Superradiant and dark exciton states in an optical lattice within a cavity

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Abstract – We study ultracold atoms trapped in a one-dimensional optical lattice prepared in a Mott insulator state of finite extent and collectively coupled to a single cavity mode. Due to resonant dipole-dipole interactions among the atoms, electronic excitations get delocalized and form excitons. These excitons can be explicitly calculated and divided into two groups: antisymmetric modes which decouple from the cavity mode called dark excitons, and symmetric modes coupled to the cavity mode called bright excitons. In a typical geometry the most uniform exciton is coupled to the cavity photons much stronger than other symmetric bright states and dominates the optical response of the atoms (superradiant state). In the strong coupling regime this superradiant state mixes with a cavity photon to form a doublet of polariton states, and the other excitons play only a minor role in the dynamics. We analytically calculate the corresponding collective Rabi splitting including the nearest-neighbor dipole-dipole induced excitonic shifts, which strongly depend on the polarization of the cavity mode with respect to the lattice orientation.

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Strong coupling of a single atomic transition to a cavity mode has been achieved experimentally in several different setups [1,2], and more extensively studied theoretically [3]. In a recent breakthrough for a Bose-Einstein Condensate of atoms (BEC) within an optical cavity one successfully demonstrated strong collective atom-field coupling [4,5]. Experiments now target to use BECs coupled to microwave strip-line resonators on atom chips [6,7], where strong coupling is expected even for magnetic coupling of dipole forbidden hyperfine transitions. Theoretically, in a first approximation the coherent coupling of \(N\) atoms of a BEC to a single cavity mode, with identical single atom-photon coupling \(f\), is well described by the Tavis-Cummings model. It leads to an effective collective coupling enhancement of \(\sqrt{N}f\) [8] for the lowest collective atomic excitation, as the cavity prototype of the Dicke model for atoms in free space microwave fields [9]. From the point of controlling atomic motion a Bose gas of ultracold atoms in an optical lattice can now be routinely prepared in the Mott insulator phase [10] as predicted by the Bose-Hubbard model [11]. These achievements together should allow the implementation of an optical lattice of ultracold atoms within a cavity. Due to the long stability and absence of atom-atom collisions, such a setup promises important improvements for a light-matter interface in quantum information processing [12] and studies of new effects of many-particle physics of quantum liquids [13,14]. In addition it could be the basis of the implementation of an ultrastable atomic lattice laser [15] on the route to an improved optical lattice clock or a combined atom-photon laser [16]. As pointed out by Lukin and coworkers [17] besides collective coupling, dipole-dipole shifts in such a lattice will lead to important modifications and limitations.

Optical lattices are formed by counter propagating off-resonant laser beams interacting with atomic motion only in a dispersive and conservative way. For atoms in such a lattice we consider here only the ground state and a single electronically excited state and we assume that the corresponding optical lattice potentials have minima at the same positions, with one atom trapped in each site and localized in the corresponding lowest Bloch band. The one-dimensional optical lattice is placed between spherical cavity mirrors, as seen in fig. 1, where only a single cavity mode is close to resonance to the previous atomic transition. Different from the standard Tavis-Cummings

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model we include dipole-dipole interactions among the atoms leading to the formation of collective electronic excitations similar to the previously studied case of a two-dimensional optical lattice, where, exploiting the lattice symmetry, we got in-plane propagating excitation waves (excitons) with in-plane wave vectors as good quantum numbers [18]. In a perfectly planar cavity translational symmetry enforces that only excitons and photons with the same in-plane wave vector are coupled and form cavity polaritons [18]. Such an idealized setup is, however, hard to implement. Hence in this work we target now a much more realistic setup involving a finite one-dimensional optical lattice in a standard finite-size spherical mirror cavity. It is now important to see how much of the polariton physics survives in this case and which important physical effects can be still observed and calculated in this truncated model.

