Migration of bosonic particles across a Mott insulator to superfluid phase interface

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We consider a boundary between a Mott insulator and a superfluid region of a Bose-Hubbard model at unit filling. Initially both regions are decoupled and cooled to their respective ground states. We show that, after switching on a small tunneling rate between both regions, all particles of the Mott region migrate to the superfluid area. This migration takes place whenever the difference between the chemical potentials of both regions is less than the maximal energy of any eigenmode of the superfluid. We verify our results numerically with DMRG simulations and explain them analytically with a master equation approximation, finding good agreement between both approaches. Finally we carry out a feasibility study for the observation of the effect in coupled arrays of micro-cavities and optical lattices.

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Introduction – Effective many-particle systems in artificial structures that can be well controlled in experiments have become an important testbed for the investigation of quantum many-particle and condensed matter physics. Extensive work with arrays of Josephson junctions [1] and ultra cold atoms in optical lattices [2] has lead to substantial progress and seminal experiments. Very recently it has been shown, that arrays of coupled micro-cavities can host effective Bose-Hubbard models for one [3] and two [4] polariton components, related polariton models [5] and effective spin Hamiltonians [6]. The phase diagrams of these models [7, 8] and the possibility of a glassy phase have been discussed [9]. As a new feature, this approach offers the possibility to control and address individual lattice sites. Besides being a prerequisite for quantum information applications, this possibility opens the door to the study of many-particle systems which are inhomogeneous or out of equilibrium. In this work we exploit these strengths of local addressability and controllability to study novel physical effects.

We consider a one-dimensional Bose-Hubbard model of $N$ sites, where sites 1 to $N_I$ are in a Mott insulator and the rest in a superfluid regime. Initially there is no particle hopping between the two areas, which are both prepared in their respective ground states with on average one particle per site. At $t = 0$, we then switch on a small hopping rate between sites $N_I$ and $N_I + 1$. As our results show, this causes all particles of the Mott region to migrate to the superfluid part, leaving the Mott part almost completely empty.

We present time dependent DMRG simulations [9] for finite systems with various parameters and an analytical approximation using a master-equation for the case where the superfluid region is large and has no particle interactions. We find good agreement between both approaches. These findings indicate that the scenario we consider could be used to experimentally study dissipative quantum dynamics [10] where a part of the employed effective many body system acts as the heat bath, the properties of which can even be controlled and tested. Finally we discuss possibilities to observe the effect in both, coupled cavities [3] and optical lattices [2].

Model and concept – We consider a Bose-Hubbard model, where the chemical potential, hopping rate and on-site interactions vary from site to site. The Hamiltonian of our model with open boundary conditions reads,

$$H = \sum_{j=1}^{N-1} \left[ U_j n_j (n_j - 1) - \mu_j n_j - J_j \left( a_j^\dagger a_{j+1} + \text{h.c.} \right) \right] \quad (1)$$

where $a_j^\dagger$ creates a particle in site $j$ and $n_j = a_j^\dagger a_j$. $\mu_j$, $J_j$ and $U_j$ are the chemical potential, hopping rate and on-site interaction at site $j$ and $J_N = 0$. We consider a scenario (c.f. figure 1) with $U_j = U$ and $\mu_j = \mu$ for $j = 1, \ldots, N_I$ and denote this part of the chain part A. The remaining sites, which we will refer to as part B, have $U_j = \bar{U}$ and $\mu_j = \bar{\mu}$ ($j = N_I + 1, \ldots, N$). The hopping rates take values $J_j = \tilde{J}$ for part A, i.e. for $j = 1, \ldots, N_I - 1$ and $J_j = \bar{J}$ for part B, i.e. for $j = N_I + 1, \ldots, N$.
$N_J+1, \ldots, N-1$, while hopping between $N_J$ and $N_J+1$ is initially zero, $J_{N_J}=0$. Parts A and B are prepared in their respective ground states with filling factor $1$, i.e. on average one particle per site in both parts. Hence, part A(B) initially contains $N_J(N-N_J)$ particles. We assume that part A is operated in a Mott insulator regime, $U \gg J$, whereas part B is operated in a superfluid regime, $\tilde{U} \ll \tilde{J}$. At $t=0$, $J_{N_J}$ is then switched to a finite but small value $J_{N_J} = J_I$, where $J_I \ll U$ and $J_I \ll \tilde{J}$.

