Localization of an impurity particle on a boson Mott insulator background

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We investigate the behavior of a single particle hopping on a three dimensional cubic optical lattice in the presence of a Mott insulator of bosons in the same lattice. We calculate the critical interaction strength between the impurity and background bosons, beyond which there is bound state (polaron) formation. We give exact results in the limit of a perfect Mott insulator, where polaron formation is equivalent to impurity localization. We calculate the effects of lattice anisotropy, higher impurity bands, and fluctuations of the Mott insulator on the localization threshold. We argue that our results can be checked experimentally by RF spectroscopy of impurity particles.

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I. INTRODUCTION

Recent experiments using cold atoms in optical lattices have displayed remarkable versatility, creating highly controllable, isolated, low temperature environments where ideas about many particle quantum mechanics can be tested. With improvement over the control of system parameters, as well as advancement of novel measurement techniques such as noise correlations, it seems plausible that a great variety of models will be realized in optical lattices. The precision of optical lattice experiments presents another challenge for theory. Measurements of effects that are beyond the simplest descriptions such as mean field theory, are becoming possible.

One of the new classes of quantum models realized by cold gas experiments is the mixture of different species of atoms. Boson-boson mixtures as well as boson-fermion mixtures have been created. It is now also possible to selectively turn on optical lattice potentials for any of the species forming the mixture.

The possibility of experimental realization of atomic gas mixtures stimulated a lot of theoretical interest. From the theory point of view, mixtures are appealing as they can display some qualitatively new physics stemming from simple ideas in many body theory. There is possibility of pairing due to mediated interactions, formation of composite particles similar to molecules, large counterflows of different species or even countersuperfluidity. There are also ideas to simulate random potentials using one species as the disorder potential for the others. Two recent experiments about boson-fermion mixtures have shown that the optical lattice experiments are advanced enough so that all these theoretical ideas may now be tested in the laboratory.

The parameter space for mixtures is very large, with many possible phases and a complicated phase diagram. The phase diagram of mixtures changes remarkably depending on the strength and type of optical lattices, number of components, nature of interactions, and the identity of the particles. While more general investigations of this parameter space, which point out novel phases, are very useful, in this paper, we concentrate on a simple limit and provide some exact results. Experimentally, it would be easy to check such results and gain a better understanding of the various effects that may be present in the system.

We investigate the limit where one bosonic species interacts with a single particle of another species. While the identity of the external particle does not matter in what follows, we refer to it as the fermion for convenience. All the results of the paper are valid for a bosonic impurity as well. We assume that both species share the same lattice potential and that the lattice potential is deep enough so that only one band of the lattice is populated. The Hubbard-type Hamiltonian for this system can be written as

$$H = -t_b \sum_{<i,j>} b_i^\dagger b_j + \frac{U_{bb}}{2} \sum_i n_i(n_i - 1) - \mu_b \sum_i n_i - t_f \sum_{<i,j>} f_i^\dagger f_j + U_{bf} \sum_i n_i f_i^\dagger f_i,$$

where $b^\dagger$, $b$ and $f^\dagger$, $f$ are the bosonic and impurity creation and annihilation operators respectively; $n_i = b_i^\dagger b_i$ is the on-site number operator for the bosons and $<i,j>$ represents a sum over nearest neighbors. The strength of the tunnelling terms are characterized by hopping matrix elements $t_b$ for bosons and $t_f$ for the fermion. $U_{bb}$ and $U_{bf}$ are the on-site interaction strengths between bosons and between a boson and a fermion respectively.

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Depending on the ratio between the tunnelling strength and the interaction for bosons, the system may either form a superfluid (SF) or a Mott insulator (MI) state [21]. While the localization problem can be studied in both regimes, we can provide exact results only for the Mott insulator case. In this paper, we concentrate on the problem in the Mott regime as the problem is qualitatively different from that of a superfluid interacting with an impurity. Thus, we consider \( t_b/U_{bb} \ll 1 \), give exact results only in the limit \( t_b/U_{bb} = 0 \) and calculate corrections due to finite boson hopping. For a Mott insulator with \( n_0 \) bosons per site, the chemical potential is constrained to
\[
U_{bb}(n_0 - 1) \leq \mu_b \leq U_{bb}n_0. \tag{2}
\]

With these considerations for bosons, the fermion can show two qualitatively different behaviors. It can either behave like a free fermion with its wavefunction stretching throughout the system, or it may create a defect in the Mott insulator and form a bound state with this defect. We calculate the critical interaction strength that separate these two regimes. In Section III we study the case of a perfect Mott insulator and obtain the phase diagram for localization of the impurity; in Section IV we generalize this exact result to an anisotropic lattice where hopping strength in one direction is different from the other two. We consider the effect of higher impurity bands in Section IV. In Section V we calculate the change in the fermion hopping strength due to fluctuations in the Mott insulator background. We summarize our results and discuss experimental methods to measure this bound state formation in Section VI.

