i^\dagger \hat{X}_j$.
\[
\hat{H}^{(1)} = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \tilde{\mu} \sum_{j} \hat{n}_j + \frac{1}{2} \tilde{U} \sum_{j} \hat{n}_j (\hat{n}_j - 1) - \frac{1}{2} \sum_{i\neq j} V_{ij} \hat{n}_i \hat{n}_j,
\]

(3)

with \(\tilde{\mu} = \mu + \kappa n_0 - E_p\), \(\tilde{U} = U - 2E_p\), and \(\tilde{T} = T / \langle \hat{X}^2 \rangle\). Here \(\langle \cdot \rangle\) denotes the average over the thermal phonon distribution and \(i, j\) are nearest neighbors. We find \(\langle \hat{X}^2 \rangle\) = \(\exp[-\sum_{\mathbf{q} \neq 0} |M_{\mathbf{q}0}|^2 (1 - \cos(\mathbf{q} \cdot \mathbf{a})) / (2N_\mathbf{q} + 1)]\), with \(\mathbf{a}\) the position vector connecting two nearest neighbor sites and \(N_\mathbf{q} = (\exp(h^2 q^2 / 2kT) - 1)^{-1}\). Thus, the hopping bandwidth decreases exponentially with increasing coupling constant \(\kappa\) and temperature \(T\).

At high temperatures \(E_p \ll k_B T \ll k_B T_c\) (with \(T_c\) the critical temperature of the BEC) inelastic scattering, in which phonons are emitted and absorbed, becomes dominant, and thus the transport of atoms through the lattice changes from being purely coherent to incoherent. We investigate this crossover by deriving a generalized master equation (GME) for a single particle starting from \(\hat{H}_{\text{eff}}\) in Eq. (1). Using the Nakajima-Zwanzig projection method [22], we find that the occupation probabilities \(P_i(t)\) at site \(i\) and time \(t\) evolve according to the GME [23]

\[
\frac{\partial P_i(t)}{\partial t} = \int_0^t ds \sum_j \{ W_{ij}(s) P_j(t-s) - W_{ji}(s) P_i(t-s) \},
\]

(4)

where the effect of the phonon bath is encoded in the memory functions \(W_{ij}(s)\), which are symmetric in \((i,j)\). To first order in \(\zeta\), thus keeping only nearest-neighbor correlations, we find

\[
W_{ij}(s) = 2 \left( \frac{J}{\hbar} \right)^2 \text{Re} \left[ \exp \left( 2 \sum_{\mathbf{q} \neq 0} |M_{\mathbf{q}0}|^2 [1 - \cos(\mathbf{q} \cdot \mathbf{a})] \right) \times \left( N_{\mathbf{q}0} + 1 \right) (\exp(-i\mathbf{q} \cdot \mathbf{r}_0) - 1) \right] \cdot \left( N_{\mathbf{q}0} + 1 \right) (\exp(-i\mathbf{q} \cdot \mathbf{r}_0) - 1) \right],
\]

(5)

and \(W_{ij}(s) = 0\) if \(i, j\) are beyond nearest neighbors. The nontrivial part of \(W_{ij}(s)\) takes the values \(2(\hbar / J)^2\) at \(s = 0\) and \(2(J / \hbar)^2\) in the limit \(s \rightarrow \infty\). In the regime \(k_B T \ll E_p\), we have \(\tilde{T} \sim J\), and the memory function \(W_{ij}(s)\) is well approximated by \(2(\hbar / J)^2 \Theta(s)\) [with \(\Theta(s)\) the Heaviside step function], which describes purely coherent hopping in agreement with \(\hat{H}^{(1)}\). For \(E_p \ll k_B T \ll k_B T_c\), we observe that \(\tilde{T} \sim J\), and \(W_{ij}(s)\) drops off sufficiently fast for the Markov approximation to be valid, as illustrated in Fig. 2(a). In this case one can replace \(P_i(t-s)\) by \(P_i(t)\) in Eq. (4) and after integration over \(s\) the GME reduces to a standard Pauli master equation \(\hat{\rho}/\partial t = -i[\hat{H}, \hat{\rho}]/\hbar\) [24] describing purely incoherent hopping.

