Novel polaron state for single impurity in a bosonic Mott insulator

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Abstract – We show that a single impurity embedded in a cold-atom bosonic Mott insulator leads to a novel polaron that exhibits correlated motion with an effective mass and a linear size that nearly diverge at a critical value of the on-site impurity-boson interaction strength. Cold-atom technology can tune the polaron’s properties and break up the composite particle into a deconfined impurity-hole and boson particle state at finite, controllable polaron momentum.

The exploration of and unprecedented control over quantum many-body systems have become central driving forces in cold-atom physics. Optical lattices (the standing-wave patterns of frequency-stable, reflected laser beams that are experienced by ultra-cold atoms as periodic potentials [1]) have unlocked strongly correlated lattice physics to cold-atom simulation. The Bose-Hubbard Hamiltonian [2] has successfully and quantitatively modeled boson atom dynamics in such optical lattices. Studies of the boson superfluid–to–Mott-insulator (MI) phase transition predicted within the Bose-Hubbard model [3] highlight the unusual cold-atom access and control: experiments observed the transition [4], revivals of inter-site superfluid coherence [5] and different integer filling-number islands in the MI phase as seen spectroscopically [6] and, more recently, by direct imaging [7–10]. In this letter, we show that by combining the control over optical lattice parameters (varying the barrier height), over the inter-particle interactions (varying an external, homogeneous magnetic field in a Feshbach resonance [11,12]), and over particle-species (creating mixtures of distinguishable kinds of atoms), cold-atom experiments can realize a novel1 and controllable polaron in the MI phase.

The polaron state is induced by an impurity atom that experiences the same (or similar) optical lattice potential as the MI bosons from which it is distinguishable. The polaron consists of the impurity and a boson that is promoted to the next Hubbard band by a strong impurity-boson repulsion. If the impurity-boson interaction is Feshbach tuned to be nearly as repulsive as the boson-boson interaction, the excited boson remains pinned to the impurity site. The boson-impurity pair propagates through the lattice with finite total momentum $K$. The linear polaron size, $\lambda_K$, or average distance between the impurity and the excited boson sensitively depends on $K$, and increases with increasing impurity-boson repulsive interaction $U_{IB}$ (see footnote 2). Surprisingly, the effective mass of the polaron increases with its size. Moreover, in the strong-coupling limit the effective mass diverges at the critical value of $U_{IB}$ above which the boson-impurity pair becomes unbound ($\lambda_0 \to \infty$). Most significantly, optical lattice experiments can create, probe and manipulate composite particles with properties that are unusual in traditional polaronic and excitonic systems.

We will model our problem with a bosonic Hubbard Hamiltonian on a hyper-cubic lattice of dimension $d$:

$$
\mathcal{H} = -t_B \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} b^\dagger_{\mathbf{r}} b_{\mathbf{r}'}, - t_I \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} c^\dagger_{\mathbf{r}} c_{\mathbf{r}'} + U_{BB} \sum_{\mathbf{r}} b^\dagger_{\mathbf{r}} b_{\mathbf{r}} c^\dagger_{\mathbf{r}} c_{\mathbf{r}} + U_{IB} \sum_{\mathbf{r}} b^\dagger_{\mathbf{r}} b_{\mathbf{r}} c^\dagger_{\mathbf{r}}. 
$$

(1)
The operator $b^\dagger_r \, (b_r)$ creates (annihilates) a boson on site $r$, while $c^\dagger_r \, (c_r)$ creates (annihilates) the impurity. $(r, r')$ indicates that $r$ and $r'$ are nearest neighbors. The statistics of $c^\dagger_r$ and $c_r$ is irrelevant because we are considering a single impurity problem.