II. LOCALIZATION IN A PERFECT MOTT INSULATOR

In this section, we calculate the critical interaction strength for bound state (polaron) formation in the limit that the boson Mott insulator is perfect, i.e. the hopping strength for bosons is zero (\( t_b/U_{bb} = 0 \)). We relax this assumption in Section V and analyze the effects of fluctuations in the Mott background. When boson hopping is neglected the Mott insulator background becomes almost inert for the fermion, presenting a spatially independent mean field energy shift. In this case the fermion will move with the dispersion relation
\[
E_k = t_f \left[ 6 - 2 \sum_{i=x,y,z} \cos(k_i a) \right], \tag{3}
\]
where \(-\pi/a < k_i \leq \pi/a\) is the crystal momentum of the fermion in the \( i \) direction and \( a \) is the lattice constant. We cannot expect this delocalized behavior of the fermion to continue if the interactions between the background bosons and the fermion become very strong. Let us assume that the fermion and the bosons attract each other, i.e. \( U_{bf} < 0 \). In this case, it would be energetically favorable to put more bosons at a lattice site and bind the fermion to these bosons. This will only happen at a critical interaction strength, beyond which the energy gained by boson-fermion attraction is larger than the sum of the kinetic energy cost of localizing the fermion and the interaction energy cost of introducing more bosons.

This critical interaction strength can then be found by investigating the single particle Hamiltonian
\[
H = -t_f \sum_{<i,j>} f_i^\dagger f_j - V f_0^\dagger f_0, \tag{4}
\]
where we take the site at which the defect is formed as the origin and assume that the defect represents a localized attractive potential \( -V \) to the fermion. We can then ask for which value of \( V \) there will be a bound state in the spectrum. This is the discrete version of the problem of existence of a bound state for a localized potential well [22]. Just like the continuum version, in one and two dimensional lattices there is a bound state for an infinitesimally small attractive potential. In three dimensions, however, there is a certain critical value below which there is no bound state. In the case of a finite attractive potential, the dispersion relation takes the following implicit form
\[
\phi_k \left[ \hat{E} + 2 \sum_i \cos(k_i a) \right] = -\hat{V} \psi_0, \tag{5}
\]
where \( \hat{E} = E/t_f \) and \( \hat{V} = V/t_f \) are the scaled quantities and \( \phi_k = \sum_i \psi_i e^{-ik \cdot r_i} \) is the Fourier transform of the particle’s wave function. We obtain the relation between the binding energy and the attractive potential by taking the Fourier transform of Eq. (5)
\[
\frac{1}{V} = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{1}{\left( 6 - 2 \sum_i \cos \theta_i \right) + \epsilon}. \tag{6}
\]
FIG. 1: Binding energy $\epsilon$ of the impurity as a function of $V/t_f$. The critical interaction strength where the localization begins can also be obtained from the figure, i.e. $\epsilon = 0$ for $V/t_f \lesssim 3.96$.

where $\theta_i = k_i a$ and we take

$$\tilde{E} = -6 - \epsilon,$$

with $\epsilon > 0$ being the binding energy. When $\epsilon = 0$, i.e. at the localization threshold, the above integral can be evaluated exactly [23] and the critical value at which the localization takes place is

$$\tilde{V}_c = \frac{2}{(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}) [\frac{3}{2} K(k_0)]^2} = 3.95678,$$

where $k_0^2 = [(2 - \sqrt{3})(\sqrt{3} - \sqrt{2})]^2$ and $K$ is the complete elliptic integral of the first kind. For nonzero $\epsilon$, the integral was evaluated by Joyce [24]. Using this result, the potential is obtained as

$$\tilde{V} = \frac{2}{(1 - \eta)^{1/2}} \frac{1}{1 - \frac{1}{4}\eta} \frac{1}{(\frac{2}{3})^2} K(k_+ K(k_-),$$

where $\eta = -16z(\sqrt{1-z} + \sqrt{1-9z})^{-2}$, $z = 1/\omega^2 = 1/(3 + \epsilon/2)^2$, and $k_\pm^2 = \frac{1}{4} \left[ \frac{1}{2} \eta \sqrt{1 - 1/4\eta} - (1 - 1/2\eta) \sqrt{1 - \eta} \right]$. In the limit of large binding energy, $\epsilon \gg 1$, we obtain a linear relation $\tilde{V} \propto \epsilon$, which is expected as the particle is strongly localized at a single lattice site.

