Exciton–polariton scattering as signature of defects in cold atom optical lattices

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Abstract. We study the effect of defects in the Mott insulator phase of ultracold atoms in an optical lattice on the dynamics of resonant electronic excitations. These excitations can be described analogous to Frenkel excitons in solids and form polaritons, when coupled to an optical resonator. Defects, which are empty sites in a singly occupied Mott insulator state or singly occupied sites for a filling factor two, change the exciton dynamics. We show that vacancies behave like hard sphere scatterers, while singly occupied sites in a doubly filled region generate either attractive or repulsive interaction potentials. We suggest cavity polaritons as tools which detect such defects and show how the scattering can be controlled by changing the exciton–photon detuning. In the case of aspherical individual lattice sites, we calculate the effective scattering potential as a function of the cavity photon polarization direction which exhibits a crossover from a repulsive into an attractive potential and should give a clearly observable signal.
1. Introduction

In one of the most significant achievements of cold atom physics in recent years, a degenerate gas of ultracold atoms loaded into an optical lattice formed by far off resonance lasers was demonstrated to undergo a quantum phase transition from a superfluid into the Mott insulator phase [1]. The Mott insulator phase constitutes a perfectly regular lattice of atoms at half the laser wavelength with a fixed number of atoms per site, which can be described by the Bose–Hubbard model [2, 3]. This artificial crystal of atoms with parameters well controllable in time and space generates a close connection between cold atoms and solid state physics, which has generated a plethora of subsequent work generalizing the model and identifying more solid state phenomena to be studied in such configurations [4]. Experimentally, strong progress has also been achieved since the original demonstration and recently even strong resonant light–matter coupling for a Bose–Einstein condensate in an optical cavity has been achieved [5].

In earlier work [6], we already exhibited the similarities of such artificial crystals and molecular or noble atom crystals, where internal molecular excitations can be described by quasi-particles, which are called Frenkel excitons. In particular for the special case of identical ground and excited state optical lattice potentials, the Mott insulator phase also allows the formation of such excitons as collective electronic excitations delocalized in the optical lattice [7, 8]. If the optical lattice is placed between cavity mirrors with a single cavity mode close to resonance with the excitons, coherent superpositions of excitons and cavity photons can form. In the strong coupling regime the corresponding system eigenstates then are cavity polaritons, which have very similar behavior in solid state and cold atom systems [7, 9]. The high control and flexibility of the atomic lattice systems offer many possibilities beyond the analogous solid state case, where new physical effects appear e.g. in the case of lattices with two atoms per site, where the on-site resonant excitations form symmetric (bright) and antisymmetric (dark) superposition states of individual excitations [10]. While the symmetric states radiate and via dipole–dipole coupling will form excitons and thus cavity polaritons, the antisymmetric states have no dipole moment, so that their excitations are long lived and stay localized at one site. Asymmetries of local lattice sites then can lead to coupling between bright and dark states and produce strongly polarization dependent spectra.

Optical lattices are spatially defined by the laser field and are thus almost perfect over long distances. Nevertheless due to imperfections in the dynamical formation of the Mott insulator phase, the appearance of some defects is unavoidable [1]. In particular there can be missing...
or extra atoms at some sites. Such defects might create decisive errors when lattices are used for parallel quantum information processing or for observing even more exotic quantum phases in such systems. Hence some suggestions to repair such defects were soon presented [11]. On the other hand defects are very hard to detect by direct observations of the atomic distribution without destruction.

In this paper, we investigate the effect of such defects on the dynamical properties of excitons and cavity polaritons. We concentrate in the case of a low defect number, where the exciton and cavity polariton picture still holds and these quasi-particles are only scattered by single defects. Namely, the distance between each of the two defects is large enough for the formation of coherent excitons and cavity polaritons, which propagate as free quasi-particles between each of the two scattering processes. In principle defects can move by hopping among the lattice sites, but the corresponding timescale is so long that they can be considered frozen. Introducing more and more defects with faster hopping would then correspond to the transition from the Mott to a superfluid atomic phase in the lattice, which will not be considered here. Hence while our theory strictly speaking treats only a single excitation, it should be valid for a low enough density of excitons.