Here we will only consider the case of strongly repulsive on-site boson-boson interaction, $U_{BB} \gg n|t_B|, |t_I|$, and integer filling factor $\nu=m_B$ to stabilize the MI state. An increase in the intensity of the optical lattice laser of wavelength $\lambda$ so that the lattice height $V_0$ significantly exceeds the recoil energy $\hbar \omega_R = h^2/(2m_B \lambda^2)$, where $m_B$ is the actual boson mass) drives the boson system deep into the MI regime. This increase tightens the trapping frequency $\omega_T$ of the optical lattice wells, $\omega_T = 2 \omega_R \sqrt{T}$, where $V = \sqrt{V_0/\hbar \omega_R}$. For fixed boson-boson scattering length $a_{BB}$, an increase in $x$, $x > 1$, enhances $U_{BB} \approx \hbar \omega_T \sqrt{\pi} (a_{BB}/\lambda)^x 4/1$, and exponentially decreases the hopping matrix element $t_{BB}$ which we estimate as $t_{BB} \approx (3/2) \hbar \omega_T e^{-(\sigma/2)^2} \sqrt{T}$. Scattering lengths take the value of a few nm whereas the optical wavelength is of the order of a micron but even for $x \sim 9, U_{BB}$ can exceed $t_B$ by an order of magnitude, whereas $t_B$ can still be of the order of 10 Hz. Thus, the MI-regime can be accessed by varying the optical lattice height, which leaves a homogeneous magnetic field tuned near a Feshbach resonant value as a control knob to vary $a_{BB}$ ($\propto U_{BB}$) or the impurity-boson scattering length $a_{IB}$ ($\propto U_{IB}$) independently. We consider the regime $U_{IB} \gg n|t_B|, |t_I|$. The eigenstates of $H$ become highly degenerate in the static limit $t_B = t_I = 0$. The lowest-energy eigenstates, illustrated in fig. 1, can be expressed as

$$|r_0, 0\rangle = c^\dagger_r |0\rangle,$$

$$|R, r\rangle = \frac{1}{\sqrt{n(n+1)}} e^{iK \cdot r} b^\dagger_R (n+1)b^\dagger_r |0\rangle \quad \text{for} \quad r \not= 0,$$

where $|0\rangle = \prod_r (n!)^{-1/2} b^\dagger_r |0\rangle$, and where $|0\rangle$ denotes the vacuum state. The states $|R, r\rangle$ correspond to the impurity at site $R$ creating a hole at the same site and relocating the removed boson to site $r$ (see fig. 1(a)). In defect theory, an impurity-hole system in which the impurity and the hole occupy the same site is called a substitutional impurity. The states of eqs. (2) and (3) then span a Hilbert space within which we construct the Hamiltonian eigenstate. In a regime of parameters space the eigenenergy is negative, corresponding to a composite particle that consists of a substitutional impurity (located at $R$) bound to the extra boson (of position coordinate $R + r$) that was expelled from the impurity site. The size of the resulting polaron is the size of the particle-hole bound state, i.e., the mean value of $r$.

The energy eigenvalues of the states (3) are given by

$$H(R, r) = (U_{BB} + U_{IB}(n - 1) + E_0) |R, r\rangle \quad \text{for} \quad r \not= 0,$$

$$H(R, 0) = (n U_{IB} + E_0) |0\rangle,$$

where $E_0 = N U/n(n-1)/2$ represents the ground state energy of the undoped MI: $H|0\rangle = E_0 |0\rangle$ ($N$ is the total number of lattice sites). The energy of any other eigenstate is of order $U_{BB}$ or $U_{IB}$ higher than the energy of the eigenstates (4). According to perturbation theory, to lowest order in the small parameters $t_B/U_{BB}$ and $t_I/U_{IB}$ ($\nu = I, B$), we can exclude those high-energy states and restrict the action of $H$ to the lowest energy subspace generated by the states (4). In this way we reduce the many-body problem to a two-body system described by the low-energy effective Hamiltonian,

$$\tilde{H} = \sum_{\langle K, K' \rangle} \tilde{H}_{0K} + \tilde{H}_{1K},$$

$$\tilde{H}_{0K} = -t_B (n+1) \sum_{<K, K'>} |K, r\rangle \langle K, r'|,$$

$$\tilde{H}_{1K} = \frac{\tau}{\sqrt{2d}} \sum_{0 \neq \langle 0, r' \rangle} |K, 0\rangle \langle K, r'| + |K, r'\rangle \langle K, 0\rangle$$