The exact evaluation of the integral above allows us to calculate not only the critical boundary but also the binding energy $\epsilon(V/t_f)$ of the bound state (Fig. 1). We now translate our one particle results to the many particle case. Let us first assume that the fermion-boson interaction is attractive, $U_{bf} < 0$. In this case the simplest defect would be to introduce one more boson, thus the attractive potential seen by the fermion will be $V = [U_{bf}].$ However, to introduce one more boson to a Mott insulator with $n_0$ particles per lattice site would cost energy, $U_{bb}n_0 - \mu$. Thus, the phase boundary between the free fermion state and the bound state of the fermion and one bosonic defect (polaron) is given by

$$\epsilon = \frac{-U_{bf}}{t_f} - \frac{U_{bb}n_0 - \mu}{t_f}.$$

This is by no means the only defect that can be created in the Mott insulator. If the boson-fermion attraction is strong enough, it becomes energetically favorable to attract more bosons and form a bound state of two bosons and one fermion. The phase boundary for such a defect can be decided by comparing the energy of this state with the energy of the bound state of one boson and one fermion. Thus, the equation for phase boundary is

$$\epsilon = \frac{-U_{bf}}{t_f} - \frac{U_{bb}(2n_0 + 1) - 2\mu}{t_f}.$$
FIG. 2: Phase diagram for $\mu = (n_0 - 1/2)U_{bb}$. Numbers in each region show how many extra particles ($U_{bf} < 0$) or holes ($U_{bf} > 0$) are attracted to the localization site. The region marked as $\geq 7$ contains all the phases with seven or more extra bosons (holes). Phase diagram for this value of $\mu$ is symmetric around $U_{bf} = 0$. For small boson-boson repulsion $U_{bb}$, even for small $|U_{bf}|$ values, large number of bosons are attracted. While this phase diagram is independent of $n_0$, the number of holes that are attracted is limited by $n_0$.

One can similarly find the boundaries for bound states with higher number of bosons.

Another kind of defect would present itself for repulsive interactions, $U_{bf} > 0$. For sufficiently strong repulsive interactions it would be preferable to create a hole in the Mott insulator state and bind the fermion to this hole. The corresponding phase boundary is given by

$$\epsilon \left( \frac{U_{bf}}{t_f} \right) = -U_{bb}(n_0 - 1) + \mu / t_f \tag{12}$$

Similar to the attractive interactions, it is possible to form bound states of the fermion with more holes. One can continue to deplete the Mott state until all the $n_0$ bosons are removed from the defect site. After this point it would be preferable to deplete bosons from the neighboring sites. We have, however, not included such states in our phase diagram. In Figs. 2, 3, and 4, we present three phase diagrams for different chemical potentials. Fig. 2 indicates that when $U_{bf}$ is close to zero, even for small $|U_{bf}|$ values, the fermion can be bound to a large number of bosons. If we take $\mu = (n_0 - 1/4)U_{bb}$ as in Fig. 3, the symmetry around $U_{bf} = 0$ is broken and for the repulsive interactions it is harder to attract holes. Fig. 4 represents the opposite case ($\mu = (n_0 - 3/4)U_{bb}$) where stronger interactions are required to attract particles.

We believe that the phase diagram can be checked experimentally. While it would be possible to modify $U_{bf}$ by an interspecies Feshbach resonance, an easier route would be to change $t_f$ which is controlled by the strength of the optical lattice. The localized impurity states can be distinguished from free fermion states as their mean field shifts would be different; in principle, RF spectroscopy \cite{25,26} would directly detect the difference in the mean field shift. Although the calculation was carried out for a single impurity, we expect these results to be quantitatively correct for a small density of fermionic impurities over a bosonic Mott insulator background. Essentially, if the inverse of Fermi momentum is much larger than the lattice spacing, then the fermions would hardly affect each other’s behavior.