As the mode spacing is typically much larger than the atom decay rate only the lowest cavity mode can be tuned to resonance with the atomic transition and we can simplify the calculations by considering only a Gaussian mode (see fig. 1). Mathematically it is represented by the Hamiltonian \( H_e = E_e a^\dagger a \), where \( a^\dagger \) and \( a \) are the creation and annihilation operators of a cavity photon with energy \( E_e = h\nu_c \), respectively. The electric-field operator across the cavity waist [1], chosen along the optical lattice axis is then defined by

\[
\hat{E}(r, z = 0) = i \sqrt{\frac{E_e}{2\epsilon_0 V}} e^{-r^2/w_0^2} \{ e \ a - e^* \ a^\dagger \},
\]

where \( e \) is the photon polarization unit vector, \( w_0 \) is the beam waist, and \( V \) is the mode volume given by \( V = \pi w_0^2 L/4 \). \( L \) is the distance between the cavity mirrors, as seen in fig. 1. In principle our considerations can also be extended to any higher order mode which would lead to more complicated mathematical expressions but should not essentially change the basic physics.

An electronic excitation of an atom in the lattice can be transferred to different lattice sites not only via the cavity mode but also due to direct dipole-dipole interaction. The corresponding excitation Hamiltonian then reads

\[
H_{ex} = \sum_n E_a \ B_n^\dagger B_n + \sum_{(n,m)} J_\theta \ B_n^\dagger B_m, \tag{2}
\]

where \( B_n^\dagger \) and \( B_n \) are the creation and annihilation operators of an electronic excitation at site \( n \) with transition energy \( E_a = h\nu_a \), respectively. At low number of electronic excitations we treat only a single excitation in a small region at a given time, so that the operators \( B_n \) can be assumed to behave as bosons with the commutation relation \( [B_n, B_m^\dagger] = \delta_{nm} \) neglecting the suppression of local double excitations. To first order we take into account only the interaction between nearest-neighbor sites. The energy transfer coupling parameter is

\[
J_\theta = \frac{\mu^2}{4\pi\epsilon_0 \bar{a}^3} (1 - 3\cos^2 \theta), \tag{3}
\]

where \( \mu \) is the magnitude of the atomic transition dipole and \( \theta \) is the angle between the transition dipole vector and the optical lattice direction. While for isotropic atomic states the magnitude of the transition dipole vector is independent of the cavity photon polarization, a particular choice of initial and final atom states fixes its direction [19]. Here \( \bar{a} \) is the lattice constant.

Let us now start the calculations with a finite lattice of \( N \) sites labeled by \( n = 1, \ldots, N \). As a calculation trick to fix the boundary condition we add two additional empty sites, \( n = 0 \) and \( n = N+1 \), as in fig. 2. In this frame the excitation Hamiltonian can be diagonalized via the transformation \( B_n = \sqrt{\frac{2}{N+1}} \sum_k \sin(\frac{n\pi}{N+1} k) \ B_k \). The resulting collective excitation modes are labeled by \( k = 1, \ldots, N \) and represent standing wave type excitons (see fig. 2). The diagonalized Hamiltonian then reads \( H_{ex} = \sum_k E_k \ B_k^\dagger B_k \), with the energy dispersion \( E_k = E_a + 2J_\theta \cos(\frac{k\bar{a}}{N+1}) \). In place of equal atomic levels the excitons have discrete energy levels spread out over a range (band) of width \( 4J_\theta \).

Let us now look at the coupling of these collective states to the cavity mode via simple electric dipole interaction \( H_I = -\hat{\mu} \cdot \hat{E} \). The dipole operator is defined by \( \hat{\mu} = \hat{\mu} \sum_n (B_n^\dagger + B_n) \), where \( \hat{\mu} \) is the transition dipole

\[
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matrix element between the ground and excited states. As the photon polarization at the waist is in a plane which includes the optical lattice direction, for an isotropic transition (e.g., \( S \rightarrow P \)) the atomic dipole direction can be chosen along the photon polarization, we define \( \mu = (\mathbf{e} \cdot \mathbf{j}) \). When the optical lattice is centered with respect to the cavity axis the atomic positions are \( r_n = n\tilde{a} - L/2 \), with the lattice length \( L = (N + 1)\tilde{a} \). For a waist size \( w_0 \) much larger than \( \tilde{L} \) we also can assume a mostly homogeneous coupling \( c^{-\gamma_0^2}/w_0^2 \approx 1 \). We need also the summation over \( n \), which is \( \sum_n \sin(\frac{\pi n}{N+1} k) = \cot(\pi k / (N+1)) \) for odd \( k \)'s, \( (k = 1, 3, \ldots) \), and zeros for even \( k \)'s, \( (k = 2, 4, \ldots) \). Finally, in the rotating-wave approximation, we get \( H_I = \sum_{k \text{odd}} (f_k |B^\dagger_a + f_k |a^\dagger B_n) \), where \( f_k = -i\sqrt{\frac{\hbar \omega_0 \mu^2}{\epsilon_0 V (N+1)}} \cot(\pi k / (N+1)) \).