$$+ U_0 |K, 0\rangle |K, 0\rangle,$$

where $\tau = t_B \sqrt{2d[n+1 - \sqrt{n(n+1)}]}$,

$$|K, r\rangle = \frac{1}{\sqrt{Nn(n+1)}} \sum_R e^{iK \cdot R} b^\dagger_R b^\dagger_r |0\rangle \quad \text{for} \quad r \not= 0,$$

$$|K, 0\rangle = \frac{1}{\sqrt{N}} \sum_R e^{iK \cdot R} c_R'^\dagger |0\rangle.$$
lattice, the impurity atom can be accelerated with forces that are invisible to the b-bosons by using the recently demonstrated species-specific dipole potentials [13,14].

One-dimensional case. Since the potential $V(r)$ can be attractive, we look for bound state solutions of $\mathcal{H}_K$. For $d = 1$, the exact ground state of $\mathcal{H}_K$ can be expressed as

$$|\psi^0_K\rangle = \alpha_K \left[ \frac{(n + 1)}{\sqrt{n(n + 1)}} |K, 0\rangle + \sum_{r \neq 0} e^{-r/\lambda_K} |K, r\rangle \right],$$

(8)

with $\alpha_K^2 = n(1 - e^{-1/\lambda_K})/(1 + n - e^{-1/\lambda_K})$, and

$$e^{1/\lambda_K} = \frac{U_K}{2t_B(n + 1)} + \sqrt{\frac{U_K^2}{4t_B^2(n + 1)^2} + \frac{(n - 1)}{(n + 1)}}.$$  

(9)

The corresponding eigenvalue is

$$e^K_b = -2t_B(n + 1) \cosh(1/\lambda_K).$$  

(10)

This equation has a physical solution $(\lambda_K > 0)$ for $U_K < U_c$ with $U_c = -2t_B$:

$$\lambda_K = \frac{2t_B}{U_c - U_K}.$$  

(11)

Note that the size of the polaron, $\lambda_0$, diverges for $U_0 \rightarrow U_c$.

The solutions for $U_K > U_c$ describe the scattering of a substitutional impurity and the extra boson particle. In the $U_K > U_c$-regime, in which the composite particle unbinds, the substitutional impurity (the impurity-hole unit) is localized with infinite mass (at least to first order in the hopping matrix element $t$) while the boson that was promoted to the next Hubbard band freely propagates. The binding-unbinding transition in a polaron-type composite particle resembles the polaron-molecule transition in a single impurity embedded in an itinerant fermion gas [15–17]. Unlike the Mott-polaron of the current manuscript, the latter system, recently observed in a cold-atom trap [18], does not depend on the Mott-phase or any other lattice physics. The solutions for $U_K > U_c$ are unbound particle-hole states: the impurity-hole item and the boson that was promoted to the next Hubbard band propagate independently while scattering in each other’s vicinity.

The attractive potential $U_K$ has to reach a critical value for the stabilization of the bound state because the hopping amplitude is smaller for the bonds that include the origin. Since we are assuming that $t_I, t_B > 0$, $e^0_K$ has its minimum at $K = 0$. The effective mass, $m^*$, of the exciton is given by the equation

$$\frac{1}{m^*} = \partial^2_{K}\epsilon_{K}|K=0|\frac{|\langle\psi^0_K|K, 0\rangle|^2}{m_I},$$  

(12)

where $m_I = (2|t_I|)^{-1}$ is the bare (lattice) mass of the impurity in units in which the unit length is given by the lattice constant and $\hbar = 1$. The identity (12) follows from the Hellmann-Feynman theorem and $\partial_K|\psi^0_K|K, 0\rangle|K=0 = 0$. By taking the large $\lambda_0$ limit, we obtain the relation between $m^*/m_I$ and $\lambda_0$ near the critical point:

$$\frac{m^*}{m_I} = \frac{n\lambda_0}{n + 1}.$$  

(13)

