Ultracold atoms in optical lattices generated by quantized light fields

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We study an ultracold gas of neutral atoms subject to the periodic optical potential generated by a high-$Q$ cavity mode. In the limit of very low temperatures, cavity field and atomic dynamics require a quantum description. Starting from a cavity QED single atom Hamiltonian we use different routes to derive approximative multiparticle Hamiltonians in Bose-Hubbard form with rescaled or even dynamical parameters. In the limit of large enough cavity damping the different models agree. Compared to free space optical lattices, quantum uncertainties of the potential and the possibility of atom-field entanglement lead to modified phase transition characteristics, the appearance of new phases or even quantum superpositions of different phases. Using a corresponding effective master equation, which can be numerically solved for few particles, we can study time evolution including dissipation. As an example we exhibit the microscopic processes behind the transition dynamics from a Mott insulator like state to a self-ordered superradiant state of the atoms, which appears as steady state for transverse atomic pumping.

I. INTRODUCTION

Laser light, far red detuned from an atomic resonance, is nowadays a standard tool in experimental quantum optics to create tunable optical potentials \cite{1} which can be loaded with ultracold atoms to provide for a plethora of possibilities to study quantum properties of many-body strongly correlated systems \cite{2}. The high level of microscopic understanding and extensive control of the light fields and atoms allow to implement genuine models like e.g. the Bose-Hubbard (BH) model \cite{3,4}. Initially originating from condensed matter physics \cite{5} it has been used to study the Mott insulator to superfluid phase transition \cite{6} in detail and in real time. Adjusting several of the lattice parameters as the intensity and the configuration of the lattice lasers provides a versatile toolbox of techniques to control the dynamics of the atoms in the lattice \cite{7}. Moreover, the collisional properties of the certain types of atoms can be tailored by means of magnetic \cite{8} or optical \cite{9} Feshbach resonances. Using extra confinement it was even possible to observe the Mott insulator to superfluid transition in 1D \cite{10,11} and 2D \cite{12}, followed by other spectacular demonstrations of condensed matter physics phenomena as the realization of a Tonks gas in 1D \cite{13,14} and the Berezinskii-Kosterlitz-Thouless phase transition in 2D \cite{15}. Theoretically many more proposals to apply these methods to spin systems and investigate further fascinating properties of strongly correlated systems were put forward (see \cite{16} for a review).

In all of these approaches, the light fields were approximated by classical, externally prescribed fields independent of the atoms. This requires intense light, far detuned from any atomic transition. Of course this assumption holds no longer if the light, which generates the optical lattice, is enhanced by an optical resonator. In this case - given a sufficient atom number $N$ and atom-field coupling $g$ - the field itself becomes a dynamical quantity \cite{17} depending on the atomic distribution. As all atoms are coupled to the same field modes, this immediately introduces substantial long range interactions, which cannot be ignored as in free space. In specially designed cases this force induces coherently driven atoms to self-organize in regular patterns as predicted in Ref. \cite{18,19} and subsequently experimentally verified \cite{20}.

In addition, in a high-$Q$ optical resonator relatively low photon numbers are sufficient to provide strong forces. This was demonstrated by trapping an atom in the field of just a single photon \cite{21,22}. Hence the inevitable photon number fluctuations induced by cavity damping generate force fluctuations on the atoms causing diffusion. At the same time as cavity photon loss constitutes a dissipation channel, it can also carry out energy and entropy of the system. This opens possibilities for cooling of atomic motion \cite{23,24,25,26}, as demonstrated by beautiful experiments in the group of Rempe \cite{27,28}. Since this cooling mechanism does not require the existence of closed optical cycles it could even be used for qubits \cite{29} or to damp quantum oscillations or phase fluctuations of a BEC coupled to a cavity field \cite{30,31}.

For low photon numbers the quantum properties of the light field get important as well and the atoms are now moving in different quantized potentials determined by the cavity photon number. Quantum mechanics of course allows for superpositions of photon numbers invoking superpositions of different optical potentials for the atoms. First simplified models to describe this new physics were recently proposed by us \cite{32} and in parallel by other authors \cite{33}. As the intracavity field itself depends on the atomic state (phase), different atomic quantum states are correlated with different states of the lattice field with differing photon number distributions. In this way quantum mechanics allows for the creation of very exotic atom-field states, like a superposition of a Mott-insulator and superfluid phase, each thereof correlated with a different photon number. Some quite exotic looking phase diagrams for this system were already discussed in Ref. \cite{34}. Without resorting to the full complex dynamics of the system, the quantum correlations between the field and the atomic wavefunctions open the possibility of non-destructively probing the atomic
state by weak scattering of coherent light into the cavity mode [34] and carefully analyzing its properties [35].

It is quite astonishing, that experimental progress in the recent years has made such systems experimentally accessible and at present already several experimental groups succeeded in loading a BEC into a high-Q optical cavity [36, 37, 38, 39, 40]. A reliable analysis of these experiments has made more thorough theoretical studies of such systems mandatory.

In this work we concentrate on the study of an ultracold gas in optical lattices including the quantum nature of the lattice potential generated from a cavity field. This extends and substantiates previous studies and predictions on such a system by us [32] as well as other authors [33]. Here we limit ourselves to the case of a high-Q cavity which strongly enhances a field sufficiently red detuned from any atomic transition to induce an optical potential without significant spontaneous emission. In particular we address two different geometric setups, where either the cavity mode is directly driven through one mirror, or the atoms are coherently excited by a transverse laser and scatter light into the cavity mode. The cavity potential can also be additionally enhanced by some extra conservative potential applied at a different frequency [11, 12]. These two generic cases leads to quite different physical behavior and allow to discuss several important aspects of the underlying physics.

This paper is organized as follows. Sec. II is devoted to a systematic presentation of our model and various simplifying approximations as adiabatic elimination of the excited states of the atoms and subsequent formulation of an effective multi-particle Hamiltonian in second quantized form. In section III we specialize on the simplest generic case of a coherently driven cavity and approximate the corresponding Hamiltonian by adiabatic elimination of the cavity field. We investigate the properties thereof, corresponding to the influence of the cavity on the Mott-insulator to superfluid quantum phase-transition and identify the regime of validity for the elimination of the cavity field. Finally, we compare these results with the dynamics of the full master equation. In Sec. IV we study the more complex case of atoms coherently driven by a laser field transversal to the cavity axis, where it is much harder to find valid analytical simplifications and one has to resort to numerical studies of few particle dynamics. Finally, we conclude in Sec. V.

II. MODEL

We start with $N$ two-level atoms with mass $m$ and transition frequency $\omega_{eg}$ strongly interacting with a single standing wave cavity mode of frequency $\omega_c$. We also consider coherent driving of the atoms at frequency $\omega_p$ and with maximal coupling strength $\hbar g_0$ and of the cavity with amplitude $\eta$ (see Fig. 1). Note that in the specific examples later we will consider only one pump laser beam at a time.

![Fig. 1](color online). Scheme of atoms inside an optical cavity, driven by two external pumping lasers. An additional conservative lattice potential, independent of the intracavity field, is realized by a far off-resonant dipole trap (FORT).

Using the rotating-wave and electric-dipole approximation, we can describe a single atom of this system by the Jaynes-Cummings Hamiltonian [43]

$$H^{(1)} = H_A^{(1)} + H_R^{(1)} + H_{Int}^{(1)}. \quad (1)$$

Explicitly the different Hamiltonians for the atoms, the field mode and the interaction read:

$$
H_A^{(1)} = \frac{\hbar^2}{2m} \ddot{a} + V_c(x) \sigma^+ \sigma^- + V_g(x) \sigma^- \sigma^+ + \hbar \omega_{eg} \sigma^+ \sigma^- - i \hbar h(x) \left( \sigma^+ e^{-i \omega_p t} - \sigma^- e^{i \omega_p t} \right), \quad (2a)
$$

$$
H_R^{(1)} = \hbar \omega_c a^\dagger a - i \hbar \eta \left( \omega_c a^\dagger e^{i \omega_p t} - a e^{-i \omega_p t} \right), \quad (2b)
$$

$$
H_{Int}^{(1)} = -i \hbar \eta g(x) \left( \sigma^+ a - \sigma^- a^\dagger \right). \quad (2c)
$$