In this section, we obtained the phase diagram for the interaction of one impurity particle with a perfect Mott insulator. In the next three sections, we investigate how this ideal situation is affected by lattice anisotropy, higher impurity bands, and fluctuations of the Mott insulator.

### III. EFFECTS OF LATTICE ANISOTROPY

In the optical lattice experiments, it is possible to change the strength of the laser beams forming the lattice, hence realize a model system where the lattice is not isotropic. For a quantitative comparison with experiment, it is
FIG. 3: Phase diagram for $\mu = (n_0 - 1/4)U_{bb}$. Symmetry in Fig. 2 is broken and particle attraction is easier than the hole attraction, since the chemical potential is increased with respect to the symmetry point. To attract a hole one needs higher boson-fermion interaction $|U_{bf}|$ for the same $U_{bb}$.

FIG. 4: Phase diagram for $\mu = (n_0 - 3/4)U_{bb}$. As opposed to Fig. 3 to attract a particle one needs higher boson-fermion interaction.

necessary to take this effect into account. We assume that the hopping strength for the fermion is different in one direction compared to the other two directions and calculate the effect of such anisotropy on the phase diagram of the previous section.

The localization threshold for the anisotropic case can also be calculated analytically. Thus, in the following discussion we need not assume that the anisotropy of the lattice is small. As a simple limit, we obtain the two dimensional lattice localization problem as the layers are decoupled. For that limit, even the smallest attraction between the fermion and bosons causes bound state formation. As the coupling between the two dimensional layers is increased the critical interaction needed for bound state formation monotonically increases.

Because of the anisotropy, the single particle Hamiltonian in Eq. (4) is modified as

$$H = -t_f \sum_{<i,j>} f_i^\dagger f_j - t'_{fz} \sum_{<i,j>} f_{iz}^\dagger f_{jz} - V f_0^\dagger f_0,$$

(13)
where we take the hopping term in the $z$ direction to be $t_f' \neq t_f$. We obtain the relation between $\tilde{V}$ and $\epsilon$ as

$$
\frac{1}{\tilde{V}} = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{1}{(2\pi)^3} \left[ 4 - 2 \sum_{i=x,y} \cos \theta_i + 2 \tau (1 - \cos \theta_z) \right] + \epsilon,
$$

where $\tilde{E} = -4 - 2\tau - \epsilon$ and $\tau = t_f'/t_f$. For $\epsilon = 0$ this integral can be evaluated exactly \cite{22}. The critical value for the localization is found to be

$$
\tilde{V}_c = \frac{2}{w} \left( \sqrt{2} \sqrt{1 + \tau - \sqrt{2 + \tau}} \left( \frac{\tau}{2} \right)^2 K [k_+ (\tau)] K [k_- (\tau)] \right).
$$

where

$$
k_\pm (\tau) = \left[ \frac{1}{\tau} \left( \sqrt{2} \sqrt{1 + \tau - \sqrt{2 + \tau}} \right) \sqrt{2 + \tau} \pm \sqrt{2} \right]^2.
$$

As $\tau$ increases, i.e. the anisotropy of the lattice increases, the critical value for the potential increases and the localization becomes more difficult (Fig. 5). As $t_f' \rightarrow 0$, the system becomes two dimensional and there is no threshold for localization, as expected. For large $t_f'/t_f$, $V_c \sim \sqrt{t_f'} t_f$, which gives $V_c \rightarrow 0$ in the one dimensional limit, $t_f \rightarrow 0$. Moreover, it is possible to evaluate the integral for nonzero $\epsilon$ \cite{22}, yielding

$$
\tilde{V} = \frac{2 \left( \sqrt{1 - (2 - \tau)^2 z} + \sqrt{1 - (2 + \tau)^2 z} \right)}{w \left( \frac{\tau}{2} \right)^2 K [k_+ (\tau)] K [k_- (\tau)]},
$$

where $w = 2 + \tau + \epsilon/2$, $z = 1/w^2$ and

$$
k_\pm^2 = \frac{1}{2} - \frac{1}{2} \left[ \sqrt{1 - (2 - \tau)^2 z} + \sqrt{1 - (2 + \tau)^2 z} \right]^{-3}
\times \left\{ \begin{array}{l}
\sqrt{1 + (2 - \tau) \sqrt{z}} \sqrt{1 - (2 + \tau) \sqrt{z}} + \sqrt{1 - (2 - \tau) \sqrt{z}} \sqrt{1 + (2 + \tau) \sqrt{z}} \\
\pm 16 z + \sqrt{1 - \tau^2 z} \left[ \sqrt{1 + (2 - \tau) \sqrt{z}} \sqrt{1 + (2 + \tau) \sqrt{z}} + \sqrt{1 - (2 - \tau) \sqrt{z}} \sqrt{1 - (2 + \tau) \sqrt{z}} \right]^2 
\end{array} \right\}.
$$