According to their spatial symmetry, the excitons can be antisymmetric with even \( k \), \( (k = 2, 4, \ldots) \) and odd number of nodes, or symmetric states of odd \( k \)'s, \( (k = 1, 3, \ldots) \) and even number of nodes. The antisymmetric excitons are decoupled from the cavity mode and denoted as dark states, while the latter are coupled to cavity photons (bright states). Now we show that the first mode \( (k = 1) \), which has no nodes, would interact with the cavity mode much stronger than the other even states \( (k = 3, 5, \ldots) \), which generally are only weakly coupled to the light. Mathematically this behavior is clearly seen from the coupling function \( \cot(\pi k / (N+1)) \), which decays very fast for small \( k \)'s, where \( |f_k|/|f_{k\neq1}| = k \). The effective oscillator strength is proportional to \( |f_k|^2 \), hence the oscillator strength of the first mode \( (k = 1) \) is stronger by a factor \( k^2 \) from the \( (k \neq 1) \) state for small \( k \)'s and the oscillator strength of the first state is 9 times stronger than the third one. As the oscillator strengths sum to one, we conclude that, for \( (N \gg 1) \), the first state \( (k = 1) \) includes about 0.81 of the sum and the second bright state \( (k = 3) \) includes 0.09.

Let us present the above results in a typical example with the following parameters. The lattice constant is \( \tilde{a} = 10^{-7} \text{[M]} \), the beam waist is \( w_0 = 3 \times 10^{-4} \text{[M]} \), the distance between the mirrors is \( L = 1.5 \times 10^{-3} \text{[M]} \), and the cavity mode volume is \( V = 10^{-10} \text{[M^3]} \). The atomic transition dipole is \( \mu = 5 \times 10^{-29} \text{[CM]} \), the angle between the dipole and the optical lattice direction at the waist is taken to be \( \theta = 0 \), and which results in an energy transfer parameter of \( J_0 / \hbar = -6.8 \times 10^7 \text{[Hz]} \). The atomic transition frequency is \( \omega_a = 4 \times 10^{14} \text{[Hz]} \). For the case of \( N = 10^3 \) sites, in fig. 3a we plot the shifted exciton dispersion \( E_k - E_a = \omega_a \) as a function of \( k \). In fig. 3b we plot the square of the exciton-photon coupling \( |f_k|^2 \) as a function of \( k \). Here the cavity photon frequency is taken to be at resonance to the first exciton mode, that is \( E_a = E_1 \). As expected the coupling decays very fast for large \( k \). For the coupling of the first exciton we have \( |f_1| / \hbar = 2.55 \times 10^7 \text{[Hz]} \), and for the third exciton we have \( |f_3| / \hbar = 8.5 \times 10^6 \text{[Hz]} \). The even modes are exactly decoupled from the light mode as they involve destructive interference of the coupling to different lattice sites [20].

Next, we study the effective coupled atom-field eigenstates. In principle the cavity mode will couple different excitons by absorption and emission of cavity photons. In the light of the above discussion, we can, however, to a first approximation neglect the coupling of the cavity photons to the other exciton states except of the coupling to the maximally coupled (superradiant) \( k = 1 \) state. In this limit the coupled photon-exciton Hamiltonian simply has the well known Jaynes-Cummings-type form:

\[
H = E_{ex} B^\dagger B + E_a a^\dagger a + f B^\dagger a + f^* a^\dagger B,
\]

where we dropped the exciton index. The coupling strength is

\[
f = -i\sqrt{\frac{E_x \mu^2}{\epsilon_0 V (N+1)}} \cot \left( \frac{\pi}{2(N+1)} \right),
\]

and the exciton energy reads

\[
E_{ex} = E_a + 2J_0 \cos \left( \frac{\pi}{N+1} \right).
\]