Here $h(x)$ denotes the mode-function of the transverse pump field, $g(x)$ denotes the cavity mode function and the field operator $a$ describes the annihilation of a cavity photon with frequency $\omega_c$. $V_c(x)$ and $V_g(x)$ are external trapping potentials for the atom in the excited and the ground state, respectively. In order to change to slowly varying variables we apply a unitary transformation with operator $U(t) = \exp[-i \omega_p t (\sigma^+ a - a^\dagger \sigma^-)]$, such that we end up with the following single-particle Hamiltonian, using the same symbols for the transformed quantities:

$$
H_A^{(1)} = \frac{\hbar^2}{2m} \ddot{x} + V_c(x) \sigma^+ \sigma^- + V_g(x) \sigma^- \sigma^+ - \hbar \Delta_c \sigma^+ \sigma^- - i \hbar h(x) \left( \sigma^+ - \sigma^- \right), \quad (3a)
$$

$$
H_R^{(1)} = -\hbar \Delta_e a^\dagger a - i \hbar \eta \left( \sigma^+ a - a^\dagger \sigma^- \right), \quad (3b)
$$

$$
H_{Int}^{(1)} = -i \hbar \eta g(x) \left( \sigma^+ a - \sigma^- a^\dagger \right), \quad (3c)
$$

where $\Delta_c = \omega_p - \omega_c$, $\Delta_e = \omega_p - \omega_{eg}$ denotes the detunings of the cavity and the atomic transition frequency from the pumping field frequency. In order to describe the situation for $N$ atoms, we use the single-particle Hamiltonian of Eq. (1) and (3) in second quantization formalism [44], i.e.,

$$
H = H_A + H_R + H_{A-R} + H_{A-P} + H_{A-A}. \quad (4)
$$
The terms in this expression correspond to the single particle terms in \(2\) and \(3\). Hence, \(H_A\) and \(H_R\) model the free evolution of the atomic and the field variables, respectively. They obey the usual bosonic commutation relations

\[
\left[ \Psi_f(x), \Psi_{f'}^{\dagger}(x') \right] = \delta^3(x - x') \delta_{f, f'},
\]

\[
\left[ \Psi_f(x), \Psi_{f'}^{\dagger}(x') \right] = \left[ \Psi_f^{\dagger}(x), \Psi_{f'}^{\dagger}(x') \right] = 0,
\]

for \(f, f' \in \{e, g\}\). The field operator remains unchanged, i.e., \(H_R = -\hbar \Delta_a a^\dagger a - i \hbar \eta (a - a^\dagger)\). The two-body interaction is modeled by a short-range pseudopotential \([13]\), characterized by the s-wave scattering length \(a_s\), leading to a Hamiltonian

\[
H_{A-A} = \frac{U}{2} \int d^3x \Psi_g^{\dagger}(x) \Psi_g^{\dagger}(x) \Psi_g(x) \Psi_g(x),
\]

where \(U = 4 \pi a_s \hbar^2 / m\). The coupling of the cavity field with the atoms inside the cavity is given by

\[
H_{A-R} = -i \hbar \int d^3x \Psi_g^{\dagger}(x) g(x) a \Psi_e(x) + \text{h.c.},
\]

whereas the interaction with the laser beam, which coherently drives the atoms, reads

\[
H_{A-P} = -i \hbar \int d^3x \Psi_g^{\dagger}(x) h(x) \Psi_e(x) + \text{h.c.}.
\]

Let us now calculate the Heisenberg equations for the various field operators, starting with the operator for the excited state, i.e.,

\[
\frac{\partial \Psi_e(x)}{\partial t} = i \left( \frac{\hbar}{2m} \nabla^2 - \frac{V_e(x)}{\hbar} + \Delta_a \right) \Psi_e(x) - \left[ g(x) a + h(x) \right] \Psi_g(x).
\]

The first term corresponds to the free evolution of the atomic state, whereas the second term describes the absorption of a cavity photon or a pump photon together with the annihilation of a ground state atom. Similarly, the equation for the ground state operator reads:

\[
\frac{\partial \Psi_g(x)}{\partial t} = i \left( \frac{\hbar}{2m} \nabla^2 - \frac{V_g(x)}{\hbar} - \frac{U}{\hbar} \Psi_g^{\dagger}(x) \Psi_g(x) \right) \Psi_g(x) + \left[ g(x) a^\dagger + h(x) \right] \Psi_e(x).
\]

Finally, the Heisenberg equation for the cavity field operator is given by:

\[
\frac{\partial a}{\partial t} = i \Delta_a a + \eta + \int d^3x g(x) \Psi_g^{\dagger}(x) \Psi_e(x).
\]

Again, the first term corresponds to the free field evolution, whereas the last two terms are driving terms of the cavity field.

As we want to treat temperatures close to \(T = 0\) we have to avoid heating and ensure weak atomic excitation, where there is only negligible spontaneous emission. In this limit we can adiabatically eliminate the excited states from the dynamics of our system. This requires large atom-pump detunings \(\Delta_a\), where we also can neglect the kinetic energy term and the trapping potential in \([10]\) compared to \(\Delta_a\). Necessarily, we assume that the field operators \(\Psi_g(x)\) and \(a\) vary on a much slower time scale than the \(1/\Delta_a\) terms, such that we obtain:

\[
\Psi_e(x, t) = -\frac{i}{\Delta_a} \left[ h(x) + g(x) a(t) \right] \Psi_g(x, t).
\]

Inserting this expression for \(\Psi_e(x)\) into \([11]\) and \([12]\) leads then to:

\[
\frac{\partial \Psi_g(x)}{\partial t} = i \left( \frac{\hbar}{2m} \nabla^2 - \frac{V_g(x)}{\hbar} - \frac{\hbar^2(x)}{\Delta_a} - \frac{g^2(x)}{\Delta_a} a^\dagger a \right.
\]

\[
- \frac{\hbar(x) g(x) a}{\Delta_a} (a + a^\dagger) - \frac{U}{\hbar} g(x) \Psi_g(x) \right] \Psi_g(x),
\]

\[
\frac{\partial a}{\partial t} = i \left[ \Delta_a - \frac{1}{\Delta_a} \int d^3x g^2(x) \Psi_g^{\dagger}(x) \Psi_g(x) \right] a
\]

\[
- \frac{i}{\Delta_a} \int d^3x h(x) \Psi_g^{\dagger}(x) \Psi_g(x) + \eta.
\]

To discuss the underlying physics in a tractable form, the trick is now to find an effective Hamiltonian \(H_{\text{eff}}\) which leads to the same dynamics as given by Eq. \([14]\) and \([15]\). Thus this Hamiltonian has to obey:

\[
i \hbar \frac{\partial \Psi_g(x)}{\partial t} = [\Psi_g(x), H_{\text{eff}}] \quad \text{and} \quad i \hbar \frac{\partial a}{\partial t} = [a, H_{\text{eff}}].
\]

From this we can easily read off a possible effective Hamiltonian of the form:

\[
H_{\text{eff}} = \int d^3x \Psi_g^{\dagger}(x) \left\{ -\frac{\hbar^2}{2m} \nabla^2 + V_g(x) + \frac{\hbar}{\Delta_a} \left[ h^2(x) + g^2(x) a^\dagger a + h(x) g(x) (a + a^\dagger) \right] \right\} \Psi_g(x)
\]

\[
+ \frac{U}{2} \int d^3x \Psi_g^{\dagger}(x) \Psi_g^{\dagger}(x) \Psi_g(x) \Psi_g(x)
\]

\[
- \frac{\hbar \eta (a - a^\dagger)}{\Delta_a} - \hbar \Delta_a a^\dagger a.
\]

The corresponding single particle Hamiltonian, which leads to this second quantized Hamiltonian is \([10]\):

\[
H_{\text{eff}}^{(1)} = \frac{\hbar^2}{2m} + V_g(x) + \frac{\hbar}{\Delta_a} \left[ h^2(x) + g^2(x) a^\dagger a + h(x) g(x) (a + a^\dagger) \right] - i \hbar \eta (a - a^\dagger) - \hbar \Delta_a a^\dagger a.
\]
This simplified effective atom-field Hamiltonian will be the basis of our further considerations. It is, however, still much too complex for a general solution and we will have to make further simplifying assumptions. Hence at this point we will restrict ourselves to 1D motion along the cavity axis. In an experimental setup this could be actually realized by a deep radial trapping potential, but we think that at least qualitatively the model should also capture the essential physics if some transverse motion of the particles was allowed. As one consequence this assumption requires a rescaling of the effective two-body interaction strength [47], which enters as a free parameter in our model anyway.

Mathematically we thus end up with a one-dimensional optical lattice, which is partly generated by the resonator field and superimposed onto a prescribed extra trapping potential \( V_g(x) = V_g(x) \). The mode function of the cavity along the axis is approximated by \( g(x) = g(x) = g_0 \cos(kx) \). Furthermore the laser field behaves as a broad standing wave \( h(x) = h_0 \cos(k_x y) \), which in one-dimensional considerations \( (y = 0) \) is just a constant term that we can eventually omit in [17].