Using this exact result, the phase diagram can be obtained for arbitrary $\tau$. In Fig. 6 we display the phase diagram for $\tau = 1.5$. Comparing Fig. 6 with Fig. 2 (isotropic case) we see that the phase boundaries are closer to the $U_{bf}$ axis.

**IV. EFFECTS OF HIGHER IMPURITY BANDS**

An important point one always has to keep in mind about the optical lattice experiments is that the effective Hubbard models, such as Eq. 4, are obtained by projecting the system into the lowest band of the lattice \cite{21}. This procedure is expected to describe the low energy physics as long as the band gaps are larger than the temperature and interaction scales in the problem. In the equivalent language of Wannier functions, this condition corresponds to requiring the Wannier function of each lattice site to be undisturbed by interactions.

In the context of the current problem, we discussed the critical hopping strength that is needed to localize the impurity particle to a small region, which is of the order of one lattice site. The precise determination of the Hubbard model parameters such as $U_{bf}$ depends on the microscopic model one starts from. For the Hubbard model to work correctly, the Wannier functions for the impurity must be unchanged even if the impurity particle is localized to one lattice site. As a localized impurity attracts (or repels) extra particles (holes) to its localization site, one may expect the on-site wave function of the localized particle to be different from the Wannier functions at other lattice sites. This is essentially considering the coupling of the localized particle to higher impurity bands, and should be a small effect controlled by the parameter $U_{bf} \Delta_f$, where $\Delta_f$ is the width of the first band gap of the impurity bands. Thus, the effect we are considering in this section would be important only if the impurity particle is highly mobile in the lattice, while the interaction between the background particles and the impurity is strong enough to localize the particle (Fig. 7).
FIG. 5: The critical value of interaction $V_c/t_f$ as a function of lattice anisotropy characterized by $t'_f/t_f$ (Eq. (15)). If the hopping parameter $t'_f$ increases, anisotropy of the lattice increases and the localization becomes more difficult. $\tau = t'_f/t_f = 1$ gives $V_c/t_f$ for the isotropic case.

FIG. 6: Phase diagram in the presence of lattice anisotropy ($\tau = t'_f/t_f = 1.5$ and $\mu = (n_0 - 1/2)U_{bb}$). To be compared with Fig. 2 ($\tau = 1$, $\mu = (n_0 - 1/2)U_{bb}$). One can see that anisotropy with $\tau > 1$ causes the localization threshold to move to higher values of $|U_{bf}|$.

FIG. 7: Schematic representation of the effect of higher impurity bands to the hopping parameter. If the localized impurity attracts extra particles (holes) to the localization site, the local wave function of the impurity particle changes. Then the hopping parameter for this site is different from that for the other sites.
FIG. 8: The critical value of interaction $V_c/t_f$ as a function of $\tau = t'_f/t_f$ (Eq. 22). As the ratio of the hopping parameters $\tau$ increases, localization occurs for smaller values of the interaction.

In such a case, the system can still be modelled by a Hubbard model where the hopping strength between the localization site and its neighbors ($t'_f$) is different from the hopping strength between any other neighboring sites in the lattice ($t_f$). These hopping strengths can once again be calculated by looking at the overlaps of the localized wavefunctions between neighboring lattice sites [20].