In the strong-coupling regime the effective mass of the MI impurity polaron is proportional to its size. This behavior, very different from that of lattice polarons induced by electrons in condensed matter, is caused by the unusual mode of transportation: the impurity can hop only when the displaced boson and the hole mutually annihilate ($r = 0$). As a consequence of this correlated motion, the effective mass is proportional to $|\langle\psi^0_K|K, 0\rangle|^2$ (see eq. (12)).

To test the validity of $\mathcal{H}$ we computed the correlation function $C_{IB}(r)$ between the positions of the impurity and the site with one additional boson by solving the original Hubbard model with the constraint of no more than two particles per site. We used the Density-Matrix Renormalization Group (DMRG)[19,20]. Figure 2 shows the comparison between the numerical results for a chain of $L = 40$ sites and the analytical results given by eq. (8). The upper curves correspond to $U_{IB} = U_{BB} + t_B$ and the lower ones correspond to $U_{IB} = U_{BB} - 2t_B$. As expected, both results coincide in the strong-coupling limit. Note that the extra boson is displaced over only a few lattice sites ($r \leq 6$), so that this physics can be realized in today’s optical lattices which typically have a linear size corresponding to 100 sites or so.

General case. The bound states of $\mathcal{H}$ can be found in any dimension by using the Green’s function formalism [21]. We construct a basis of states that diagonalizes $\mathcal{H}_{K\Gamma}$ and we separate $\mathcal{H}_K$ into three terms, $\mathcal{H}_K = \mathcal{H}_{0K} + \mathcal{H}_{K+} + \mathcal{H}_{K-}$, where

$$\mathcal{H}_{\pm} = \epsilon_{\pm}[K, \psi^\pm](K, \psi^\pm),$$  

(14)

$$\epsilon_{\pm} = (U_K \pm \zeta_K)/2, \zeta_K = \sqrt{U_K^2 + 4\tau^2},$$  

$$|K, \psi^\pm\rangle = u_{\pm}|K, 0\rangle \mp u_{\pm}|\psi_s\rangle, |\psi_s\rangle = \frac{1}{\sqrt{Z}} \sum_{(0, r')} |K, r\rangle,$$  

where

$$L = 40, N_b = 40, N_I = 1, t_b = 1.0, t_I = 2.0$$  

- $U_{BB} = 40$
- $U_{BB} = 60$
- $U_{BB} = 200$
- Analytic

![Fig. 2: (Colour on-line) Correlation function between the positions of the impurity and the site with one additional boson for $n = 1$. The dashed line is the analytical result of eq. (8). The full lines were obtained by solving $\mathcal{H}$ (with a constraint of no more than two particles per site) by means of the DMRG method in a chain of $L = 40$ sites. The upper (lower) curves correspond to $U_{IB} = U_{BB} + t_B$ ($U_{IB} = U_{BB} - 2t_B$).](image-url)
and \( u_\pm = (1 \pm U_K/\xi_K)^{1/2}/\sqrt{2} \). By introducing the Green operators
\[
G^0_K(z) \equiv \frac{1}{z - \mathcal{H}_0K}, \quad G^+_K(z) \equiv \frac{1}{z - \mathcal{H}_0K - \mathcal{H}^+_K},
\]
\[
G^-_K(z) \equiv \frac{1}{z - \mathcal{H}^-_K}, \quad (15)
\]
we obtain the \( G^+_K(z) \)-operator from \( G^0_K(z) \) by expanding in \( \mathcal{H}^+_K \):
\[
G^+_K = G^0_K + G^0_K[K, \psi^+] \frac{\epsilon^+}{1 - \epsilon^+ G^0_K(\psi^-, \psi^+)(K, \psi^+)} G^0_K
\]
with \( G^0_K(\psi^+, \psi^+) = (K, \psi^+|G^0_K|K, \psi^+) \). Similarly, by considering \( \mathcal{H}^-_K \) as the unperturbed Hamiltonian and expanding in the perturbation \( \mathcal{H}^-_K \), we find
\[
G^-_K = G^+_K + G^+_K[K, \psi^-] \frac{\epsilon^-}{1 - \epsilon^- G^+_K(\psi^-, \psi^-)(K, \psi^-)} G^+_K
\]
with \( G^+_K(\psi^-, \psi^-) = (K, \psi^-|G^+_K|K, \psi^-) \). The exact dispersion relation of the bound state is obtained from the poles of \( G_K(0, 0) \equiv (K, 0|G_K|K, 0) \).