As we consider external pumping of atoms and mode, we essentially treat an open system and we have to deal with dissipation as well. Such dissipation processes are modeled by Liouvillean terms \( \mathcal{L} \) appearing in the master equation for the atom-field density operator, i.e.,

\[
\dot{\rho} = \frac{1}{i\hbar}[H_{\text{eff}}, \rho] + \mathcal{L}\rho. \tag{19}
\]

As mentioned above, we assume large atom-pump detuning \( \Delta_a \), suppressing spontaneous emission to a large extent. However, we still have to deal with the cavity loss \( \kappa \), which will thus be the dominant dissipation process. Hence the corresponding Liouvillean using a standard quantum optics approach [50] reads:

\[
\mathcal{L}\rho = \kappa \left( 2a a^\dagger - a^\dagger a - \gamma a^\dagger a \right). \tag{20}
\]

Equivalently in the corresponding Heisenberg equation for the field operator, cavity loss leads to damping terms and fluctuations, so that it then reads:

\[
\dot{a} = \left\{ i \left[ \Delta_c - \frac{g_0^2}{\Delta_a} \int dx \Psi_g^\dagger(x) \cos^2(kx) \Psi_g(x) \right] - \kappa \right\} a
- i \frac{g_0 h_0}{\Delta_a} \int dx \Psi_g^\dagger(x) \cos(kx) \Psi_g(x) + \eta + \Gamma_{\text{in}}. \tag{21}
\]

Since we will be mainly interested in normally ordered quantities and assume vacuum \((T=0)\) outside the cavity, the input noise operators \( \Gamma_{\text{in}} \) will not enter in the dynamics, such that we will omit them later.

Let us now proceed and transform the Hamiltonian into a more commonly known form. Following standard procedures, one constructs maximally localized eigenfunctions at each site and expands the atomic field operator \( \Psi_g(x) \) in terms of single atom Wannier functions [49]

\[
\Psi_g(x) = \sum_n \sum_k b_{n,k} w_n(x - x_k), \tag{22}
\]

where \( b_{n,k} \) corresponds to the annihilation of a particle in the \( n \)-th energy band at site \( k \). Since we assume the involved energies to be much smaller than the excitation energies to the second band, we are able to keep only the lowest vibrational state in the Wannier expansion, i.e.,

\[
\Psi_g(x) = \sum_k b_k w(x - x_k), \text{ where } w(x) = w_0(x). \tag{20}
\]

This yields to the following Hamiltonian:

\[
H = \sum_{k,l} E_{kl} b_k^\dagger b_l^\dagger + (\hbar U_0 a^\dagger a + V_a) \sum_{k,l} J_{kl} b_k^\dagger b_l^\dagger
+ \hbar \eta_{\text{eff}} (a + a^\dagger) \sum_{k,l} J_{kl} b_k^\dagger b_l^\dagger - i \hbar (a - a^\dagger)
+ \frac{1}{2} \sum_{i,j,k,l} U_{ijkl} b_i^\dagger b_j^\dagger b_k b_l - \hbar \Delta_a a^\dagger a, \tag{23}
\]

where the addendum \( \text{eff} \) of the Hamiltonian is omitted. Here we introduced an important characteristic parameter of atomic cavity QED, namely the refractive index \( U_0 \) of a single atom at an antinode, which is given by \( U_0 = \frac{g_0^2}{\Delta_a} \). It gives the frequency shift of the cavity mode induced by a single atom at an antinode and also corresponds to the optical lattice depth for an atom per cavity photon [17]. Similarly, the parameter \( \eta_{\text{eff}} = g_0 h_0 / \Delta_a \) describes the position dependent effective pump strength of the cavity mode induced by the scattered light from a single atom at an antinode.

Note that the Wannier state expansion Eq.\( \text{[22]} \) depends on the potential depth. Thus the Wannier functions and the corresponding matrix elements depend on the cavity field and thus in principle are dynamic quantities. However, they keep the same functional form with a few changing parameters, which have to be determined consistently. This is of course consequently also true for the various coupling parameters in the Hamiltonian. The above model thus can only be valid as long as the single band approximation stays valid during the system dynamics and the parameters dont change to rapidly. In the special but rather interesting case, where the atoms are trapped solely by the cavity field [21][22] this is not valid for very low photon numbers. Here a single photon number jump will induce excitation to higher bands, which induces nonlinear dynamics beyond the single band model.

In practise this problem can be circumvented by adding an additional external trapping potential \( V_g(x) \) to the model, which guarantees a minimum potential depth even in the case of zero cavity photons. Experimentally this is feasible, for instance, with a far detuned, off-resonant dipole trap (FORT) [21], i.e., \( V_g(x) = V_g \cos^2(k_x x) \), where \( k_F \) denotes the wave number of the FORT field. In the experimental realization, the frequency of the corresponding laser field \( \omega_F \) is only very few free spectral ranges separated from the main cavity frequency \( \omega_c \) [27][52][53]. Hence, in the vicinity of the cavity center, the coincidence of the FORT field and the cavity field is very good, and we can replace in good agreement \( \cos^2(k_F x) \) with \( \cos^2(k x) \).

Let us remark here that by including this extra potential, we can keep our model and allow for further analyti-
an adjustment of the scattering length dimensional on-site interaction strength, originating from the cavity field operators in the Hamiltonian. Explicitly they read as:

\[ E_{kl} = \int dx \, w(x-x_k) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) w(x-x_l), \]

\[ J_{kl} = \int dx \, w(x-x_k) \cos^2(kx)w(x-x_l), \]

\[ \tilde{J}_{kl} = \int dx \, w(x-x_k) \cos(kx)w(x-x_l). \]

The on-site elements \( J_{kk} \) and \( E_{kk} \) are independent of the lattice site \( k \), whereas \( \tilde{J}_{kl} \) changes sign periodically, i.e., \( \tilde{J}_{k,k+1} = 0 \). Note that the existence of this term implies that two adjacent wells acquire different depths forcing us to re-arrange that for the case of the directly pumped atom the on-site terms \( \eta \) are only a small perturbation of the condensate density. As the next-nearest elements are typically two orders of magnitude smaller than the nearest-neighbor term they can safely be neglected (tight-binding approximation). Hence we label the site-independent on-site matrix elements with \( \eta \) and field mediated atom-atom interaction, which appear complex we need some further approximations at this point in order to catch some qualitative insight.

III. CAVITY PUMP

Let us now turn to the conceptually simplest case and restrict the pumping only to the cavity, where only a single mode is coherently excited (cavity pumping). This mode will generate an optical potential in addition to the prescribed external potential. For large enough photon numbers the external potential can even be omitted and the particles are trapped solely by the cavity field. As essential ingredient in the dynamics, the identical coupling of all atoms to this same field mode induces a long-range interaction between the atoms independent of their positions. Setting \( \eta = 0 \), the Hamiltonian \( (26) \) is reduced to:

\[ H = E_0 \hat{N} + \hbar \hat{B} + (\hbar U_0 a^\dagger a + V_C) \left( J_0 \hat{N} + J B \right) \]

\[ - \hbar \Delta_c a^\dagger a - i\eta (a - a^\dagger) + \frac{U}{2} \hat{C}. \]

Here we introduced \( \hat{C} = \sum_k \hat{n}_k (\hat{n}_k - 1) \) for the operator of the two-body on-site interaction. Still we see that the corresponding Heisenberg equation for the cavity field:

\[ \dot{a} = \left\{ i \left[ \Delta_c - U_0 \left( J_0 \hat{N} + J B \right) \right] - \kappa \right\} a + \eta. \]

depends on atom number and coherence. For very weak fields this yields an atom statistics dependent cavity transmission spectrum, which was studied in some detail in Ref. \[33\]. Here we go one step further and study the dynamical back action of the field onto atomic motion and field mediated atom-atom interaction, which appear at higher photon number. As the model is still rather complex we need some further approximations at this point in order to catch some qualitative insight.
A. Field-eliminated Hamiltonian

Although the influence of the cavity field on the atoms is equal on all particles, their common interaction generates a dynamics much more complex than for a Bose-Hubbard model with prescribed external potential. This is more analogous to real solid state physics where the state of the electrons also acts back on the potentials. To exhibit the underlying physics, we will now derive an approximate Hamiltonian, which solely depends on particle variables by adiabatically eliminating the field \( J \). This should be valid when the damping rate \( \kappa \) of the cavity generates a faster time scale than the external atomic degree of freedom. Actually as tunneling is mostly a very slow process (much slower than the recoil frequency), this will be almost always the case in practical experimental setups. To this end, we simply equate \( 2\kappa \) to zero and obtain formally \( a = \eta J \). In the following we constrain ourselves to the case of a fixed number of atoms, i.e., \( N = N_{\text{f}} \). The very small tunneling matrix element \( J \) can be used as an expansion parameter, leading to:

\[
a \approx \frac{\eta}{\kappa - i\Delta_c} \left[ 1 - i \frac{U_0 J}{\kappa - i\Delta_c} \hat{B} - \frac{(U_0 J)^2}{(\kappa - i\Delta_c)^2} \hat{B}^2 \right].
\]

(30)

where we introduced a shifted detuning \( \Delta_c' = \Delta_c - U_0 J_0 N \).