Here, we concentrate on the type of defects which are induced by a missing atom: in the case of one atom per site this corresponds to vacant sites, while for two atoms per site a defect is a singly occupied site. In calculating the exciton and cavity polariton elastic scattering amplitude of such defects, the two cases behave even qualitatively very different. As a consequence of this defect scattering we show how cavity polaritons can be used as observation tools to detect defects in the Mott insulator phase.

The paper is organized as follows. In section 2, we investigate the exciton scattering off a vacancy in an optical lattice in the Mott insulator with filling factor one, which is generalized to the scattering of cavity polaritons in section 3. The scattering of excitons and cavity polaritons off a defect in the Mott insulator case with two atoms per site is treated in section 4, where we also treat the special case of an optical lattice with asymmetric sites.

2. Exciton scattering of a vacancy in an optical lattice

We consider first a two-dimensional (2D) optical lattice at the magic wavelength filled with one, two-level atom per site in the Mott-insulator phase. Including dipole–dipole interactions resonant excitations of the atoms can be represented as quasi-particles called Frenkel excitons [6]. A single atom missing at the origin (\(r_i = 0\)) then creates an impurity in the artificial lattice of ultracold atoms, which for sufficient lattice depth stays localized and will not hop among the lattice sites as shown in figure 1. We will now consider scattering of these excitons at such a missing atom (hole). As the scattering time is much shorter than the hopping time, the impurity is assumed to be localized during the scattering process.

Adding the impurity to the ideal atom crystal just needs a small change in the system Hamiltonian \(H = H_0 + V\) derived in [6], whose components now read:

\[
H_0 = \sum_k \hbar \omega_{\text{ex}}(k) B_k^\dagger B_k, \quad V = -\hbar \omega_A B_0^\dagger B_0. \tag{1}
\]

\(H_0\) represents free excitons due to the resonant electronic excitation transfer among lattice sites induced by dipole–dipole interactions including the lattice symmetry. \(B_k^\dagger\) and \(B_k\) are the creation and annihilation operators of an exciton with in-plane wavevector \(k\), respectively, and \(\omega_{\text{ex}}(k)\) is
the exciton dispersion. \( V \) is the impurity Hamiltonian at the origin, where \( \hbar \omega_A \) is the atomic transition energy. To get the above form, we add to and subtract from the whole Hamiltonian \( H \) the impurity Hamiltonian \( V \), that is \( H = H - V + V \), and then define the ideal case Hamiltonian by \( H_0 = H - V \).

For an exciton the impurity thus appears as a potential well located at the origin, with depth \( \hbar \omega_A \) and radius \( a \). Here, we will not try to find the self-consistent eigenstates of \( H \) but consider only the scattering problem. We can neglect trapping of an exciton in the impurity potential as a vacant site cannot absorb the trapping energy. Hence we consider only the scattering process of an exciton off the impurity.

In the following, we calculate the scattering amplitude of an exciton off an impurity. The initial exciton has wavevector \( k \) very far from the impurity, is scattered elastically and found with wavevector \( k' \) also very far away, and for elastic scattering we have \( |k'| = |k| \). As the impurity is very deep with depth \( \hbar \omega_A \), in order to calculate the scattering amplitude, we need to go beyond the Born approximation \[12\] even though the perturbation is confined to a radius \( a \).

The eigenstates of the free exciton Hamiltonian are \( H_0|\phi_k\rangle = E(k)|\phi_k\rangle \), and the full Hamiltonian eigenstates obey \( H|\psi\rangle = E|\psi\rangle \). The excitation eigenstates in the quasi-momentum space \( |\phi_k\rangle \) are related to the lattice space eigenstates by \( |\phi_k\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ik \cdot r_i} |\phi_i\rangle \), where \( N \) is the number of lattice sites. The eigenstates form a complete basis, with the closure relation \( \sum_i |\phi_i\rangle \langle \phi_i| = \hat{1} \). A general state \( |\psi\rangle \) can be expanded by \( |\psi\rangle = \sum_i \psi_i |\phi_i\rangle \), with the expansion amplitude \( \psi_i = \langle \phi_i | \psi \rangle \).