This Hamiltonian can be easily diagonalized using the transformation \( A_{\pm} = X^{\pm}B + Y^{\pm}a \), to get \( H = \sum_r E_r' A_r^\dagger A_r \), with the two polariton eigenenergies \( E_{p'} = (E_e + E_{ex})/2 \pm \Delta \), where \( \Delta = \sqrt{\delta^2 + |f|^2} \), with the detuning \( \delta = (E_e - E_{ex})/2 \). The eigenstates are coherent superpositions of the exciton and the cavity photon. The exciton amplitudes are \( X^{\pm} = \pm \sqrt{(\Delta \mp \delta)/2\Delta} \), and the cavity photon amplitudes are \( Y^{\pm} = f/\sqrt{2(\Delta \mp \delta)} \). In fig. 4a we plot the shifted polaron dispersion \( E_{p'} - E_{ex} \) as a function of the detuning \( \delta \), in using the previous numbers. In fig. 4b we plot the excitonic and photonic weights for the lower and upper branches. It is seen that at the exciton-photon intersection point the polaron becomes half exciton-half photon. But for large positive detuning the lower branch becomes exciton and the upper becomes photon, and vice versa for the negative detuning.
The vacuum Rabi splitting $\Omega_0$ vs. the atom number $N$, for interacting (full line), and non-interacting (dashed line), optical lattice ultracold atoms. The difference increases with the atom number.

We define the collective excitation operator $B_n = \frac{1}{\sqrt{N}} B_n$, $B = \frac{1}{\sqrt{N}} \sum_n B_n$, to get

$$H = E_0 B^\dagger B + E_c a^\dagger a + \tilde{f} B^\dagger a + \tilde{f}^* a^\dagger B,$$

where

$$\tilde{f} = -i \sqrt{\frac{h \mu \mu^2 N}{2 \epsilon_0 V}}.$$

The Hamiltonian (8) exhibits a relative energy shift $E_0 - E_{ex} = -2J_0 \cos(\frac{\pi}{N+1})$ which is about $1.35 \times 10^8$ [Hz] for $N = 10^3$ and $\theta = 0$ and $|\tilde{f}|/h = 2.8 \times 10^7$ [Hz] for the case of resonance $E_c = E_0$. In fig. 6 we compare the vacuum Rabi splitting $\Omega_0 = 2|\tilde{f}|/h$ as a function of the atom number for the two cases. It is seen that for large atom number the vacuum Rabi splitting for independent atoms is larger than that of interacting atoms. The difference is about $5 \times 10^6$ [Hz] for $N = 10^3$ atoms. We conclude that the vacuum Rabi splitting is reduced by the dipole-dipole interactions. This difference can partly account for the deviation of the vacuum Rabi splitting from a square root dependence at large atom number $N$, as it was observed experimentally for a BEC within a cavity [4].

For more comparison we plot the generalized Rabi splitting for the two cases. We consider the case with $E_0 = E_c$. Then for atoms without dipole-dipole interaction we have $\delta = 0$, and then $\Omega = 2|\tilde{f}|/h$, which is a square root function of $N$, and $\theta$ independent. For the case with dipole-dipole interactions, we consider only the superradiant state to get the generalized Rabi splitting, which is $\Omega = 2\Delta/h$, where

$$\Delta = \sqrt{J_0^2 \cos^2 \left(\frac{\pi}{N+1}\right) + |\tilde{f}|^2},$$

and which is $N$ and $\theta$ dependent. In fig. 7a we plot the generalized Rabi splitting as a function of $\theta$ for the two cases, and with $N = 10^3$. It is clear that around $\theta = 54.74^\circ$ the generalized Rabi splitting for interacting case is lower than the non-interacting case, where around $\theta = 54.74^\circ$ the dipole-dipole interaction is zero, that is $J_0 \approx 0$. In fig. 7b we plot the generalized Rabi splitting as a function of $N$ for the two cases, where for the interacting case we plot for the angles $\theta = 0^\circ, 54.74^\circ, 90^\circ$. 

Fig. 6: The vacuum Rabi splitting frequency $\Omega_0$ vs. the atom number $N$, for interacting (full line), and non-interacting (dashed line), optical lattice ultracold atoms. The difference increases with the atom number.