In order to obtain an effective Hamiltonian, where the cavity degrees of freedom are eliminated, we replace the field terms in (28), by the steady state expressions (30), as well as in the Liouville super operator (20). Note, that this is more appropriate than the naive approach of a replacement just in the Hamiltonian, as has been done in our former work [32]. If we consider terms up to order \( \propto J^2 \), the exchange in the Hamiltonian yields:

\[
H_{\text{ad}} = (E + J V_c) \hat{B} + \frac{U}{2} \hat{C} \\
+ \frac{\hbar U_0 J \eta^2}{\kappa^2 + \Delta_c^2} \left( \frac{\Delta_c^2 - \kappa^2}{\kappa^2 + \Delta_c^2} \hat{B} - \frac{3 \hbar U_0 J \Delta_c'}{\kappa^2 + \Delta_c^2} \hat{B}^2 \right).
\]

(31)

Next, by applying the same procedure to the Liouville equation - again up to terms \( \propto J^2 \) - we obtain an adiabatic Liouville operator:

\[
\mathcal{L}_{\text{ad}} = -i \left[ \frac{2 \hbar U_0 J \eta^2}{(\kappa^2 + \Delta_c^2)^2} \left( \hat{B} + \frac{2 \Delta_c' \hbar U_0 J}{\kappa^2 + \Delta_c^2} \hat{B}^2 \right), \theta \right] \\
+ \frac{\kappa \hbar^2 J \eta^2}{(\kappa^2 + \Delta_c^2)^2} \left( 2 \hat{B} \theta \hat{B} - \hat{B}^2 \theta - \theta \hat{B}^2 \right).
\]

(32)

The Lindblad terms in the second line are real, corresponding to dissipation, whereas the first, imaginary term corresponds to a unitary time evolution and has therefore to be added to the adiabatic Hamiltonian, i.e.,

\[
H_{\text{ad}} = H_{\text{ad}} + \frac{2 \hbar U_0 J \eta^2}{(\kappa^2 + \Delta_c^2)^2} \left( \hat{B} + \frac{2 \Delta_c' \hbar U_0 J}{\kappa^2 + \Delta_c^2} \hat{B}^2 \right).
\]

Altogether, we end up with a Hamiltonian, where the cavity field has been eliminated:

\[
H_{\text{ad}} = (E + J V_c) \hat{B} + \frac{U}{2} \hat{C} \\
+ \frac{\hbar U_0 J \eta^2}{\kappa^2 + \Delta_c^2} \left( \hat{B} + \frac{U_0 J \Delta_c'}{\kappa^2 + \Delta_c^2} \frac{\kappa^2 - 3 \Delta_c^2}{\kappa^2 + \Delta_c^2} \hat{B}^2 \right).
\]

(33)

The loss rate of the cavity is described by the remaining dissipative part of (32):

\[
\mathcal{L}_{\text{ad}} \theta = \frac{\kappa \hbar^2 J \eta^2}{(\kappa^2 + \Delta_c^2)^2} \left( 2 \hat{B} \theta \hat{B} - \hat{B}^2 \theta - \theta \hat{B}^2 \right).
\]

(34)

Note, that the above adiabatic elimination procedure is not completely unambiguous due to ordering freedom. Nevertheless it should give a qualitatively correct first insight. An alternative way of deriving an effective Hamiltonian, depending solely on particle observable is similar to (10) and (17). This amounts to a replacement of the field variables with (30) in the Heisenberg equation for the external atomic degrees of freedom, which read as follows:

\[
b_k = \frac{1}{\hbar} \left[ (E + J V_{cl}) (b_{k-1} + b_{k+1}) - U \hat{n}_k b_k \right].
\]

(35)

A naive replacement of the field operator \( a \) and its adjoint \( a^\dagger \) by (30) in the above expression leads to an equation for \( b_k \), which cannot be generated from an effective adiabatic Hamiltonian in the form \( b_k = -i \hbar [b_k, H_{\text{ad}}] \). Hence, before substituting the adiabatic field operators, we have to symmetrize the expression containing the field term in (35) in the form

\[
b_k = - \frac{1}{\hbar} \left[ (E + J V_{cl}) (b_{k-1} + b_{k+1}) - U \hat{n}_k b_k \right] \\
- \frac{i \hbar U_0 J}{2} \left[ a^\dagger a (b_{k-1} + b_{k+1}) + (b_{k-1} + b_{k+1}) a^\dagger a \right].
\]

(36)

This form enables us to describe the dynamics of \( b_k \) by a Heisenberg equation with an effective Hamiltonian, which up to second order in \( J \) reads:

\[
H_{\text{ad}} = (E + J V_c) \hat{B} + \frac{U}{2} \hat{C} \\
+ \frac{\hbar U_0 J \eta^2}{\kappa^2 + \Delta_c^2} \left( \hat{B} + \frac{U_0 J \Delta_c'}{\kappa^2 + \Delta_c^2} \frac{\kappa^2 - 3 \Delta_c^2}{\kappa^2 + \Delta_c^2} \hat{B}^2 \right).
\]

(37)

The terms in the second line stem from the field terms in (33). Although this Hamiltonian looks a bit different from the first version derived before (33), their properties are - within their regime of validity - in very good agreement as long as hopping is slow compared to damping.

To exhibit the physical content of this Hamiltonian one can look at its eigenstates. As first step we calculate the Mott insulator state (see Eq. (48)) fraction of the
density operator in powers of \( \epsilon \) is supposed to be constant. This allows to expand the site interaction energy for different values of \( \Delta' \). This will indicate changes of position and behavior of the Mott insulator superfluid transition (see Fig. 1). To compare the two approximate Hamiltonians in Fig. 2 we plot the difference of the Mott insulator fraction of the ground state of (33) and (37), as well as the difference of the steady state photon number. Obviously the two Hamiltonians, converge in the limit of large cavity decay \( \kappa \). This can also be seen in Fig. 2 where the dashed-dotted line depicts the case of a smaller \( \Delta' \) (which is equivalent to an enlarged \( \kappa \)), showing a strongly enhanced coincidence.

### B. Field-eliminated density operator

Let us now use a further and somehow more systematic alternative approach to eliminate the cavity field dynamics from the system evolution directly from the Liouville equation by following a method proposed by Wiseman and Milburn [53], which is valid for large \( \kappa \) and low photon numbers. In this case we have

\[
\frac{|\langle H_{at} \rangle|}{\kappa} \sim \frac{|hU_{0}(a^\dagger a)|}{\kappa} = \epsilon \ll 1, \quad (38)
\]

where \( H_{at} \) is the atomic part of (28), i.e., \( H_{at} = (E + V_{4}J) \hat{B} + U \hat{C}/2 \). Again the total atom number \( N \) is supposed to be constant. This allows to expand the density operator in powers of \( \epsilon \), corresponding to states with increasing photon number:

\[
\rho = \varrho_{0} \otimes |0\rangle_{a}\langle 0| + (\varrho_{1} \otimes |1\rangle_{a}\langle 0| + h.c.) + \varrho_{2} \otimes |1\rangle_{a}\langle 1| + (\varrho_{2}' \otimes |2\rangle_{a}\langle 0| + h.c.) + O(\epsilon^{3}). \quad (39)
\]

Here \( \varrho_{i} \) are density operators for the particle variables, corresponding to the order \( i \) of magnitude in the expansion parameter \( \epsilon \). We substitute this expression into the Liouville equation (19) with the Hamiltonian from (28), which leads to the following set of equations:

\[
\dot{\varrho}_{0} = \frac{1}{i\hbar} [H_{at}, \varrho_{0}] - \eta \left( \varrho_{1} + \varrho_{1}^\dagger \right) + 2\kappa \varrho_{2}, \quad (40a)
\]

\[
\dot{\varrho}_{1} = \frac{1}{i\hbar} [H_{at}, \varrho_{1}] - \eta \left( \sqrt{2} \varrho_{2}' + \varrho_{2} - \varrho_{0} \right) - \kappa \varrho_{1}(40b)
\]

\[
+ i \left[ \Delta_{c} - U_{0} \left( J_{0}N + J\hat{B} \right) \right] \varrho_{1} + \kappa O(\epsilon^{4})
\]

\[
\dot{\varrho}_{2} = \frac{1}{i\hbar} [H_{at}, \varrho_{2}] + \eta \left( \varrho_{1} + \varrho_{1}^\dagger \right) - 2\kappa \varrho_{2}, \quad (40c)
\]

\[
- iU_{0} \left[ J_{0}N + J\hat{B}, \varrho_{2} \right] + \kappa O(\epsilon^{4})
\]

\[
\dot{\varrho}_{2}' = \frac{1}{i\hbar} [H_{at}, \varrho_{2}'] + \sqrt{2} \varrho_{0} \varrho_{2}' - 2\kappa \varrho_{2}' \quad (40d)
\]

\[
+ 2i \left[ \Delta_{c} - U_{0} \left( J_{0}N + J\hat{B} \right) \right] \varrho_{2}' + \kappa O(\epsilon^{4})
\]

Now we adiabatically eliminate the off-diagonal elements \( \varrho_{1} \) and \( \varrho_{2}' \). Setting their derivations in (40b) and (40d)
to zero and neglecting terms with respect to the assumption \( [38] \), we obtain:

\[
\dot{\varphi}_2 = \frac{\eta}{\sqrt{2A}} \varphi_1 + O(\varepsilon^3). \tag{41}
\]