In the scattering problem the incoming exciton is prepared in a delocalized unperturbed exciton state \( |\phi_k\rangle \) and the scattered exciton is also observed very far from the impurity. Hence, the whole system eigenstates \( |\psi\rangle \) need to obey the boundary condition \( |\psi\rangle \rightarrow |\phi_k\rangle \) as \( V \rightarrow 0 \). The required solution is given by the Schwinger–Lippmann equation \[12\]

\[
|\psi\rangle = |\phi_k\rangle + G_0 V |\psi\rangle,
\]

where

\[
G_0 = \lim_{\eta \rightarrow 0^+} \left( \frac{1}{E - H_0 + i\eta} \right).
\]

The sign of \(+i\eta\) is chosen in such a way to ensure that the scattered exciton propagates far from the impurity. In multiplying the equation from the left by the bra vector \( \langle \phi_i | \) and inserting the above identity operator between \( G_0 \) and \( V \), we get

\[
\langle \phi_i | \psi \rangle = \langle \phi_i | \phi_k \rangle + \sum_j \langle \phi_i | G_0 | \phi_j \rangle \langle \phi_j | V | \psi \rangle.
\]
The calculations using the above definitions yields:

\[
\psi_i = \frac{1}{\sqrt{N}} e^{i k \cdot r_i} - \frac{E_a}{N} \lim_{\eta \to 0} \frac{e^{i k' \cdot r_i}}{E - E(k') + i \eta} \psi_0, \tag{5}
\]

where \( E_a = \hbar \omega_A \). This represents the scattered wave amplitude at site \( i \) very far from the impurity. The first term is for the non-scattered wave, and the second is for the scattered wave. For the impurity site amplitude, at \( r_0 = 0 \), we get

\[
\psi_0 = \frac{1}{\sqrt{N}} \left\{ 1 + \frac{E_a}{N} \sum_{k'} \lim_{\eta \to 0} \frac{1}{E - E(k') + i \eta} \right\}^{-1}. \tag{6}
\]

As the scattering is elastic the energy \( E \) can be replaced by the incident exciton energy and we have \( E = E(k) \). We get

\[
\psi_i = \frac{1}{\sqrt{N}} \left\{ e^{i k \cdot r_i} + \frac{E_a I_{os}}{1 - E_a I_{st}} \right\}, \tag{7}
\]

where we defined the oscillating and static summations

\[
I_{os} = - \frac{1}{N} \sum_{k'} \lim_{\eta \to 0} \frac{e^{i k' \cdot r_i}}{E(k) - E(k') + i \eta}, \quad I_{st} = - \frac{1}{N} \sum_{k'} \lim_{\eta \to 0} \frac{1}{E(k) - E(k') + i \eta}. \tag{8}
\]

Our main aim now is to calculate the two sums in the case of small wavevector scattering excitons, that is \( k a \ll 1 \). For this we can use the parabolic approximation for the dispersion of the excitons, \( \omega_{ex}(k) = \omega_{ex}(0) + \hbar k^2/2m_{ex} \), where \( m_{ex} \) is the exciton effective mass. For isotropic atoms in a square lattice of cubic symmetry, and in including only nearest neighbor interactions with coupling parameter \( J \), we get \( m_{ex} = -\hbar / (2J a^2) \), and \( \omega_{ex}(0) = \omega_A - 2J \). For a large enough 2D optical lattice, the sum over \( k' \) can be approximated by a 2D integral given by

\[
\frac{1}{N} \sum_{k'} \to \left( \frac{a}{2\pi} \right)^2 \int d^2 k'. \tag{9}
\]

We get the two integrals

\[
I_{os} = - \frac{2m_{ex}}{\hbar^2} \left( \frac{a}{2\pi} \right)^2 \int d^2 k' \lim_{\eta \to 0} \frac{e^{i k' \cdot r_i}}{k^2 - k'^2 + i \eta}, \quad I_{st} = - \frac{2m_{ex}}{\hbar^2} \left( \frac{a}{2\pi} \right)^2 \int d^2 k' \lim_{\eta \to 0} \frac{1}{k^2 - k'^2 + i \eta}, \tag{10}
\]

as shown in the appendix. The scattered exciton, following the definition in [13], is given by

\[
\psi_i = \frac{1}{\sqrt{N}} \left\{ e^{i k \cdot r_i} - f(k) \sqrt{\frac{i \pi}{2kr}} e^{i k \cdot r_i} \right\}, \tag{11}
\]

where \( r = |r_i| \) is the distance of the \( i \) site from the origin. We defined the scattering amplitude by