**Numerics** — We numerically calculated the initial state and the time evolution for chains of finite length using the TEBD algorithm [9] with matrices of dimension $20$, timesteps $dt = \frac{0.005}{\alpha}$ and a 4th order Trotter formula. Truncation errors at each timestep were $<10^{-6}$.

As parts A and B are initially decoupled and both in their respective ground states, we calculate this initial state via an evolution in imaginary time, exp($-\beta H$) with $\beta \to \infty$ and $H$ given by eq. (1) with $J_{N_J}=0$. The imaginary time evolution starts from a state with exactly one particle in each site, $|1,1,\ldots,1\rangle$, and since it conserves the total number of particles in both parts independently, our initial state has unit filling with $N_I$ particles in part A and $N-N_I$ particles in part B.

We then simulate the time evolution, exp($-iHt$), of this initial state, where $H$ is given by eq. (1) but now with $J_{N_J}=J_I$. Figure 2 shows the evolution of the number densities in each site, $(n_j)(t)$ for a chain of length 40. Sites 1 - 20 are in a Mott insulator regime with $U = 1.0$, $J = 0.1$, $\mu = 0$ and $J_I = 0.1$. For the remaining sites, $\tilde{U} = 0.2$, $\tilde{\mu} = 0$ and $\tilde{J} = 1.0$. The initial evolution is plotted separately with higher resolution in figure 3A and shows that particles close to the boundary leave the Mott insulator region first. The total number of particles in part A, $N_A = \sum_{j=1}^{20} \langle n_j \rangle$ is shown to decay to zero in figure 3B. Initially $N_A$ decays fast by one particle as the particle that is already next to the boundary leaves part A first. All further particles first need to travel to the boundary resulting in a slower decay of $N_A$. Since part B has a finite size, one should expect recurrences in $N_A$. Whereas these appear on short time scales for small chains, the simulated time range in figure 2 is not long enough to see them.

**Analytical approach** — Here we give an analytical approximation for the case where part B has no interactions, $\tilde{U} = 0$, and is very large, $N-N_J \gg 1$. To this end we derive a master equation [11] for the reduced density matrix of part A, $\sigma = \text{Tr}_B(\rho)$, which reads, $\frac{d\rho}{dt} = -i[H_I,\sigma] - \int_0^t ds \text{Tr}_B \{[H_I, [H_I(t-s),\langle GS|GS\rangle\langle GS|\sigma]|s]\}$. Here, $\langle GS \rangle$ is the ground state of part B, $H_I = -J\sum_{j=1}^{N_I-1} (a_j^\dagger a_{j+1} + \text{h.c.})$, $H_I = -J_{N_J} (a_{N_{J+1}}^\dagger a_{N_{J+1}+1} + \text{h.c.})$ and $H_I(t) = e^{iH_{0}t} H_I e^{-iH_{0}t}$ with $H_{0} = \sum_{j=1}^{N_J} j_n (n_j - 1) - \mu \sum_{j=1}^{N_I} j_n - \tilde{\mu} \sum_{j=N_{J+1}}^{N-I} j_n - J_{N_J} (a_{N_{J+1}}^\dagger a_{N_{J+1}+1} + \text{h.c.})$. The equation is valid up to second order in $J$ and $J_I$, we thus focus on the regime where $U, J_I \gg J, J_I$.