The hopping rate is of the form \(w_{ij} \sim J^2 \exp(-E_a/k_B T_0) / (\hbar \sqrt{\kappa T_0})\) [4,20], where \(E_a \sim E_p\) is the activation energy.

The temperature-dependent crossover from coherent to diffusive hopping in a quasi-one-dimensional (1D) system is apparent in the evolution for a time \(\tau \sim 1/w_{ij}\) of a particle initially localized at lattice site \(j = 0\). The mean-squared displacement of the lattice atom, \(\langle \hat{r}^2 \rangle = \sum_i f_i P_i(t)\), can be decom-
FIG. 3. (Color online) (a) Energy spectrum of three polarons in a 1D optical lattice. The solid line shows the lowest energy band $E_k(k)$ characterizing off-site three-polaron clusters. The lattice (wavelength $\lambda=790$ nm, $M=31$ sites, periodic boundary conditions) contains $^{133}$Cs atoms with $J=7.5 \times 10^{-3}E_R$, $U=50E_p$, and $\kappa/E_p\lambda=1.05 \times 10^{-2}$. The BEC consists of $^{87}$Rb atoms with $n_0=5 \times 10^6$ m$^{-3}$ and $g/E_p\lambda=4.5 \times 10^{-2}$. (b) Probability of finding a three-polaron cluster (solid line) or a two-polaron cluster (dashed line) versus temperature. The parameters are $g/E_p\lambda=6.5 \times 10^{-2}$, $\kappa/E_p\lambda=1.32 \times 10^{-3}$, $U=2.2E_p$, $M=27$, and the rest as for (a).

significantly increased $P_2$ compared to the values shown in Fig. 3(b).

The clustering of polarons leads to their mutual exponential localization. This is illustrated by the density-density correlations $\langle \hat{n}_i\hat{n}_j \rangle$ for the three-polaron cluster in Fig. 4(a). With increasing attractive interaction $V_{ij}$, the mutual localization gets stronger, leading to an increased broadening of the momentum distribution, as shown in Fig. 4(b). This allows polaron clusters to be identified in time of flight experiments. We note that the transition from a superfluid to a Mott insulator also leads to broadening of the momentum distribution as, e.g., observed in [10]. However, using Bragg spectroscopy [9] would allow the unambiguous distinction of boson clustering from this transition.

![Energy spectrum of three polarons](image1)

![Probability of finding a three-polaron cluster](image2)

FIG. 4. (Color online) (a) Density-density correlation in a system of three polarons indicating the formation of off-site three-polaron clusters. (b) Corresponding momentum distribution $\langle n_j \rangle$. $\kappa/E_p\lambda=\{0.4, 0.6, 1.8, 10.1, 12.1\} \times 10^{-2}$ where a higher value corresponds to a more localized correlation in (a) and a more spread distribution in (b). The other parameters are $g/E_p\lambda=6.5 \times 10^{-2}$, $M=27$, $U=3E_p$, and the rest as in Fig. 3(a).

We have demonstrated that the dynamics of bosonic impurities immersed in a BEC is accurately described in terms of polarons. We found that spatial coherence is destroyed in hopping processes at large BEC temperatures, while the main effect of the BEC at low temperatures is to reduce the coherent hopping rate. Furthermore, the phonons induce off-site interactions leading to the formation of stable clusters, which are not affected by loss due to inelastic collisions. Using the techniques introduced in this paper, qualitatively similar phenomena can also be shown to occur for fermionic impurities. In either case these effects can be controlled by external parameters and lie within the reach of current experimental techniques.

M.B. thanks Danail Obreschkow for fruitful discussions. This work was supported by the U.K. EPSRC through QIP IRC (Grant No. GR/S82176/01) and Project No. EP/ C51933/1, the EU through the STREP project OLAQUI, the Berrow Society (M.B.), and the Keble Association (A.K.).