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Coupling of polaritons to vibrational modes of ultracold atoms in an optical lattice

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A B S T R A C T

The coupling of internal electronic excitations to vibrational modes of the external motion of ultracold atoms in an optical lattice is studied here in using a perturbation expansion in small atomic displacements. In the Mott insulator case with one atom per site, the resonance dipole–dipole coupling between neighboring sites can induce emission and absorption of vibrational quanta. Within a cavity in the strong exciton–photon coupling regime such coupling results in polariton–vibration interactions, which create a significant thermalization mechanism for polaritons toward their minimum energy, and leading to motional heating of the lattice atoms.

1. Introduction

The superfluid to the Mott insulator quantum phase transition in a system of ultracold boson atoms in an optical lattice has been first predicted theoretically [1], and then realized experimentally [2]. The optical lattice is formed off standing waves of counter propagating laser beams with lattice constant of half laser wave length. The ultracold atoms are loaded into such optical lattice, and in varying the laser intensity the superfluid-Mott insulator phase transition can be achieved, and in the Mott insulator phase a fixed number of atoms per site is obtained, where the transition is well described by the Bose–Hubbard model [1]. For deep optical lattice potentials the on-site lowest motional states can be described by harmonic oscillators, and the transitions of the atoms between these vibrational states are usually induced by Raman scattering of light or via scattering interactions during atom hopping among different sites [3]. We study here a different mechanism for the excitation and de-excitation of vibrational modes which is induced by resonance dipole–dipole interactions. The discussion is limited to two-level atoms in a deep optical lattice prepared in the Mott insulator phase with one atom per site, and we assume ground and excited state optical lattice potentials with minima at the same positions but with different depth.

We already studied collective electronic excitations (excitons [4]) in such a system for the cases of one and two atoms per site. For an optical lattice, which is located between two cavity mirrors [5], we showed that in the strong coupling regime, excitons and photons are coherently mixed to form cavity polaritons [6–8]. In these works we considered only the case of atoms localized in the lowest vibrational state, i.e. the first Bloch band. However, in more realistic optical lattices, dynamical excitation of atoms to higher vibrational states will occur. In the present work we aim to include higher vibrational states which are induced through their coupling to excitons. As optical lattices in the Mott insulator phase are similar to molecular crystals, the formalism adopted here is in the spirit of the coupling of Frenkel excitons and optical phonons in molecular crystals [9,10], but some caution is needed to identify the correct physical analogies between optical phonons in molecular crystals and the vibrational states in optical lattices. In our case the interaction is mediated by resonance dipole–dipole coupling and is treated in the perturbation theory. Furthermore, polariton–vibration interactions emerge through the polariton excitonic part, and serve as a significant source of polariton relaxation toward their minimum energy, and as an important mechanism for excitation and de-excitation of vibrational modes.

The paper is organized as follows. In Section 2 we present electronic excitations and vibrational modes of cold atoms excited to higher Bloch bands in an optical lattice. And in Section 3 we derive the coupling of electronic excitations to vibrational modes. We derive the cavity–polaritons coupling to the vibrational modes in Section 4. A summary appears in Section 5.

2. Electronic excitations and vibrational states for an optical lattice

The electronic excitations for ultracold atoms of an optical lattice in the Mott insulator phase can be represented by the

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Hamiltonian

$$H = \sum_i \hbar\omega_A B_i^\dagger B_i + \sum_{i,j} \hbar J_{ij} B_i^\dagger B_j, \tag{1}$$

where $B_i^\dagger, B_i$ are the creation and annihilation operators of an excitation at lattice position i. In the case of a single electronic excitation, the operators can be taken to obey the Bose commutation relation $[B_i, B_j^\dagger] = \delta_{ij}$. The internal atomic transition frequency is ω_A. An internal electronic excitation can be exchanged among atoms at different sites i and j, which is induced by dipole–dipole interactions and can be parametrized by a coupling integral J_{ij}. It is now essential to note that this coupling depends on the atomic displacements $\mathbf{u}_i^{\lambda m}$ and thus on the local vibrational excitation. Here $\mathbf{u}_i^{\lambda m}$ is the average change of the atomic size at site i, of position $\mathbf{n}_i$, in the λ internal state, for the ground and excited state energies ($\lambda = e, g$), due to the excitation of the atom to a higher vibrational state with m quanta, and where $\mathbf{u}_i^{\lambda m}$ is measured relative to $\mathbf{u}_i^{\lambda 0}$ of the vibration-less state. The dependence of the on-site transition energy $\hbar\omega_A$ on the vibrational state is neglected. As long as $\mathbf{u}_i^{\lambda m}$ is a small distance relative to the lattice constant a, which is the case for the lowest vibrational modes, to lowest orders in this small perturbation we can split the Hamiltonian in the form $H = H_{ex} + H_{vib} + H_{ex-vib}$. Here H_{ex} is the internal excitation Hamiltonian, which is obtained for atoms in the ground vibrational states, H_{vib} is the atom vibration Hamiltonian, for excited and ground state atoms, and the coupling Hamiltonian H_{ex-vib} is derived perturbatively for atoms excited to higher vibrational states.

To zeroth order, for atoms in the ground vibrational states, we thus get

$$H_{ex} = \sum_i \hbar\omega_A B_i^\dagger B_i + \sum_{i,j} \hbar J_{ij}^0 B_i^\dagger B_j, \tag{2}$$

where J_{ij}^0 is the transfer parameter among atoms in the lowest vibrational states.