The Hamiltonian of part B is diagonalized via the transformation $a_j = \sqrt{\frac{2}{N-N_{J+1}} \sum_{i=1}^{N-N_{J+1}} \sin \left(\frac{\pi j}{N-N_{J+1}}\right)} b_i$ so that $-\tilde{J} \sum_{j=N_{J+1}}^{N-I} (a_j^\dagger a_{j+1} + \text{h.c.}) = \sum_{i=1}^{N-N_{J+1}} \omega_i b_i$ with $\omega_i = -2J \cos \left(\frac{\pi j}{N-N_{J+1}}\right)$. Then we find $\langle GS|a_{N_{J+1}}(t) a_{N_{J+1}}^\dagger|GS\rangle = \langle GS|a_{N_{J+1}}(t) a_{N_{J+1}}^\dagger|GS\rangle = \langle J_I \rangle^{-1} J_{I_1}(2J_I)$, where $J_{I_1}$ is a Bessel function of the first kind and we neglected terms of order $\frac{2\pi}{(N-N_{J+1})}$. These correlations decay sufficiently fast ($\propto t^{-3/2}$) and the time integral in the master equation can (after a transformation of the integration variable) be extended to the range $(-\infty,0)$ and the equation becomes an ordinary differential equation $\frac{d}{dt} \sigma_{nm} = -i(n_{N_J} [H_I, \sigma]|m_{N_J}) - (n_{N_{J+1}} m_{N_{J+1}} - i n_{N_{J+1}} m_{N_{J+1}} + \sqrt{n+m+1} (\Gamma_{n+1} + \Gamma_{m+1} - i \Theta_{m+1} + i \Theta_{n+1}) \sigma_{nm+1,m+1},$ and $|n_{N_J}\rangle$ is the state of site $N_J$ with $n$ particles and...
The energy shifts $\Theta_n$ are given by $\Theta_n = -(J_n^2/J)\chi_n$ for $|\chi_n| < 1$ and $\Theta_n = -(J_n^2/J)\chi_n\sqrt{1-\chi_n^2}$ otherwise, whereas the decay rates $\Gamma_n$ are given by $\Gamma_n = \text{Re}\left((J_n^2/J)\sqrt{1-\chi_n^2}\right)$ with $\chi_n = (U/J)(n-1) - (\mu - \tilde{\mu})/(2J)$. There is thus a particle flow from part A to part B whenever $|\chi_n| < 1$. One can identify two scenarios in which this flow is blocked: If the chemical potential is larger in part B, $\tilde{\mu} > \mu$, all $\Gamma_n$ are zero for $\mu - \tilde{\mu} < -2J$. If on the other hand, the chemical potential is larger in part A, $\mu < \tilde{\mu}$, $\Gamma_1$ is zero if $\mu - \tilde{\mu} > 2J$, whereas other $\Gamma_n$ with $n$ such that $\mu - \tilde{\mu} - 2J > 2U(n-1)$ remain nonzero.

Hence, if part A is deep in the Mott insulator regime with $U \gg J$ and states $|n_{N_A}\rangle$ with $n_{N_A} > 1$ have very small occupation, the decay channels $\Gamma_n$ with $n > 1$ do not contribute and the particle flow vanishes whenever $|\mu - \tilde{\mu}| > 2J$, that is if the difference of the chemical potentials in parts A and B is larger than the maximal energy of any eigenmode of part B, i.e. $|\mu - \tilde{\mu}| > \max(|\omega_l|)$. Nonetheless, for $\mu - \tilde{\mu} > 2J$ and moderate ratios $U/J$, there is a slow flow of particles from part A to B, which becomes more and more suppressed with increasing $U/J$. For $U \gg J$ we thus approximate $\Theta_n$ and $\Gamma_n$ by the values for $n = 1$ and obtain,

$$\frac{d\sigma}{dt} = -i \left[ H_1 + \Theta_n a_{N_A}^\dagger a_{N_A}, \sigma \right] + \Gamma \left( 2a_{N_A}^\dagger \sigma a_{N_A}^\dagger - a_{N_A}^\dagger a_{N_A} \sigma - \sigma a_{N_A}^\dagger a_{N_A} \right).$$

We numerically tested the accuracy of eq. (2) for chains of $N = 20$ and $N = 50$ sites, where sites 1, \ldots, 4 form part A and the remaining sites part B. Figure 3 shows the results for various parameters. In the upper row, we plot the total number of particles in part A, $N_A = \sum_{j=1}^{N} |n_j|$, as given by the numerics whereas the lower row shows differences between $N_A$ as given by the numerics and $N_A$ as given by the master equation, $[N_A]_{\text{numerics}} - [N_A]_{\text{master}}$. We find good agreement between both approaches.

The applicability of the master equation approach, which we have confirmed with our numerics, shows that the superfluid region behaves like bath and the Mott insulator like a quantum system under dissipation. Experimental implementations of these scenarios would thus also allow to investigate processes as described by e.g. the spin boson model and its relation to the Kondo problem. Moreover the properties of the bath could even be controlled and tested in these experiments.