To observe the system we need to couple the cavity mode to the external radiation field [18]. We do this by considering a non-perfect cavity mirror with the coupling parameter $\gamma$, and by including the cavity photon damping rate $\Gamma_c$ and similarly the atomic decay rate $\Gamma_a$. For an incident field with a fixed polarization one can simply calculate reflected, transmitted, and absorbed fields. The reflection spectrum is $R(\nu) = 1/[1 + i\gamma \Lambda(\nu)]^2$, the transmission spectrum is $T(\nu) = \gamma^2 [\Lambda(\nu)]^2/[1 + i\gamma \Lambda(\nu)]^2$, and the absorption spectrum is obtained from $R(\nu) + T(\nu) + A(\nu) = 1$. We defined $\Lambda(\nu) = \sum_r [Y^r]^2/(\nu - \nu_r)$. We used the damping frequencies $\Gamma_a = \Gamma_c = \gamma = 10^7$ [Hz]. The two peaks show the energies of the two polaron states for zero detuning and $\theta = 0$, where $|X^\pm|^2 = 1/2$ and $|Y^\pm|^2 = 1/2$.

To show the relevance of an excitonic interpretation of the dynamics we compare it to the case without dipole-dipole interactions [5]. The electronic excitation is described now by the Hamiltonian $H_{ex} = \sum_n E_n B_n^\dagger B_n$ (as before, for low excitations the operators $B_n$ are taken to be bosonic). The excitation-photon coupling Hamiltonian reads $H_1 = \sum_n (f B_n^\dagger a + f^* a^\dagger B_n)$, where the coupling parameter is $f = -i \sqrt{\frac{h \mu \mu^2}{2 \epsilon_0 V}}$. The total Hamiltonian is given by

$$H = \sum_n E_n B_n^\dagger B_n + E_c a^\dagger a + \sum_n (f B_n^\dagger a + f^* a^\dagger B_n).$$

Fig. 5: The transmission spectra showing the two peaks of the polariton doublet at $\delta = 0$.

To show the double-peaked feature as shown in fig. 5. We used the damping frequencies $\Gamma_a = \Gamma_c = \gamma = 10^7$ [Hz]. The two peaks show the energies of the two polaron states for zero detuning and $\theta = 0$, where $|X^\pm|^2 = 1/2$ and $|Y^\pm|^2 = 1/2$.

Fig. 4: (a) The shifted polariton dispersions ($E_p^\pm - E_{ex})/h$ vs. the detuning $\delta/h$. The vacuum Rabi splitting is obtained at $\delta = 0$. (b) The excitonic and photon weights, $|X^\pm|^2, |Y^\pm|^2$, vs. the detuning $\delta/h$, for the lower and upper branches. At $\delta = 0$ the branches are half exciton-half photon. For large positive detuning the lower branch becomes exciton and the upper becomes photon, and vice versa for negative detuning.
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Fig. 7: (a) The generalized Rabi splitting frequency $\Omega$ vs. $\theta$, for the interacting case (full line), and the non-interacting case (dashed line), with $N = 10^3$. The non-interacting case is $\theta$ independent. (b) The generalized Rabi splitting frequency $\Omega$ vs. $N$, for the interacting case (full lines) at the angles $\theta = 0^\circ, 54.74^\circ, 90^\circ$, and the non-interacting case (dashed line). Around $\theta = 54.74^\circ$ the interacting case splitting is smaller than the non-interacting one.

In summary, we calculated the dipole-dipole interactions induced shifts of the coupled atom-field eigenmodes of a quantized cavity mode strongly coupled to collective excitations (excitons) of ultracold atoms in an optical lattice. For a typical cavity the interaction is dominated by a single almost maximally coupled exciton mode so that the linear optical response creates a doublet of eigenstates. The resonances show a significant polarization angle dependent shift. Analogous results also hold for any chain of electromagnetic active materials, e.g. a lattice of quantum dots within a cavity. Such dipole-dipole shifts enter in the effective transition frequency of an atomic lattice clock. While in principle for a perfectly filled lattice they can be explicitly calculated and thus accounted for, they will lead to errors if there is an uncertainty in the atom number or defects with unknown positions in the lattice. If one allows for atomic tunneling would increase the atom number fluctuations in the lattice and couple different exciton states. These unknown energy shifts of excitons will also limit the coherence time of an atomic lattice quantum memory. As a next step towards even more realistic results one should include several cavity eigenmodes and more weakly coupled excitons in the dynamics.

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