\[
f(k) = \frac{\pi E_a/2 \Delta_{ex}}{1 + (\pi E_a/2 \Delta_{ex}) \left[ \ln \left( ka/\pi \right) - i(\pi/2) \right]}, \tag{12}
\]
and the effective exciton bandwidth is defined by

$$\Delta_{\text{ex}} = \frac{\hbar^2 \pi^2}{2 m_{\text{ex}} a^2}. \quad (13)$$

The dipole–dipole interaction energy between different sites in optical lattices is small, and hence the excitons have a small bandwidth. In our case we have the limit of $E_a \gg \Delta_{\text{ex}}$ so that the scattering amplitude is $f(k) \approx \frac{1}{\ln(ka/\pi)}$, which exactly reproduces the result for the scattering off a hard disk of radius $a$ [14], with the scattering cross-section defined by $\sigma(k) = 2\pi |f(k)|^2$.

We thus conclude that an impurity generated by a missing atom in an optical lattice acts effectively like a hard disk of radius $a$. As the scattering is elastic, for an incident exciton with a fixed and small wavevector $k$ we get a scattered exciton with a wavevector $k'$, which is equal in magnitude to the incident one, namely $|k| = |k'| = k$. Hence if a large number of incident excitons with identical wavevector are scattered off the impurity, we get a ring of radius $k$ of scattered excitons.

The scattering amplitude is plotted in figure 2 as a function of wavevector, $k$, for lattice constant $a = 2000$ Å. The singularity at $k = 0$ is the 2D signature.

**3. Cavity polariton scattering of a vacancy in an optical lattice**

We now add cavity mirrors to our lattice as described in [6], where in the strong coupling regime, the system eigenstates are cavity polaritons. As a polariton is a coherent superposition of an exciton and a photon it can scatter off the impurity due to its excitonic part. The corresponding Hamiltonians then read:

$$H_0 = \sum_{kk'} \hbar \Omega_r(k) A_{kk'}^\dagger A_{kk'}, \quad V = -E_a B_0^\dagger B_0, \quad (14)$$

![Figure 2. The scattering amplitude versus wavevector $k$, for zero detuning.](http://www.njp.org/)
where $\Omega_\pm (k)$ are the upper and lower polariton branch dispersions, given by: $\Omega_\pm (k) = \frac{\alpha_{\text{ex}g}(k) + \alpha_{\text{ex}a}(k)}{2} \pm \Delta_k$. Here, $\Delta_k = \sqrt{\delta^2_k + |g_k|^2}$, and the exciton–photon detuning is defined by $\delta_k = \frac{\alpha_{\text{ex}a}(k) - \alpha_{\text{ex}g}(k)}{2}$. The parameter $g_k$ is for the exciton–photon coupling, which is taken to be of the electric dipole interaction. The cavity-photon dispersion is given by $\omega_{\text{cav}}(k) = \frac{\epsilon}{\sqrt{\epsilon}} \sqrt{k^2 + (\pi/L)^2}$, where $L$ is the distance between the cavity mirrors, and $\epsilon$ is the cavity medium dielectric constant, which here is taken to be a vacuum with $\epsilon = 1$. The polariton operators are defined by $A_{k \pm} = X_k^\pm B_k + Y_k^\pm a_k$, with $a_k$ the cavity photon operator. $X_k^\pm$ and $Y_k^\pm$ are the exciton and photon amplitude, respectively, which are given by $X_k^\pm = \pm \sqrt{\frac{\delta_k + \Delta_k}{2\Delta_k}}$, and $Y_k^\pm = \frac{g_k}{\sqrt{\delta_k + \Delta_k}}$ (more details are found in [6]).

We now calculate the polariton scattering off such an impurity. Again the scattering is elastic so that an incident polariton in branch $r$ with wavevector $k$ will scatter into a polariton with wavevector $k'$ in the same branch.