We consider \( \epsilon^0_b, \lambda_0 \) and \( m^* \) near the critical point, \( U_0 = U_c \). Identifying \( \lambda_K \) in \( d \)-dimensions from the asymptotic behavior of the bound state wave function: \( \langle \psi^0_b|K, r \rangle \sim e^{-r/\lambda_{K}}/r^{(d-1)/2} \) for \( r = (r, 0, 0, \cdots) \) and \( r \gg 1 \), we obtain
\[
\epsilon^0_b = -2t_B(n+1) \left[ d - 1 + \cosh(\lambda_{K}^{-1}) \right]. \tag{17}
\]

Thus, \( \lambda_0 \propto \Delta_b^{-1/2} \) where \( \Delta_b \equiv -2dt_B(n+1) - \epsilon^0_b \) is the composite particle binding energy. From eq. (12), we obtain the effective mass, \( m^* \),
\[
\frac{m^*}{m^0} = \left. \frac{d\epsilon^0_b}{d\mathcal{H}^-_K} \right|_{K=0}. \tag{18}
\]

Near the critical point, the large polaron size washes out the dependence on specifics that occur on the scale of the lattice constant. Hence, we expect the binding energy to vanish with the same scaling laws as the binding of a single impurity \([21]^3\):
\[
\Delta_b(0) \propto (U_0 - U_c)^2 \text{ for } d = 1 \text{ and } 3,
\]
\[
\Delta_b(0) \propto \exp \left[ \frac{C}{U_0 - U_c} \right], \text{ for } d = 2, \tag{19}
\]
where the constant \( C \) depends on microscopic details of \( \mathcal{H} \). These equations lead to the relation between \( m^* \) and \( \lambda_0 \):
\[
\frac{m^*}{m^0} \propto \lambda_0 \text{ for } d = 1 \text{ and } 3,
\]
\[
\frac{m^*}{m^0} \propto \lambda_0^2/(\ln \lambda_0)^2 m^0 \text{ for } d = 2.
\]

\( ^3 \)The impurity only affects the diagonal energy of the site at the origin.

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![Fig. 3: (Colour on-line) (a) \( K_r \) dependence of spectral weight for the simple cubic lattice \( \epsilon_B = t_1 = 1, n = 1, K_r = K_y = 0, \) and \( U_{BB} - U_{IB} = 7 \). Each line is shifted by \( K_x/\pi \) for visualization. We use \( \eta = 2^{-10} \) as an infinitesimal constant. (b) \( U_0 \) dependences of the bound state energy \( \epsilon^0_b \) (top), linear size of the polaron \( \lambda_0 \) (middle), and ratio of effective and bare masses \( m^*/m^0 \) (bottom) for \( n = 1 \). The dashed line indicates \( U_0 = U_c \).](Image)
the hopping $t$) while the boson freely propagates. Binding transition has been also reported in studies of the Fermi polaron problem [18,22].