In this case, we take the single particle Hamiltonian as

$$H = -t_f \sum_{\langle i,j \rangle} f_i^\dagger f_j - (t'_f - t_f) \sum_{\langle i,m \rangle} f_i^\dagger f_m (\delta_{i0} + \delta_{m0}) - V f_0^\dagger f_0.$$  \hspace{1cm} (19)

Calculations similar to those performed in the previous sections yield

$$\tilde{V} = \frac{1 - \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{d\theta_x d\theta_y d\theta_z}{(2\pi)^3} \frac{2(\tau - 1)}{6-2} \sum_i \cos \theta_i}{\int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{d\theta_x d\theta_y d\theta_z}{(2\pi)^3} \frac{1}{6-2} \sum_i \cos \theta_i + \epsilon},$$  \hspace{1cm} (20)

where $\tilde{E} = -6 - \epsilon$. Evaluating this integral exactly [27], we obtain the relation

$$\tilde{V} = \frac{2\tau}{(1-\eta)^{1/2} \omega \left(1 - \frac{1}{4\eta}\right)^{1/2} \left(\frac{2}{\pi}\right)^2 K(k_+)K(k_-)} - 2(\tau - 1) \omega,$$  \hspace{1cm} (21)

where $\eta = -16z(\sqrt{1-z} + \sqrt{1-9z})^{-2}$, $z = 1/\omega^2 = 1/(3 + \epsilon/2)^2$, and $k_+^2 = \frac{1}{2} \left[1 \pm \eta \sqrt{1 - \frac{1}{4\eta} - (1 - \frac{1}{2}\eta) \sqrt{1 - \eta}}\right]$. When $\epsilon = 0$, the critical value for the potential is found to be

$$\tilde{V}_c \approx 3.95678[1 - 0.51622(\tau - 1)].$$  \hspace{1cm} (22)

As can be seen in Fig. 8, the coupling to higher impurity bands can substantially change the critical value for localization. If $U_{bf} < 0$, we expect a narrowing of the local wave function (as in Fig. 7), then $t'_f < t_f$ and consequently localization is harder $V_c(\tau) > V_c(\tau = 1)$. Similarly if $U_{bf} > 0$ we expect easier localization. In general one would then expect each different polaron state to have a different $\tau$ value. Still to gain a basic understanding of this effect we obtain the phase diagram (Fig. 9) using constant value of $\tau = 1.5$.

V. EFFECTS OF FLUCTUATIONS OF THE MOTT INSULATOR

The ideal Mott insulator state is achieved only when the boson hopping term in the Bose-Hubbard Hamiltonian is zero. When there is a small but nonzero hopping probability for the bosons, the ground state of the MI contains
virtual particle and hole excitations. When $t_b/U_{bb}$ gets larger, these excitations gain more amplitude and will finally destroy the order in the MI, and cause a transition to the SF state.

In the previous sections, we considered the MI to be a perfect insulator by setting boson hopping to zero. In this section, we consider the effects of small but nonzero hopping on our calculations. We always work in the limit that the boson hopping $t_b$ is the smallest energy scale of the system and require that the system be away from the MI-SF transition boundaries. Under these conditions, we can use perturbation theory to investigate the effects of particle and hole fluctuations on the localization of the impurity particle.

There are two main consequences of turning on the boson hopping. First, the compound object formed by the impurity and the extra bosons (polaron) will become mobile. The width of the polaron band will be proportional to $t_f t_b^\delta$, where $\delta$ is the number of extra bosons (or holes) forming the polaron. As $t_b$ is the smallest energy scale in the problem, this polaron mobility effect will be small, especially for polarons containing more than one boson or hole. In other words as $t_f \gg t_b$, the fermion is much more mobile than the boson (or the combined polaron). The mobility of the polaron will then have a small effect on the localization problem considered above.

The second effect is the change of effective mass (or effective hopping $t_f$) of the impurity particle due to scattering from the fluctuations of the MI. The first contribution to such processes will be proportional to $(U_{bf}/U_{bb})^2$ for the fermion to scatter from a particle-hole pair, and $(t_b/U_{bb})^2$ for the pair to be excited. Because of the presence of $U_{bf}^2$, which is large in the limit that we are interested in, this second effect will be dominant over polaron mobility. We should also mention that it is only lowest orders of the perturbation theory that these two effects can be considered separate processes.

To the lowest order in $t_b/U_{bb}$, the boson wavefunction can be written as: $| \Psi \rangle = |MI\rangle + \frac{t_b}{U_{bb}} \sum_{<i,j>} b_i^\dagger b_j |MI\rangle$. The state of the system without boson-fermion interaction is then $| \Psi \rangle | k \rangle$, where $| k \rangle$ is the wavefunction of a fermion moving with lattice momentum $\vec{k}$.