The free eigenstates obey $H_0|\phi_{kr}^{\text{pol}}\rangle = E_r(k)|\phi_{kr}^{\text{pol}}\rangle$, and the whole system eigenstates obey $H|\psi\rangle = E|\psi\rangle$, where $E_r(k) = h\Omega_r(k)$. The cavity photon eigenstate is defined by $|\alpha_{\text{cav}}\rangle = |\phi_{k}^{\text{cav}}\rangle$, and the exciton eigenstate in quasi-momentum space is defined by $B_k|\text{vac}\rangle = |\phi_{k}^{\text{ex}}\rangle$. The r polariton eigenstate is defined by $A_{k}^{\text{r}}|\text{vac}\rangle = |\phi_{kr}^{\text{pol}}\rangle$, and in terms of exciton and photon states we get $|\phi_{kr}^{\text{pol}}\rangle = X_k^\pm |\phi_{k}^{\text{ex}}\rangle + Y_k^\pm |\phi_{k}^{\text{cav}}\rangle$. In terms of real lattice space, we get $|\phi_{kr}^{\text{pol}}\rangle = \frac{X_k}{\sqrt{N}} \sum \psi^{i\text{r}} |\phi_{kr}^{\text{ex}}\rangle + \psi^{i\text{c}} |\phi_{kr}^{\text{cav}}\rangle$. A general state $|\psi\rangle$ can be expanded as $|\psi\rangle = \sum_k \psi_k^{\text{cav}} |\phi_{kr}^{\text{cav}}\rangle + \sum_i \psi_i^{\text{ex}} |\phi_{kr}^{\text{ex}}\rangle$.

As above the scattered polariton state is given by the Schwinger–Lippmann equation $|\psi\rangle = |\phi_{kr}^{\text{pol}}\rangle + G_0 V |\psi\rangle$, where we used the free Green function operator in equation (3). We multiply the equation from the left by the lattice exciton eigenstate $\langle \phi_i^{\text{ex}} \rangle$, and insert the previous identity operator between $G_0$ and $V$, to get

$$\langle \phi_i^{\text{ex}} | \psi \rangle = \langle \phi_i^{\text{ex}} | \phi_{kr}^{\text{pol}} \rangle + \sum_j \langle \phi_j^{\text{ex}} | G_0 | \phi_j^{\text{ex}} \rangle \langle \phi_j^{\text{ex}} | V | \psi \rangle. \quad (15)$$

Using the above definitions, we get the scattered polariton excitonic part amplitude by

$$\psi_i^{\text{ex}} = \frac{X_k}{\sqrt{N}} e^{ikr} \frac{E_a}{N} \sum_{k_n} \lim_{\eta \rightarrow 0} \frac{|X_k|^{2}}{E_r(k) - E_s(k') + i\eta} \psi_{0}^{\text{ex}}. \quad (16)$$

where due to energy conservation we replaced the energy $E$ by the initial energy $E_r(k)$, and $|X_k|^2$ is the exciton weight in the polariton. For the impurity site amplitude we have

$$\psi_0^{\text{ex}} = \frac{X_k}{\sqrt{N}} \left\{ 1 + \frac{E_a}{N} \sum_{k_n} \lim_{\eta \rightarrow 0} \frac{|X_k|^2}{E_r(k) - E_s(k') + i\eta} \right\}^{-1}. \quad (17)$$

We thus obtain

$$\psi_i^{\text{ex}} = \frac{X_k}{\sqrt{N}} \left\{ e^{ikr} + \frac{E_a I_{\text{os}}}{1 - E_a I_{\text{st}}} \right\}, \quad (18)$$

New Journal of Physics 10 (2008) 023001 (http://www.njp.org/)
where we defined oscillating and static sums. For a large optical lattice size the \( k \)-space can be assumed to be continuous and the sums converted to the integrals

\[
I_{os} = - \sum_{s} \left( \frac{a}{2\pi} \right)^2 \int \frac{d^2k'}{\eta - 0} \lim_{\eta \to 0} \frac{|X_k^s|^2 e^{i k' r}}{E_r(k) - E_s(k') + i\eta},
\]

\[
I_{st} = - \sum_{s} \left( \frac{a}{2\pi} \right)^2 \int \frac{d^2k'}{\eta - 0} \lim_{\eta \to 0} \frac{|X_k^s|^2}{E_r(k) - E_s(k') + i\eta}.
\] (19)