This is consistent with the assumption \( \dot{\varphi}_2 \sim O(\varepsilon^2) \). Here we defined \( A = \kappa - i\Delta_c^1 + iU_0J\tilde{B} \). Putting \( \dot{\varphi}_1 \) into \( \dot{\varphi}_2 \) and neglecting the terms consistent with the order of the expansion, such that \( \varphi_1 \sim O(\varepsilon) \), it follows that:

\[
\varphi_1 = \frac{\eta}{A + \eta^2/A} (\varphi_0 - \varphi_2) + O(\varepsilon^4). \tag{42}
\]

We simplify this expression, \( \varphi_1 = \eta A^{-1}(\varphi_0 - \varphi_2) \), which is consistent with the above expansion and substitute it into \( [40a] \) and \( [40c] \):

\[
\dot{\varphi}_0 = \frac{1}{i\hbar} \left[ H_{\text{at}}, \varphi_0 \right] + 2\kappa \varphi_2 \\
- \eta^2 \left[ A^{-1}(\varphi_0 - \varphi_2) + (\varphi_0 - \varphi_2)A^{-1} \right] \tag{43a}
\]

\[
\dot{\varphi}_2 = \frac{1}{i\hbar} \left[ H_{\text{at}}, \varphi_2 \right] - iU_0 \left[ J_0N + J\tilde{B}, \varphi_2 \right] - 2\kappa \varphi_2 \\
+ \eta^2 \left[ A^{-1}(\varphi_0 - \varphi_2) + (\varphi_0 - \varphi_2)A^{-1} \right]. \tag{43b}
\]

In order to formulate a master equation for the particle variables we have to use the reduced density operator, where we trace over the field variables, i.e., \( \dot{\varphi}_{\text{at}} = \text{tr}(\varphi) = \varphi_0 + \varphi_2 + O(\varepsilon^4) \). With \( [43a] \) and \( [43b] \) we see that:

\[
\dot{\varphi}_{\text{at}} = \frac{1}{i\hbar} \left[ H_{\text{at}}, \varphi_{\text{at}} \right] - iU_0 \left[ J_0N + J\tilde{B}, \varphi_{\text{at}} \right]. \tag{44}
\]

As a further approximation, which is also consistent with the expansion order of the assumption \( [38] \), we set \( \kappa \) to zero and neglect \( [H_{\text{at}}, \varphi_2] \) and all other terms smaller than \( O(\varepsilon^3) \). Then we can express \( \varphi_2 \) through \( \varphi_0 \):

\[
\varphi_2 = \frac{\eta^2}{2\kappa} \left[ A^{-1}\varphi_0 + \varphi_0 A^{-1} \right]. \tag{45}
\]

Within this order of magnitude of \( \varepsilon \) we can replace \( \varphi_0 \) with \( \varphi_{\text{at}} \), leading us finally to the following master equation for the reduced density operator of the particle variables:

\[
\dot{\varphi}_{\text{at}} = \frac{1}{i\hbar} \left[ H_{\text{at}}, \varphi_{\text{at}} \right] - iU_0 \left[ \frac{\eta^2}{2\kappa} \left[ A^{-1}\varphi_0 + \varphi_0 A^{-1} \right] \right]. \tag{46}
\]

Note that this model also contains a damping part, since the operator \( A \) is not hermitian. Let us investigate this damping, by expanding the inverse of \( A \) up to first order in \( J \), which is consistent with the order of magnitude in \( [49] \). Hence we replace \( A^{-1} \) and its adjoint in this equation by

\[
A^{-1} \approx \frac{1}{\kappa - i\Delta_c^1} \left( 1 - iU_0J \frac{\kappa}{\kappa - i\Delta_c^1} \right). \tag{47}
\]

and its adjoint. Since we are restricted on a subspace of constant atom number, the Liouville equation reads as follows:

\[
\dot{\varphi}_{\text{at}} = \frac{1}{\hbar} \left[ H_{\text{at}} + \frac{\hbar U_0}{\kappa^2 + \Delta_c^1} \left( \frac{J\tilde{B} + U_0\Delta_c^1\varphi_{\text{at}}}{\kappa^2 + \Delta_c^1} \right)^2, \varphi_{\text{at}} \right] - \frac{(JU_0)\eta^2}{\kappa^2 + \Delta_c^1} \left[ \tilde{B}, \left[ \tilde{B}, \varphi_{\text{at}} \right] \right]. \tag{48}
\]

Obviously, the non-dissipative part of this equation agrees perfect with our adiabatically eliminated Hamiltonian \( [37] \) and the structure of the dissipative part is of the same Lindblad form as \( [33] \). Note that an expansion of \( A^{-1} \) to higher order in \( J \) would also provide us the correct next-order term of \( [37] \) plus an extra term in the Liouville-equation, which does not correspond to unitary time evolution, as described by a Hamiltonian. This confirms the usefulness of the naive elimination method, also used in Ref. \( [32] \).

C. Quantum phase transitions in an optical lattice

In section \( \text{III A} \) we derived two approximate Hamiltonians \( [33] \) and \( [37] \) describing our system of cold atoms in an optical lattice. To a large extend they still implement the well known BH model, but with parameters controllable via cavity detuning and some additional nonlocal interaction terms. Let us now investigate their properties in some more detail. One of the key features of optical cavities is the feedback mechanism between atoms and cavity field. Hence, computations are a subtle issue, since the matrix elements in the BH Hamiltonian depend on the field amplitude, which itself depends on the atomic positions. In principle a rigorous treatment would consist of calculating the matrix elements \( [24] \) for every photon Fock state and treating the parameters of the BH model as operators. To avoid the full complexity of such an approach we will first assume only a weak dependence of the Wannier functions on the mean cavity photon number \( \langle \hat{a}\hat{a}' \rangle \), which allows us to proceed analytically. For any set of operating parameters we then calculate the matrix elements in a self-consistent way replacing the photon number operator by its average in the iteration process. Explicitly this is implemented by starting from some initial guess \( \hat{a}\hat{a}' \) in the Hamiltonian \( [37] \), from which we calculate the ground state \( \langle \psi(0) \rangle \). By use of this state we obtain an initial mean photon number \( \langle \hat{a}\hat{a}' \rangle \), which allows us to proceed analytically. For any set of operating parameters we then calculate the matrix elements in a self-consistent way replacing the photon number operator by its average in the iteration process. Explicitly this is implemented by starting from some initial guess \( \hat{a}\hat{a}' \) in the Hamiltonian \( [37] \), from which we calculate the ground state \( \langle \psi(0) \rangle \). By use of this state we obtain an initial mean photon number \( \langle \hat{a}\hat{a}' \rangle \), which allows us to proceed.
cavity photon number (cf. Fig. 3), which occurs for \( \Delta_c = U_0 J_0 N - \kappa \), especially for large \( U_0 \). Introducing some damping in the iteration procedure easily resolves this issue, though. As we mentioned already before, we restrict the model on a subspace \( \mathcal{H}_N \) of a fixed total particle number \( N \) in an optical lattice of \( M \) sites. A basis of \( \mathcal{H}_N \) consists of the states \( |N,0,0,\ldots,0\rangle,|N-1,1,0,\ldots,0\rangle,\ldots,|0,0,\ldots,0,N\rangle \). Since we are interested in the quantum phase transition between the Mott insulator (MI) and the superfluid (SF) state occurring during the variation of certain external parameters, we investigate the contributions of these specific states to the ground state of the atomic system. The Mott insulator state is a product of Fock states with uniform density distribution, i.e.,

\[
|\text{MI}\rangle = |n,n,\ldots,n\rangle,
\]

with \( n = N/M \). In contrast, in a SF state each atom is delocalized over all sites. It is given by a superposition of Fock states, namely of all possible distributions of the atoms in the lattice sites, i.e.,

\[
|\text{SF}\rangle = \sum_{k_1,k_2,\ldots,k_M} \frac{N!}{\sqrt{M^N} \sqrt{k_1!k_2!\cdots k_M!}} |k_1,k_2,\ldots,k_M\rangle,
\]

with \( \sum_{i=1}^{M} k_i = N \). Although the density in the superfluid state is also uniform \( \langle \hat{n}_i \rangle_{\text{SF}} = N/M \) and therefore equal to the Mott insulator state, its properties are fundamentally different. This manifests especially in the spectra and angle dependence of scattered light, providing for new, non-destructive probing schemes for the atomic phases \([34-35]\).