The Hamiltonian can be diagonalized by using the transformation into the quasi-momentum space

$$B_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{n}_i} B_{\mathbf{k}}, \tag{3}$$

where N is the number of sites and $\mathbf{k}$ is the in-plane wave vector for 2D optical lattice. We obtain the exciton Hamiltonian [6]

$$H_{ex} = \sum_{\mathbf{k}} \hbar\omega_a(\mathbf{k}) B_{\mathbf{k}}^\dagger B_{\mathbf{k}}, \tag{4}$$

where the exciton dispersion is $\omega_a(\mathbf{k}) = \omega_A + \sum_{\mathbf{L}} J(\mathbf{L}) e^{i\mathbf{k}\cdot\mathbf{L}}$, with $\mathbf{L} = \mathbf{n}_i - \mathbf{n}_j$ and $J(\mathbf{L}) = J_{ij}^0$. The condition for the energy transfer among lattice sites, and hence the formation of collective electronic excitations (excitons), is to have a dipole–dipole coupling larger than the excited state line width Γ, that is $J > \Gamma$, (more details in Ref. [6]).

Vibrational excitations of atoms at the ground and excited states are described by the two harmonic oscillator Hamiltonians

$$H_{vib} = \sum_i \hbar\omega_v^g b_i^\dagger b_i + \sum_i \hbar\omega_v^e c_i^\dagger c_i, \tag{5}$$

where ω_v^g and ω_v^e are the vibration frequency for ground and excited state atoms, respectively. $b_i^\dagger, b_i$ and $c_i^\dagger, c_i$ are the creation and annihilation operators of a vibration mode at site i for ground and excited state atoms, respectively. The atomic displacement operators are

$$\hat{x}_i^g = \sqrt{\frac{\hbar}{2m\omega_v^g}}(b_i + b_i^\dagger), \quad \hat{x}_i^e = \sqrt{\frac{\hbar}{2m\omega_v^e}}(c_i + c_i^\dagger), \tag{6}$$

where m is the atomic mass.

Here, ground and excited state atoms are considered as two different kinds of bosons [11], where each has its own optical lattice potential. In the transition between the ground and the excited state one kind of bosons is destroyed and another created. Hence we use two independent harmonic oscillators for the ground and excited vibrational excitations. Note that if we have physical allowed initial states, then the system dynamics due to the following interaction Hamiltonian, derived in the perturbation theory, will not couple to any un-physical states present in the Hilbert space.

3. Interactions of electronic excitations to vibrational states

To first order in the perturbation series with respect to $\mathbf{u}_i^\lambda$, we derive an approximative excitation–vibration coupling Hamiltonian H_{ex-vib}. Processes in first order include only single vibrational quantum, and we drop the index (m). To treat processes of more than a single vibrational quantum one needs to consider higher order terms of this perturbation series. The present perturbation method [12] allows one to include any number of vibrational quanta (up to the limit of the harmonic oscillator approximation).

The interaction Hamiltonian of the transfer term then reads

$$H_{ex-vib}^{II} = \sum_{i,j} \hbar [F_{ij}^{ei} c_i^\dagger + F_{ij}^{gi} b_i + F_{ij}^{ej} c_j + F_{ij}^{gj} b_j^\dagger] B_i^\dagger B_j, \tag{7}$$

where the coupling parameter is

$$F_{ij}^{\lambda i} = \sqrt{\frac{\hbar}{2m\omega_v^\lambda}} \left\{ \frac{\partial J_{ij}}{\partial \mathbf{u}_i^\lambda} \right\}_{\mathbf{u}_i^\lambda = 0}, \tag{8}$$

which is related to the derivative of J_{ij}. Furthermore, we assume the excitation–vibration coupling parameters to be site independent, by defining $F_{ij}^\lambda \equiv F_{ij}^{\lambda i}$. The excitation–vibration coupling Hamiltonian is written as

$$H_{ex-vib} = \sum_{i,j} \hbar [F_{ij}^e (c_i^\dagger + c_j) + F_{ij}^g (b_i + b_j^\dagger)] B_i^\dagger B_j. \tag{9}$$

This term describes creation and destruction of vibrations, induced by excitation transfer among different sites. Two of the four processes are plotted in Figs. 1 and 2. The process in Fig. 1 shows emission of ground state vibration at site j. While the process in Fig. 2 shows absorption of excited state vibration at site j. In the process of Fig. 1, the initial states are $|g_i, 0_v^g\rangle$ and $|e_j, 0_v^e\rangle$ with a dipole–dipole coupling, say, J_l. The final states are $|e_i, 0_v^e\rangle$

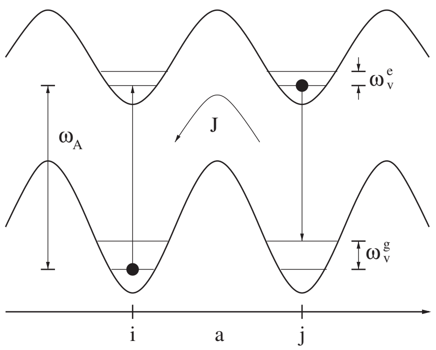

Fig. 1. The term $F_{ij}^g B_i^\dagger B_j b_j^\dagger$, represents the process of the emission of ground state vibration at site j.