We calculate first the oscillating integral in the case of scattering of small wavevector polaritons, that is in the limit \( ka \ll 1 \) in the lower branch. In this limit the polariton dispersion can be considered approximately parabolic with a polariton effective mass of \( m_p \). This is of the order of the cavity photon effective mass \( m_p \approx (\hbar \pi)/(c L) \). Hence, the lower polariton branch dispersion is taken to be \( E_r(k) = E_s(k) + (\hbar^2 k^2/2m_p) \). The scattered states will also have small wavevectors due to the energy conservation. As the upper branch has higher energies its contributions are negligibly small here. Also the upper branch for larger wavevectors is mainly photonic with small excitonic part and thus only weakly contributes to the scattering of impurities. We consider the case around zero detuning between the excitons and photons. Therefore the excitonic weight \( |X^-|^2 \) will change from half around zero wavevector up to one for large wavevectors, where the lower branch becomes excitonic. The weight \( |X^-|^2 \) is a smooth function of \( k \), and in the present case can be taken out of the integral, and fixed with the initial polariton excitonic weight value. From this point on we neglect the contribution of the upper polariton branch, both as initial and scattered states, and also as intermediate scattering state. We will drop the branch index and summation, and all the parameters will be only for the lower branch.

The integral now reads:

\[
I_{os} = -X^2 \frac{2m_p}{\hbar^2} \left( \frac{a}{2\pi} \right)^2 \int \frac{d^2k'}{\eta - 0} \lim_{\eta \to 0} \frac{e^{i k' r}}{k^2 - k'^2 + i\eta}.
\] (20)

This is similar to the case of excitons of the previous section except for the factor \( |X_k^s|^2 \) and the involvement of the much smaller polariton effective mass in place of the exciton mass. Hence we have \( m_p \ll m_\text{ex} \) and the integration (see the appendix) gives

\[
I_{os} = -\frac{\pi X^2}{2\Delta_p} \sqrt{\frac{i\pi}{2kr}} e^{ikr},
\] (21)

where we defined the polariton effective bandwidth \( \Delta_p = \hbar^2 \pi^2/2m_p a^2 \).

We now turn to the second static integral. Here no oscillating exponent appears, and hence all wavevectors along the lower branch contribute, so that the intermediate scattering state can be anywhere along the lower branch. Again for energy reasons we neglect the contribution of the upper branch. The integral then can be simplified by using a model for the lower branch dispersion in place of the real one [15]. The lower branch is divided into two parts. The first part between \( 0 \leq k \leq k_0 \) is taken to be of a parabolic dispersion with a polariton effective mass, where \( E(k) = E(0) + (\hbar^2 k^2)/(2m_p) \); and the second part between \( k_0 \leq k \leq \pi/a \), where \( \pi/a \) is the Brillouin boundary, is taken to be dispersionless with energy equal to the exciton energy at zero wavevector, where we have \( k_0 \ll \pi/a \). The intersection point between the two parts is fixed by \( \hbar^2 k_0^2/(2m_p) = E_0 - E(0) \). The integration as shown in the appendix gives

\[
I_{st} = -\frac{\pi X^2}{2\Delta_p} \left[ \ln \left( \frac{k}{k_0} \right) - i\frac{\pi}{2} \right] + \frac{\pi}{4\Delta_p},
\] (22)
where $\Lambda_k = E_0 - E(k)$. The first term is the contribution of the parabolic part and the second originates from the flat part. The $\ln(k/k_0)$ is large in the limit $ka \ll 1$, but for a laterally confined 2D optical lattice, and for the smallest wavevector $k_m$ which is different from zero, due to the fact that $\Delta_p \gg E_a$, the term $(\pi X_{k_m}^2/2\Delta_p \ln((k_m/k_0))$ is much smaller than one and can be neglected. Hence $I_{\text{st}} \approx \pi/(4\Lambda_k)$.

The scattered polariton excitonic part reads

$$\psi_{i,x} = \frac{X_i}{\sqrt{N}} \left\{ e^{ikr_i} - f(k)\sqrt{\frac{i\pi}{2kr}} e^{ikr} \right\},$$

where the scattering amplitude is given by

$$f(k) = \frac{X_k^2 (\pi E_a/2\Delta_p)}{1 - (\pi E_a/4\Lambda_k)}.$$  

As $E_a > \Lambda_k$, we have $(\pi E_a)/(4\Lambda_k) > 1$, and the scattering amplitude is negative, that is $f(k) < 0$. Also the above impurity effective potential is repulsive for the polaritons.