Let us now investigate the influence of the cavity on position and shape of the well-known “classical” MI-SF-transition \([34,35]\). To do so, we compare the two cases of a pure quantum field, i.e., \( V_{cl} = 0 \) in \([37]\), and a classical field \( (\eta = 0) \) provided by \( V_{cl} \) for generating the optical potential. We choose \( \eta \) in such a way, that at zero on-site interaction, \( g_{1D} = 0 \), both potentials are equally deep. As depicted in Fig. 4, the influence of the cavity strongly depends on the detuning \( \Delta_c \). Two contributions arise from the quantum nature of the potential. On the one hand the potential depth and therefore the matrix elements depend on the atomic state. For a classical potential this is clearly not the case. On the other hand the cavity mediates long-range interactions via the field, which corresponds to the \( \hat{B}^2 \)-term in \([37]\). If a potential depth near the phase transition point for the quantum case is associated with some certain average photon number \( \bar{n} \), then \( \bar{n} \pm 1 \) are associated with different atomic phases. This means that the ground state of the quantized cavity field contains contributions of different atomic states, each of them correlated with the corresponding photon number. In this sense photon number fluctuations drive particle fluctuations. Depending on parameters the former or the latter effect contributes more. In Fig. 4, this is shown for four atoms in four wells, where we calculated the occupation probability for the Mott insulator \( p_{\text{MI}} = |\langle \psi | \text{MI} \rangle|^2 \) and the superfluid state \( p_{\text{SF}} = |\langle \psi | \text{SF} \rangle|^2 \) as a function of the dimensionless one-dimensional on-site interaction strength \( g_{1D}/(\kappa \omega_R) \) for a purely classical and a purely quantum case. For \( \Delta_c - U_0 J_0 N = \kappa \), photon number fluctuations enhance particle fluctuations, shifting the superfluid to Mott insulator transition to higher values of the on-site interaction [Fig. 4(a)]. However, if we choose \( \Delta_c - U_0 J_0 N = -\kappa \), the influence of the atomic state on the potential depth exceeds the cavity-mediated long-range interactions, strongly shifting the transition to lower values of \( g_{1D} \) [Fig. 4(b)]. Note, that for this behavior, the cavity loss rate must be - although within the bad cavity limit - small enough. For larger \( \kappa \) the quantum effects disappear and the ground states for classical and quantum potential coincide.

To correctly address the long-range interactions, corresponding to the \( \hat{B}^2 \) term in \([37]\), we calculate the contribution of the Mott insulator state to the ground state of this adiabatic Hamiltonian including and omitting the \( \hat{B}^2 \) part, respectively. Although, in the situation of Fig. 4(b) the net effect enhances the phase transition, the cavity mediates long-range coherence via \( \hat{B}^2 \), which can be seen by enlarged particle number fluctuations as shown in Fig. 4. Although the effect is not too strong as it depends on \( J^2 \) is has infinite range and will get more important for large particle numbers.

Finally, we exhibit the transition from a cavity field with quantum properties towards a classical optical lattice. This relies on the assumption that a very bad cavity should be almost like no cavity and increasing \( \kappa \), but keeping the potential depth constant, approaches the classical limit. Hence, the effects of the quantum nature and feedback of lattice potential should disappear and the ground states for classical and quantum potential coincide. The adiabatic eliminated Hamiltonian then has to approach the classical Bose-Hubbard Hamiltonian. This is shown in Fig. 5 for a system of four atoms in four wells, where we simultaneously increase \( \kappa \) and \( \eta \), keeping
FIG. 4: (color online) Cavity influence of the Mott insulator to superfluid transition by means of a comparison of the occupation probabilities $p_{MI}$ and $p_{SF}$ for a purely quantum field, i.e., $V_{cl} = 0$, and a purely classical field, i.e., $\eta = 0$, as a function of the dimensionless one-dimensional on-site interaction strength $g_{1D}/(dE_R)$. We choose $\eta$ such that both potentials are of equivalent depth, $V = 5.5E_R$, for zero on-site interaction ($g_{1D} = 0$). The quantum and classical case is depicted with solid and dashed lines, respectively. In (a) we set $(U_0, \kappa, \eta) = (-1, 1/\sqrt{2}, \sqrt{5.5})\omega_R$ and $\Delta_c - U_0J_0N = \kappa$. (b) The same as (a) but with $\Delta_c - U_0J_0N = -\kappa$.

$U_0\eta^2/\kappa^2 = -6E_R$ fixed. For every $\kappa$ we calculated the value of the on-site interaction $g_{1D}$, where the contributions of the Mott state and the superfluid state to the ground state of the Hamiltonian are equal, i.e., $|\langle \psi | \text{MI} \rangle| = |\langle \psi | \text{SF} \rangle|$. This is compared with the corresponding value of the interaction strength at the same intersection point of a purely classical Bose-Hubbard model with a potential depth of $V_{cl} = -6E_R$. We see that the transition occurs already at a cavity linewidth of only an order of magnitude larger than the recoil frequency, where the deviation is small already. Thus one needs quite good resonators to see the quantum shift in the phase transition.

D. Comparison with the full dynamics of the master equation

Using the approximate adiabatic model with eliminated field we have found important changes in the physics so far. Even stronger effects are to be expected in the limit of less and less cavity damping and stronger atom field coupling. Let us now investigate some first
signs of this and test the range of validity of the above model in this limit. To do so we have to resort to numerics and compare solutions of the full master equation (19) with the ground states of the adiabatically eliminated Hamiltonian (37). Obviously solving the full master equation is a numerically demanding task. Nevertheless, by constraining to few atoms in few wells we are able to solve the equations and reveal the essential physical mechanisms. The limit of the band model description is of course reached for atoms coupled strongly to a cavity field with only very few photons and no additional classical potential $V_C$ present. Here very strong changes in the tunneling amplitudes occur whenever a photon leaks out of the cavity and reduces the momentary potential depth. This leads to strongly enhanced particle hopping. For instance, one can think of the situations “one photon present” and “no photon present”, where the atoms can freely move within the cavity in the absence of an external trap. On the other hand one extra photon can almost block hopping. Note that in this case the ground state atomic configuration can be close to superfluid for a low photon number and close to an insulator state for a higher photon number. As our matrix elements depend only on the mean photon number $\langle \alpha | \alpha \rangle$, these differences cannot be taken into account in an adiabatic model.

We can explicitly show this behavior by reducing the coupling strength $U_0$, but keeping the average potential depth fixed (equal matrix elements), by means of a higher average cavity photon number, which leads to strongly reduced photon number fluctuations. The most simple situation to discuss this issue is one atom loaded in a lattice consisting of only two wells. Here, $|l\rangle (|r\rangle)$ means the left (right) of the two wells, with a potential minimum at $x = 0$ ($x = \pi$). The hopping operator $\hat{B}$ then describes tunneling from the left well to the right well and vice versa. In Fig. 7 we show this tunneling behavior by plotting the mean position of the single atom $\langle kx(t) \rangle$.

The atomic ground state of this system is the symmetric state $|\psi_0\rangle = (|l\rangle + |r\rangle)/\sqrt{2}$ having a mean position of $\langle kx \rangle_{\psi_0} = \pi/2$. Decreasing $U_0$, increasing $\eta$ and adjusting $\Delta_c$, yields different mean photon numbers $\langle \alpha | \alpha \rangle$, but equal average lattice potential depth $V = U_0 \langle \alpha | \alpha \rangle$. (We do not consider an additional classical potential here.) If only few photons are present, we observe large fluctuations of the field and the system damps fast to the ground state. As the photon number increases, the potential approximates a classical potential as expected, where there is no dephasing. The (nearly) equal oscillation frequencies show that the matrix elements coincide for the different photon numbers. This is an interesting feature corresponding to the quantum nature of the potential.

In contrast to the Bose-Hubbard model for a classical optical lattice, lattice depth and interaction strength are not the only important system parameters. Quantum fluctuations of the potential are an additional source of atomic fluctuations, playing an essential role in the evolution of the system. Obviously, if only an external potential is present and the atom is no longer coupled to the cavity field ($U_0 = 0$), the system is undamped, due to the lack of the only dissipation channel present, cavity loss. In this case the Hamiltonian (28) reduces to $H = (E + JV_C) \hat{B} + U/2 \hat{C}$, and the atom, initially not in the symmetric state, oscillates between the left and right well. Note that a more rigorous treatment of operator-valued matrix elements - as described in the previous section - would be capable of describing this behavior correctly. Alternatively for few atoms Monte-Carlo wave function simulations of the full Hamiltonian could be performed, allowing for processes, where the particle leaves the lowest band (35).