The control offered by cold-atom technology over polaron size and mass hints at the intriguing prospect of studying the quantum phase transition between a “confined” gas of boson-impurity polarons and two “deconfined” gases of substitutional impurities and bosons in the next Hubbard band. The driving parameter of this transition is the difference $U_{1B} - U_{BB}$. By reducing the ratio $U_{1B}/t_B$, while keeping $U_0$ fixed, it would be possible to vary the polaron mass near the transition. The competition between potential and kinetic energies could also lead to an intermediate crystallization of polarons in the large $m^*$ regime. Bosonic impurities exhibit qualitatively different behavior in the superfluid state [23]. Therefore, impurities can be used as a probe of the superfluid-Mott transition. Moreover, the sensitivity of the binding-unbinding transition to the polaron momentum could be used as an independent characterization of the system’s parameter values.

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REFERENCES

[1] Greiner M. and Fölling S., Nature, 453 (2008) 736.
[2] Jaksch D., Bruder C., Cirac J. I., Gardiner C. W. and Zoller P., Phys. Rev. Lett., 81 (1998) 3108.
[3] Matthew P. A., Fisher Peter B., Weichman G. and Daniel S. Fisher, Phys. Rev. B, 40 (1989) 546.
[4] Greiner M., Mandel O., Esslinger T., Hänsch T. W. and Bloch I., Nature, 415 (2002) 39.
[5] Greiner M., Mandel O., Hänsch T. W. and Bloch I., Nature, 419 (2002) 51.
[6] Campbell G. K., Mun J., Boyd M., Medley P., Leinhardt A. E., Marcassa L. G., Pritchard D. E. and Ketterle W., Science, 313 (2006) 649.
[7] Bakr W. S., Gillen J. I., Peng A., Fölling S. and Greiner M., Nature, 462 (2009) 74.
[8] Bakr W. S., Peng A., Tai M. E., Ma R., Simon J., Gillen J. I., Folling S., Pollet L. and Greiner M., Science, 329 (2010) 547.
[9] Hung Chen-Lung, Zhang Xibo, Gemelke Nathan and Chin Cheng, Phys. Rev. Lett., 104 (2010) 160403.
[10] Sherson J. F., Weitenberg C., Endres M., Cheneau M., Bloch I. and Kuhr S., Nature, 467 (2010) 68.
[11] Bloch I., Dalibard J. and Zwerger W., Rev. Mod. Phys., 80 (2008) 885.
[12] Inouye S., Andrews M. R., Stenger J., Miesner H., Inouye S., Andrews M. R., Stenger J., Miesner H. and Wieman C., Phys. Rev. Lett., 81 (1998) 3108.
[13] Catani J., Barontini G., Lamporesi G., Rabatti F., Thalhammer G., Minardi F., Stringari S. and Inguscio M., Phys. Rev. Lett., 103 (2009) 140401.
[14] Lamporesi G., Catani J., Barontini G., Nishida Y., Inguscio M. and Minardi F., Phys. Rev. Lett., 104 (2010) 153202.
[15] Bruun G. M. and Massignan P., Phys. Rev. Lett., 105 (2010) 020403.
[16] Prokof’ev N. and Svistunov B., Phys. Rev. B, 77 (2008) 020408(R).
[17] The polaron-molecule transition is also expected in two-dimensional impurity-fermion systems, see Koschorreck M., Pertot D., Vogt E., Fröhlich B., Feld M. and Köhl M., arXiv:1203.1009v1; Parish M. M., Phys. Rev. A, 83 (2011) 051603; Zollner S., Bruun G. M. and Pethick C. J., Phys. Rev. A, 83 (2011) 021603.
[18] Schirotzek A., Wu C. H., Sommer A. and Zwierlein M. W., Phys. Rev. Lett., 102 (2009) 230402.
[19] White Steven R., Phys. Rev. Lett., 69 (1992) 2863.
[20] White Steven R., Phys. Rev. B, 48 (1993) 10345.
[21] Economou E. N., Green’s Functions in Quantum Physics, 3rd edition (Springer-Verlag, Berlin) 2006.
[22] Koschorreck M., Pertot D., Vogt E., Fröhlich B., Feld M. and Köhl M., arXiv:1203.1009v1.
[23] Cuccietti F. M. and Timmermans E., Phys. Rev. Lett., 96 (2006) 210401.