In the case of zero detuning, that is $\delta_0 = 0$, we have for small wavevectors $X_k^2 = 1/2$, and $\Lambda_k$ is of the order of the exciton–photon coupling, $|g_k|$, where $E_a \gg \Lambda_k$, and we get $f(k) \approx -\Lambda_k/\Delta_p$. This scattering amplitude equals that of the scattering from an effective potential of a square barrier potential of height $\Lambda_k$ and width $a$.

For the case of negative detuning, in the limit of $E_a \gg \delta_0$, where $\Lambda_k$ is of the order of the exciton–photon detuning, the scattering amplitude is $f(k) \approx -(2X_k^2\Lambda_k)/\Delta_p$. This scattering amplitude equals that of the scattering from an effective potential of a square barrier potential of height $2X_k^2\Lambda_k$ and width $a$. Hence, we find that the scattering amplitude can be controlled by changing the exciton–photon detuning.

In using the following numbers: for an atomic energy $E_a = 2\text{eV}$, exciton–photon coupling $\hbar|g| = 0.0001 \text{ eV}$, and lattice constant $a = 2000 \text{Å}$, the scattering amplitude is plotted in figure 3.
as a function of the exciton–photon detuning, for approximately normal incident waves, where we used $k = 10^{-6}$ Å. It is clear that maximum scattering is obtained for zero detuning. As the detuning increases, both positively and negatively, the $k \approx 0$ polaritons become more photonic and they scatter off the impurity much less. As the atomic energy $E_a$ is much larger than the coupling energy $\hbar g$, the scattering amplitude only shows a negligibly small asymmetry for negative and positive detunings, but we expect a clear resonance of the scattering amplitude around resonance $\delta_0$. Considering a stream of incident polaritons with the same wavevector $k = k\hat{k}$ we then should see a ring of radius $k$ of scattered polaritons.

4. Exciton and polariton scattering of a vacancy in two-atoms per site optical lattices

We will now study the scattering of excitons and polaritons in a doubly occupied optical lattice where one atom is missing in one site (called the origin site). The corresponding exciton polariton picture for an ideal lattice is discussed in [10]. Here resonant electronic excitation transfer occurs among the two on-site atoms with transfer parameter $J_0$ and also among the nearest neighbor sites with transfer parameter $J_1$. The on-site interaction can be diagonalized to form symmetric and antisymmetric localized excitation with frequencies $\omega_s = \omega_A + J_0$, and $\omega_a = \omega_A - J_0$, respectively. The symmetric state transition dipole is the sum of the two atom dipoles, while the antisymmetric one is their difference. Hence, only the symmetric states have a significant dipole moment and thus form excitons through resonant coupling. The symmetric exciton dispersion in the limit $ka \ll 1$ then reads $\omega_s(k) = \omega_A + J_0 + 8J_1 + (\hbar k^2/2m_{\text{eff}})$, with the effective mass $m_{\text{eff}} = -\hbar/(4J_1a^2)$ and, up to a rescaling, is analogous to the previous case. Naturally within a cavity only the symmetric excitons are coupled to the photons to form cavity polaritons (for details see [10]). We will show that the defect, plotted schematically in figure 4, which in this case constitutes a single atom as compared to two, here acts substantially differently from the simple no atom hole in the case of a single occupied lattice. Physically this can be understood from the fact that a single atom can store almost the same amount of energy as a pair if only one photon excitation is considered.

Let us now calculate the scattering amplitude of excitons and polaritons of this impurity. The scattering is for the symmetric excitons, and for the polariton excitonic part. The antisymmetric states are not involved in the scattering process, as they are on-site localized and posses no dipole moment.

Figure 4. An impurity in 1D optical lattice.
We concentrate on the scattering of long wavelength excitons with a parabolic dispersion described by an effective mass. The scattering amplitude is found to be

\[
f(k) = \frac{\pi J_0/2\Delta_{ex}}{1 + (\pi J_0/2\Delta_{ex}) [\ln (ka/\pi) - i\pi/2]}.
\]  

(25)

For negative on-site energy transfer, \(J_0 < 0\), the scattering is of an effective potential of a square barrier of height \(|J_0|\) and width \(a\). One needs to compare between the on-site transfer parameter \(|J_0|\) and the exciton bandwidth \(\Delta_{ex}\). In the limit of \(|J_0| \gg \Delta_{ex}\) the scattering is identical to that from an effective potential of a hard disk with radius \(a\) (see figure 2), that is \(f(k) \approx \frac{1}{\ln(ka/\pi)}\).