![FIG. 7: (color online) Mean position $\langle kx(t) \rangle$ of a single atom in two wells. We adjusted $U_0, \eta, \Delta_c$ in such a way, that the mean number of cavity photons increases, but the lattice depth stays nearly constant: $V = \hbar U_0 \langle \alpha | \alpha \rangle = -8 E_R$. Starting with $(U_0, \eta, \Delta_c) = (-50, 10, 25)$ (in units of $\omega_R$) and $\Delta_c = J_0 U_0$, followed by a successive reduction of $U_0$ by a factor of 5, together with an increase of $\eta$ by a factor of $\sqrt{5}$ and a proper adjustment of $\Delta_c$, this leads to mean photon numbers of 0.16 (solid line), 0.8 (dashed line), and 4 (dashed-dotted line). Initially, the atom is in the right well.](image)

Obviously, this enhancement of atom fluctuations for low photon numbers also affects the dynamics of several atoms. We demonstrate this for the case of two atoms in two wells. We assume strong coupling with few cavity photons and a strong on-site interaction, which - in principle - inhibits tunneling and drives the system deeply into the Mott insulator regime. However, starting from a state slightly perturbed from the ground state of the adiabatically eliminated Hamiltonian (37), the system does not evolve towards this Mott-like ground state but towards some other, drastically different state. Increasing the photon number, while keeping the lattice depth constant, reduces the atom fluctuations and keeps the system near its adiabatic ground state. This is shown in Fig. 8(a), where the probability for the system being in the Mott insulator regime $p_{\text{MI}} = |\psi_{\text{MI}}(t)|^2$ is plotted. Again we observe that, the larger the intracavity photon number is, the more the potential approaches a purely classical one and the more significant the ground state
probabilities of $|57\rangle$ are. Hence we see that including the photon number fluctuations strongly suppresses the Mott insulator state by allowing the particles to hop during photon number fluctuations. This is also a strong restriction for the use of our adiabatic model Hamiltonian, where only average photon numbers enter the model parameters.

Clearly, some added external classical potential diminishes this problem as it can ensure the existence of a bound state, independent of the number of cavity photons, giving an upper limit to the hopping rate. This is demonstrated in Fig. 8(b), where a classical potential of $V_{cl} = -5E_R$ is added. Here for $\langle a^\dagger a \rangle = 1.44$ the deviations from the adiabatic ground state are of the same order as for $V_{cl} = 0$ for $\langle a^\dagger a \rangle = 4.8$ [Fig. 8(a)]. Nevertheless, for not too leaky cavities ($\kappa$ is in an intermediate regime), the regime of validity of the adiabatically eliminated Hamiltonian $|57\rangle$ is limited to case where either a large purely classical potential or a large photon number is given.

Finally, we investigate the other limit of validity, where a rather large external classical potential, but only a very low photon number is given, i.e., a weakly driven cavity. Here the ground state properties of our model resemble to a very high degree those of the ordinary Bose-Hubbard model. As mentioned above, an atomic ensemble interacting with a purely classical potential, has no channels of dissipation in the absence of spontaneous emission. So unless we prepare the system in its groundstate, it will show undamped oscillation. In strong contrast the coupling of the atoms to an even small intracavity field with a very low photon number opens a dissipation channel. Although the enhancement of atom number fluctuations due to fluctuation induced tunneling is small, this damping still can drive the system into a steady state, very closely to the adiabatic ground state of $|57\rangle$. This is shown in Fig. 9 for the case of two atoms in two wells. Here we prepare, for different values of on-site interaction, the atoms in a state perturbed from the ground state of $|57\rangle$ with initially no photon in the cavity and a given value of the classical potential $V_{cl} = -10E_R$. For $g_{1D} = 0$, the ground state is the superfluid state, so Fig. 9(a) is the generalization of Fig. 7 to two atoms. Although the photon number is only $\langle a^\dagger a \rangle = 1.3 \times 10^{-4}$, the system is driven into its ground state. For increasing interaction strength, the Mott insulator state becomes more and more favored. Still, the interaction with the tiny intracavity field enables damping of the atomic evolution towards a steady state, very close to the adiabatic ground state.

This leads to the conclusion, that, although the cavity field may not lead to significant modifications of the ground state of the system, the cavity is a useful tool for faster preparing a system of atoms in its ground state by opening a dissipation channel, so that it decays towards an eigenstate of the adiabatically eliminated Hamiltonian $|57\rangle$.

![Figure 8](image)

**FIG. 8**: (color online) Probability of the Mott insulator state $|\psi_{MI}(t)\rangle^2$ for two atoms in two wells. Parameters and procedure as in Fig. 4, but due the second atom the photon numbers are increased. The on-site interaction is $U = 0.32E_R$. (a) $V_{cl} = 0$. The curves correspond to a mean photon number of 0.19 (solid line), 0.97 (dashed line), 4.8 (dashed-dotted line) and 24.2 (dotted line). (b) $V_{cl} = -5E_R$ and corresponding photon numbers of 0.05 (solid line), 0.28 (dashed line), 1.44 (dashed-dotted line).

### IV. ATOM PUMPING

Let us now return to our starting Hamiltonian $|24\rangle$ and consider a second generic model, where the pump laser is not injected through the cavity mirrors, but directly illuminating the atoms. This rather small change has a drastic influence on the physical behavior of this system. In the case of cavity pumping, all atoms are simultaneously coupled to the same mode. In this way the cavity field depends on the atomic distribution and long range order interactions are mediated via the cavity field, influencing the Mott-insulator to superfluid phase transition. In the new geometry, only the directly excited atoms coherently scatter photons in the cavity mode. Due to the position-dependent coupling, the scattered field amplitude and phase for each atom is strongly position dependent. Atoms located at nodes are not coupled to the field, leading to no scattering, whereas atoms at antinodes
are maximally coupled, leading to maximum scattering. Atoms in adjacent wells are separated by half a wavelength and scatter with opposite phases, such that their contributions to the scattered field interfere destructively. Naively one would thus immediately conclude that atoms forming a state with a homogeneous density scatter no field at all so that nothing happens [34, 35]. Nevertheless, fluctuations of the density still can allow for reorganization. To study this effect we assume the coherent pump field to be a broad plane wave propagating transversally to the cavity axis (see Fig. 1) replacing the empty one. Hence this changes the translational periodicity of the optical lattice from \( \lambda/2 \) to \( \lambda \). Such bistable behavior was observed by Vušetić and coworkers [20] and explained in a semiclassical treatment [18].

Let us now turn to a quantum treatment of atoms and field. Naive adiabatic elimination encounters a first difficulty, as the operators \( \hat{B}, \hat{B}^\dagger \) do not commute, \( [\hat{B}, \hat{B}^\dagger] \neq 0 \). Hence this already creates an ordering problem in the formal steady-state solution of (52), which gets even more difficult when it comes to the replacement of the field operators to obtain an effective Hamiltonian (51). Unfortunately also the second approach used in the case of cavity pumping, namely reading off an effective Hamiltonian from the particle operator Heisenberg equation does not resolve this problems. Replacing \( a \) with the steady-state expression in (53) leads to a rather complex form, so that there is no simple way to find a suitable effective Hamiltonian \( H_{ad} \), with \( \{ \hat{b}, \hat{B}^\dagger \} = \{ \hat{b}_k, H_{ad} \} \).

Hence we see that the occupation number difference drives the cavity field, which then in turn starts to dephase neighboring atom sites via the first term in the second line of Eq. (53). Note that this interesting part of the dynamics even survives for deeper lattices when \( J \) is negligibly small and \( \tilde{\eta}_0 \) is of order unity. This will be discussed in more detail using various approximations below.

A. Field-eliminated Hamiltonian

Adiabatic elimination of the field variables is a bit more subtle here as compared to the cavity pump case discussed before. The scattering amplitude of light into the cavity mode here depends strongly on the atomic positions. Hence even small position changes have a large influence on the cavity field dynamics. The maximum photon number is established when all the atoms are well localized at either only odd or only even lattice sites. For red atom field detuning this increases the lattice depth and forces the atoms into one of two stable patterns, where the wells where atoms are located are deeper than the empty ones. Hence this changes the translational periodicity of the optical lattice from \( \lambda/2 \) to \( \lambda \). Such bistable behavior was observed by Vušetić and coworkers [20] and explained in a semiclassical treatment [18].

At \( T = 0 \) quantum fluctuations still can trigger this reorganization. To study this effect we assume the coherent pump field to form a broad plane wave propagating to the cavity axis (see Fig. 1) replacing cavity pumping. This means that we set \( \eta = 0 \) and the Hamiltonian (50) for constant atom number \( N \) reads as follows:

\[
H = \left( E + jV_{cl} \right) \hat{B} + \hbar (U_0 J_0 N - \Delta_c) \hat{a}^\dagger \hat{a} + \frac{U}{2} \hat{\tilde{C}} + jU_0 J_0 \hat{a}^\dagger \hat{a} \hat{B} + \hbar \eta_{eff} (\hat{a} + \hat{a}^\dagger) \tilde{\eta}_0 \tilde{D}.
\]

Here we introduced the operator \( \tilde{D} = \sum_k (-1)^{k+1} \hat{n}_k \) describing the difference in atom number between odd and even sites. The corresponding Heisenberg equation for the cavity field (27) reads as follows:

\[
\dot{a} = \left\{ i \left[ \Delta_c - U_0 \left( J_0 N + j \tilde{D} \right) \right] - \kappa \right\} a - i \eta_{eff} \tilde{\eta}_0 \tilde{D}.
\]

Consequently the Heisenberg equation for the particle operators is:

\[
\dot{b}_k = (E + jV_{cl} - iU_0 J a^\dagger a) (b_{k+1} + b_{k-1}) - i \eta_{eff} \tilde{\eta}_0 (a + a^\dagger) (-1)^{k+1} b_k + U \hat{n}_k b_k.
\]
\[ \dot{a} = (i\Delta'_c - \kappa) a - i\eta_{\text{eff}} \hat{J}_0 \hat{D}. \]  