By treating the boson-fermion interaction as a perturbation

$$\hat{V} = U_{bf} \sum_i n_i f_i^\dagger f_i,$$

we can write the second order energy shift as

$$\Delta^{(2)} = \sum_{\alpha \neq \beta, k'} \left| \langle k' | \langle MI | b_i^\dagger b_j \hat{V} [ | MI \rangle + \frac{t_b}{U_{bb}} \sum_{<i,j>} b_i^\dagger b_j | MI \rangle ] | k \rangle \right|^2,$$

where the only non-vanishing term is
\[ \langle k' \mid MI \mid b_\beta^\dagger b_\gamma^\dagger t_b \sum_{<i,j>} b_i^\dagger b_j \mid MI \mid k \rangle = \frac{t_b}{U_{bb}} \frac{U_{bf}}{N} n_0(n_0 + 1) [e^{i(k^\prime - k) \cdot r_\beta} - e^{i(k^\prime - k) \cdot r_\alpha}]. \tag{25} \]

Again considering the lowest non-vanishing order contribution we get:

\[
\Delta^{(2)} = \frac{t_b^2 U_{bf}^2}{U_{bb}^2 N^2} n_0^2(n_0 + 1)^2 \sum_{<\alpha, \beta>, k'} \frac{2 - 2 \cos[(k^\prime - k) \cdot (\vec{r}_\beta - \vec{r}_\alpha)]}{\varepsilon_k - (U_{bb} + \varepsilon_{k'})}
\]
\[\rightarrow U_{bf}^2 t_b^2 n_0^2(n_0 + 1)^2 \int_{-\pi}^{\pi} \frac{d^3k'}{(2\pi)^3} \frac{12 - 4 \sum_i \cos[(k^\prime - k)_i]}{2t_f \sum_i \cos(k_i) - \cos(k_i)} - U_{bb} \]
\[\simeq -U_{bf}^2 t_b^2 n_0^2(n_0 + 1)^2 \left[ 12 - 28 \frac{t_f}{U_{bb}} \sum_i \cos(k_i) \right], \quad \frac{t_f}{U_{bb}} \ll 1. \tag{26} \]

Hence, we see that the first effect of the fluctuations of the MI is to renormalize the hopping strength of the impurity particle to

\[ t_f \rightarrow t_f \left( 1 - 14n_0^2(n_0 + 1)^2 \frac{U_{bf}^2 t_b^2}{U_{bb}^4} \right). \tag{27} \]

Essentially a decreasing \( t_f \) means the effective mass of the particle is larger, and it becomes easier to localize the particle. Thus, the effects of boson hopping on all the situations discussed in previous sections can be obtained by scaling the phase diagrams by the renormalized value of \( t_f \).

**VI. CONCLUSIONS**

We study the localization of a single impurity particle in a lattice containing a Mott insulator of bosons. This is a simple limit of the complex physics of the Bose-Hubbard model for mixtures of different atomic species. The impurity particle has two distinct types of behavior; it may either move freely throughout the lattice or may choose to localize at a certain lattice site by attracting extra bosons or holes. In the limit of a perfect Mott insulator, we calculate the boundary between these two phases as well as the number of extra bosons (holes) forming the bound state exactly. Our result for the phase diagram is given in Fig. 2.

We believe that this phase diagram can be checked experimentally. In recent experiments boson-fermion mixtures were created in the parameter regimes that we consider in this paper. If the density of fermions is small enough, one can disregard the many-particle nature of the fermions and consider the localization problem for one of them. To determine whether a fermion is localized, RF spectroscopy would be an ideal tool. The mean-field shift of the fermion becomes of the order of few lattice sites. Thus, we expect our calculations to accurately reflect the transition boundaries, especially for transitions between different polaron states.

The calculations presented in this paper were carried out with the assumption of a homogenous infinite system. In cold gas experiments there is always a confining trap, which in general complicates the correspondence between the infinite system predictions and experimental results. However, when a lattice boson system is driven deep into the MI regime, the density profile of the system consists of MI plateaus separated by thin SF regions. Within each MI region, the fermion would see a flat interaction potential, and when the fermion is localized, the width of the wavefunction of the fermion becomes of the order of few lattice sites. Thus, we expect our calculations to accurately reflect the transition boundaries, especially for transitions between different polaron states.