**Experimental tests** - As possible experiments we analyze here two realizations, polaritonic systems in coupled cavities and cold atoms in optical lattices. With the possibility to manipulate and measure individual lattice sites, coupled cavities suggest themselves as an ideal implementation of effective many-body systems for observing the effect under consideration. One way to initially separate part A and B is to generate a large, negative chemical potential in one cavity. This cavity thus stays empty and suppresses any particle tunneling or coupling between both parts. This chemical potential is then switched off and the particles start to migrate from the Mott insulator to the superfluid part. Figure 4 shows numerical results for such a scenario. Here sites 1 to 10 are in a Mott and the rest in a superfluid regime. Site 10 has initially a chemical potential $\mu_{10} = -4$ and thus no particle in it. As this chemical potential $\mu_{10}$ is switched off during the evolution, particles start to flow into the superfluid part. The left plot shows number densities $\langle n_j \rangle(t)$ whereas the right plot shows $N_A(t)$ (blue) and $\mu_{10}(t)$ (green). In cavities the local number statistics can be measured using resonance fluorescence.

A related experiment with cold atoms in optical lattices could be done by applying a magnetic field across the lattice. At first this field is constant and the system

![Figure 5](image-url)

**Figure 5**: A Mott insulating and a superfluid region that are initially separated by a strongly negative chemical potential in site 4. $U = 1$, $J = 0.1$, $\tilde{U} = 0.1$, $\tilde{J} = 1$ and $\mu_1 = 0$ except for $j = 10$. Number densities $\langle n_j \rangle(t)$ look similar as in figure 2 $N_A(t)$ (blue) and $\mu_{10}(t)$ (green).
is prepared in the ground state of the corresponding homogeneous model with \( U_j = U_0, J_j = J_0 \) and \( \mu_j = \mu_0 \) for all \( j \). Then a magnetic field gradient is ramped up such that there is a spatially varying field across the lattice. Since \( U_j / J_j \propto \exp(2\sqrt{V_j} / E_c) \) (\( V_j \) is the lattice potential at site \( j \) and \( E_c \) the recoil energy of the atoms) and furthermore \( V_j \propto B_j^{-1} \), where \( B_j \) is the magnetic field at site \( j \), the ratio \( U_j / J_j \) at each site can be tuned by the magnetic field. Hence a magnetic field gradient across the lattice can result in \( U_j / J_j \gg 1 \) at one end of the lattice and \( U_j / J_j \ll 1 \) at the opposite end.

Figure 6 shows a numerical simulation for such an experiment. At \( t = 0 \), we set \( U_j = J_j = 0.5 \) and \( \mu_j = 0 \) for all \( j \) (\( N = 20 \)) and prepare the system in the corresponding unit filling ground state. Then we tune the interactions and hopping rates according to \( U_j(t) = 0.5(1 + 10^{-4}(j - N/2))t \) and \( J_j(t) = 0.5(1 - 10^{-4}(j - N/2))t \). The particles move towards the site with minimal \( U_j / J_j \).

Several quantities are accessible to measurements for cold atoms in optical lattices. Time-of-flight measurements reveal the number distribution in momentum space \( S(k) = \frac{1}{N} \sum_{j=1}^{N} \left| \langle \alpha_j | \alpha_j \rangle \right|^2 \), where \( \alpha_j \) is the initial state at \( t = 0 \) and the final state at \( t = 1000 \) (green line) and the difference between both, \( S(k)|_{t=0} - S(k)|_{t=1000} \) (red line). Although the average ratio \( U_j / J_j \) remains constant, the peak broadens. In an inhomogeneous magnetic field, microwave pulses on field selective transitions can be used to selectively address atoms that experience a certain magnetic field and hence the density profile of the atoms can be measured.

Summary and outlook — We have considered an interface between a superfluid and a Mott insulator. Both parts were initially decoupled and cooled to their unit filling ground states. As a tunneling rate between both parts is switched on, all particles of the Mott region migrate into the superfluid part. This effect which we confirm numerically by DMRG simulations and analytically with a master equation is caused by the high density of states of the superfluid region, whereas in Mott insulating area there is only one state in the accessible energy range. Our results also show how effective many body systems could be used to experimentally study dissipative quantum dynamics where the properties of the bath may be tested and controlled. Experimental observations appear feasible in arrays of micro-cavities and optical lattices.

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