(54)

The steady-state solution of this equation is immediately at hand and free of ordering ambiguities of noncommuting operators.

\[ a = \frac{i\eta_{\text{eff}} \hat{J}_0}{i\Delta'_c - \kappa} \hat{D}. \]  

(55)

Also the particle operator equation is much simpler within this approximation:

\[ \dot{b}_k = (E + JV_{\text{cl}})(b_{k-1} + b_{k+1}) - i\eta_{\text{eff}} \hat{J}_0 (a + a^\dagger)(-1)^{k+1}b_k + U\hat{n}_k b_k. \]  

(56)

In this form one then can find a well defined effective Hamiltonian only containing particle operators. Let us thus proceed as in Sec. 11.2 and simply substitute (55) and its adjoint into (51). This yields the effective Hamiltonian:

\[ H_{\text{ad}} = (E + JV_{\text{cl}}) \hat{B} + \frac{U}{2} + \frac{h\hat{J}_0^2\eta_{\text{eff}}^2\Delta'_c}{\kappa^2 + \Delta'_c^2} \hat{D}^2. \]  

(57)

Within first order in \( J \) the replacement of the field variables in the Liouvillian part of the master equation (20) in this case does not provide an extra terms to be included in the Hamiltonian. So the effective cavity decay induced dissipation of the atomic dynamics takes the simple and intuitive form:

\[ \mathcal{L}_{\text{ad}} \theta = \frac{\kappa^2 \eta_{\text{eff}}^2 \hat{J}_0^2}{\kappa^2 + \Delta'_c^2} \left( 2\hat{D} \theta - \hat{D}^2 \theta - \theta \hat{D}^2 \right). \]  

(58)

Note that Eq. (57) with the replacement of the field operator by its steady-state expression also leads to the same time evolution as induced by (56) after symmetrizing with respect to the field terms. The two approaches thus lead to identical predictions, which we will exhibit in some more detail in the following.

**B. Self-organization of atoms in an optical lattice**

In this section we investigate the microscopic dynamics of self-ordering near zero temperature and compare the results of the general model Hamiltonian (57) and the corresponding effective Hamiltonian (51). In order to simplify things, we keep the approximation from above and neglect \( JU_0 a^2 / a \) in the model, i.e.,

\[ H = (E + JV_{\text{cl}}) \hat{B} - \hbar \Delta'_c a^\dagger a + \frac{U}{2}\hat{C} + h\eta_{\text{eff}} \hat{J}_0 \hat{D} (a + a^\dagger), \]  

(59)

with \( \Delta'_c = \Delta_c - U_0 J_0 N \). Let us point out here, that the Hamiltonian in this approximative form is equivalent to a Hamiltonian describing 1D motion along an optical lattice transverse to the cavity axis. Such a lattice can e.g. be generated by the pump laser itself as it was studied in [54, 57] to investigate the onset of the self-organization process [18, 19, 20] at zero temperature.

Similar to that case, the effective Hamiltonian Eq. (59) for moderate coupling reproduces quite well the results of a full Monte-Carlo wavefunction simulation. We have checked this for a rather small system of two atoms in two wells with periodic boundary conditions. This is the minimal system to study self-organization but in general sufficient to capture the physics. In this special case the operator \( B \) simply couples the ordered \( \{11\} \) state to the state \( 1/\sqrt{2}(\{20\} + \{02\}) \), while the operator \( \hat{D}^2 \) leaves all the basis states \( \{11, 20, 02\} \) unchanged. It simply leads to a relative energy shift. Hence starting from a perfectly ordered atomic state (the analog of the Mott insulator state) the Hamiltonian part of the time evolution of the system couples it to the symmetric superposition of ordered states. In an adiabatic limit those ordered states are correlated with a coherent field \( \pm \alpha \) in the cavity. Thus without damping the evolution would simply read:

\[ |\psi(t)\rangle = \cos (2\omega t) |11, 0\rangle + \frac{i}{\sqrt{2}} \sin (2\omega t) (|20, 2\alpha\rangle + |02, -2\alpha\rangle). \]  

(60)

where the frequency \( \omega \) is given by the \( (E + JV_{\text{cl}})/\hbar \). Here \( |11, 0\rangle \) is the state with one atom in each well and zero photons, whereas \( |20, \alpha\rangle \) (\( |02, -\alpha\rangle \)) corresponds to the state with both atoms in the left (right) well, and the cavity field being in a coherent state with amplitude \( 2\alpha \) (\(- 2\alpha \)). The factor 2 is due to constructive interference of the fields, scattered by the ordered atoms. In the Mott state, the scattering fields cancel each other.

Note that such an entangled superposition of different atomic states and fields cannot be reproduced by any classical or mean field evolution and requires a genuine quantum description. If on-site interaction is added the amplitude of this oscillations decreases due to extra relative different phase changes of the self-ordered and the Mott state.

Of course we now have to add the effect of dissipation via cavity loss. We will see that even single cavity photon decay events strongly perturb the system evolution. This can be immediately seen by applying the photon annihilation operator to the entangled atom-field state, i.e.,

\[ |\psi(t)\rangle \propto a |\psi(t)\rangle \propto |20, 2\alpha\rangle - |02, -2\alpha\rangle. \]  

(61)

This procedure projects out the Mott contributions to the state as they are connected to zero photons. Surprisingly in addition it also blocks further tunneling by introducing a minus sign between the two ordered states. At this point coherent atomic time evolution stops until a second photon escapes and re-establishes the plus sign. This then allows tunnel coupling back to the Mott state.
insulator state again. In this sense self-ordering is an instantaneous projective process here, where the cavity acts as measurement apparatus asking a sort of yes/no ordering question.

The fact, that for transverse pumping the adiabatic field state associated with the Mott insulator is an intracavity vacuum decouples this state from further dynamics even in the presence of dissipation. This creates numerical difficulties and prohibits an approximation of the dissipative dynamics by the adiabatic ground state values of (57) only. As soon as a photon leaks out of the cavity, the contribution of the Mott-insulator state is canceled, no matter how large it, corresponding to a given on-site interaction, might be. Hence, every initial state evolves into a superposition of the ordered states and the ground state values of the effective Hamiltonian do not make much sense. Nevertheless, including the damping via the effective Liouvillean (58) approximately reveals the complete dynamics. In Fig. 10 we show the results of a Monte-Carlo simulation of the dynamics of the Mott and the superfluid contribution, corresponding to (59) and compare it with a solution of the master equation, consisting of the Hamiltonian (57) and Liouvillean (58), where the field variables are eliminated. Furthermore, the restriction of the Hilbert space to the two states of (61) and (11, 0), allows for a proof of the accuracy of our assumption, concerning the fast evolution of the cavity field. We use the coefficients c(t), ˜c(t) (calculated with the Monte Carlo simulation) of |ψ(t)⟩ = ˜c(t)|11⟩ + c(t)|(20) ± |02⟩ to construct a purely atomic state |ψ(t)⟩ = ˜c(t)|11⟩ + c(t)|(20) ± |02⟩. Then the mean photon number, calculated with the effective photon operator (55), agrees very well with the real mean photon number, i.e.,

$$\frac{\eta_{\text{eff}}^2 J_0^2}{\Delta^2 + \kappa^2} \langle \varphi(t) | \hat{D}^2 | \varphi(t) \rangle = \langle \psi(t) | a^\dagger a | \psi(t) \rangle. \quad (62)$$

V. CONCLUSIONS

Based on an approximative Bose-Hubbard type model descriptions, we have shown that quantum characteristics of light fields generating optical potentials lead to shifts in quantum phase transition points and play a decisive role in the microscopic dynamics of the transition process. While many physical aspects can be already captured by effective Hamiltonians with rescaled parameters, cavity mediated long-range interactions also play an important role and add a new nonlocal element to optical lattices dynamics for atoms. In that context even small modifications in the setup, from cavity pump to transverse pump, have a drastic influence on the behavior of the system on a microscopic level. We have seen that the Bose-Hubbard Hamiltonian for the former system can, in a certain parameter regime, be significantly simplified by adiabatically eliminating the field variables. Although the cavity has influence on its shape, the Mott
insulator to superfluid phase transition occurs similar to classical optical lattices. For transverse pumping this is not the case. Here, the fields scattered by the atoms in the uniform Mott state cancel and completely suppress scattering. In parallel new ordered states with maximal coupling of pump and cavity field appear and the dynamics favors a superposition of these two ordered states correlated with coherent field states with phase difference $\pi$. Hence the dynamics generates strong atom field entanglement and large effective optical nonlinearities even in the limit of linear weak field scattering.

Of course the various approximations used to derive our effective Hamiltonians still leave a lot of room for improvements and we could only touch a very small part of the physical effects and possibilities contained in these model. Fortunately the experimental progress in this field is spectacularly fast and several groups now have set up optical lattices with cavity fields and intriguing potential applications of such systems were already proposed, so that one can expect a fast and exciting further development of this field.

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