After the ideal case, we consider three effects which may play a role in the experiments. The first case we consider is the possibility of tunnelling anisotropy. As the strength of the lattice is determined by the laser intensity (and beam waist), experiments occasionally have such anisotropy. We generalize the exact results to this case and find that it becomes easier to localize the impurity when the system becomes more two dimensional, as expected. Next, we consider the effect of higher bands of the impurity particle. We argue that this effect can be taken into account by modifying the hopping strengths between the localization site and its neighbors, and obtain the phase diagram. Finally, we consider the effect of small but finite tunnelling strength for the bosons forming the MI, and calculate the effective hopping strength for the impurity particle in the presence of fluctuations.

We believe that our exact results about impurity localization on a Mott insulator background provide a starting point for the investigation of the complex phase diagram of mixtures in optical lattices.
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[1] M. Greiner, O. Mandel, T. Esslinger, T.W. Hansch, and I. Bloch, Nature 415, 39 (2002)
[2] B. Paredes, A. Widera, V. Murg, O. Mandel, S. Folling, I. Cirac, G.V. Shlyapnikov, T.W. Hasch, and I. Bloch, Nature 429, 277 (2004)
[3] J.K. Chin, D.E. Miller, Y. Liu, C. Stan, W. Setiawan, C. Sanner, K. Xu, and W. Ketterle, Nature 443, 961 (2006)
[4] T. Stoferle, H. Moritz, K. Gunter, M. Kohl, and T. Esslinger, Phys. Rev. Lett. 96, 030401 (2006)
[5] M. Anderlini, P.J. Lee, B.L. Brown, J. Sebby-Strabley, W.D. Phillips, and J.V. Porto, Nature 448, 452 (2007)
[6] K.D. Nelson, X. Li, and D.S. Weiss, Nature Phys. 3, 556 (2007)
[7] E. Altman, E. Demler, and M.D. Lukin, Phys. Rev. A 70, 013603 (2004)
[8] I. Bloch, J. Dalibard, and W. Zwerger, arXiv:07043011
[9] J. Goldwin, S.B. Papp, B. DeMarco, and D.S. Jin, Phys. Rev. A 65, 021402(R) (2002)
[10] H. Ott, E. de Mirandes, F. Ferlaino, G. Roati, G. Modugno, and M. Inguscio, Phys. Rev. Lett. 92, 160601 (2004)
[11] K. Melmer, Phys. Rev. Lett. 80, 1804 (1998)
[12] H. Heiselberg, C.J. Pethick, H. Smith, and L. Viverit, Phys. Rev. Lett. 85, 2418 (2000)
[13] A. Albus, F. Illuminati, and J. Eisert, Phys. Rev. A 68, 023606 (2003)
[14] A.B. Kuklov and B.V. Svistunov, Phys. Rev. Lett. 90, 100401 (2003)
[15] M. Lewenstein, L. Santos, M.A. Baranov, and H. Feirnmann, Phys. Rev. Lett. 92, 050401 (2004)
[16] U. Gavish and Y. Castin, Phys. Rev. Lett. 95, 020401 (2005)
[17] K. Sacha and E. Timmermans, Phys. Rev. A 73, 063604 (2006)
[18] K. Gunter, T. Stoferle, H. Moritz, M. Kohl, and T. Esslinger, Phys. Rev. Lett. 96, 180402 (2006)
[19] S. Ospelkaus, C. Ospelkaus, O. Wille, M. Succo, P. Ernst, K. Sengstock, and K. Bongs, Phys. Rev. Lett. 96, 180403 (2006)
[20] D. Jaksch, C. Bruder, J.I. Cirac, C.W. Gardiner, and P. Zoller, Phys. Rev. Lett. 81, 3108 (1998)
[21] M.P.A. Fisher, P.B. Wuchman, G. Grinstein, and D.S. Fisher, Phys. Rev. B 40, 546 (1989)
[22] L.D. Landau and L.M. Lifshitz, Quantum Mechanics vol 3 , (Pergamon Press) p.162
[23] R.T. Delves and G.S. Joyce, J. Phys. A: Math. Gen. 34, L59 (2001), and references therein
[24] G.S. Joyce, J. Phys. A: Math. Gen. 5, L65 (1972)
[25] M.W. Zwierlein, Z. Hadzibabic, S. Gupta, and W. Ketterle, Phys. Rev. Lett. 91, 250404 (2003)
[26] C. Chin, M. Bartenstein, A. Altmeyer, S. Riedl, S. Jochim, J.H. Denschlag, and R. Grimm, Science 305, 1128 (2004)
[27] G.S. Joyce, J. Phys. A: Math. Gen. 35, 9811 (2002)