For polaritons the scattering of the impurity is only for their excitonic part. We consider the scattering of long wavelength lower branch polaritons with a parabolic dispersion and an effective polariton mass \(m_p\). The scattering amplitude is given by

\[
f(k) = \frac{X_k^2 (\pi J_0/2\Delta_p)}{1 - (\pi J_0/4\Lambda_k)}.
\]  

(26)

Here \(\Lambda_k = E_0 - E(k)\), where \(E_0 = \hbar\omega_A + \hbar J_0\), and where \(J_0 \gg J_1\).

In the limit of \(|J_0| \gg \Lambda_k\) we get \(f(k) \approx -X_k^2(2\Lambda_k/\Delta_p)\), where, for \(J_0 < 0\), the scattering acts like a square barrier of height \(2X_k^2\Lambda_k\) and width \(a\). Similarly in the opposite limit of \(|J_0| \ll \Lambda_k\) we get \(f(k) \approx X_k^2(\pi J_0/2\Delta_p)\), and the scattering, for \(J_0 < 0\) mimics a square barrier of height \(\pi |J_0|X_k^2/2\) and width \(a\). As shown in the previous chapter, the polariton scattering of an impurity can be modulated by controlling the exciton–photon detuning. As we change \(\delta_k\), then \(X_k^2\) and \(\Lambda_k\) are strongly changed, and as a result the scattering amplitude \(f(k)\) and the effective potential strength are changed.

Introducing the numerical examples used in the previous section with transfer energy \(\hbar J_0 = -0.001\) eV the scattering amplitude is plotted in figure 5 as a function of the exciton–photon detuning, for incident waves, namely \(k \approx 0\). It is clear that maximum scattering is obtained for zero detuning. As here the transfer energy \(\hbar J_0\) is smaller than, and close to, the
coupling energy $\hbar g$, the scattering amplitude asymmetry for negative and positive detuning is much more pronounced relative to the case of the previous section. For $k = 0$, at zero detuning, the lower branch polariton is half exciton and half photon. For negative detuning, at $k = 0$, the lower branch polariton is more photonic than excitonic; while for positive detuning it is the opposite: the lower branch polariton is more excitonic than photonic. Therefore, the positive detuning scattering amplitude is larger than the negative one.

4.1. An impurity in an asymmetric optical lattice

One of the phenomena for excitons in doubly occupied lattices appears in the case of asymmetric optical lattice sites [10]. We get a strong polarization dependence of the exciton and polariton energies. Here, we discuss the consequence of this for their scattering amplitudes off impurities.

If one of the orthogonal pairs of counter propagating lasers forming the lattice potentials has a different intensity, the potential is elongated in one direction, e.g. $x$. Hence the two atoms at one site will have a larger average distance $R$ in the $x$-direction as shown in figure 6. The atomic transition dipole induced by the cavity photon is assumed to be in the $(x, y)$-plane $\vec{\mu} = \mu(\cos \theta, \sin \theta)$, where $\theta$ is the angle between the dipole $\vec{\mu}$ and the $x$-axis. The resonance dipole–dipole interaction between the two on-site atoms is $\hbar J_0(\theta) = \hbar \tilde{J} (1 - 3 \cos^2 \theta)$, where $\hbar \tilde{J} = \mu^2 / 4 \pi \epsilon_0 R^3$. We have $\hbar J_0(\theta = 0) = -2 \hbar \tilde{J}$, and $\hbar J_0(\theta = 90) = \hbar \tilde{J}$, with $\hbar J_0(\theta \approx 54.74) = 0$. The detuning energy between symmetric and antisymmetric states thus will change sign at some angle, where the polarization even vanishes.

The long wavelength polariton scattering amplitude as a function of the relative transition dipole direction now is

$$f_k(\theta) = \frac{X^2_k(\theta) \left( \frac{\pi J_0(\theta)}{2 \Delta_p} \right)}{1 - \left( \frac{\pi J_0(\theta)}{4 \Delta_k(\theta)} \right)}.$$  \hspace{1cm} (27)

We plot this scattering amplitude as a function of $\theta$ for different values of $\tilde{J}$, and for $k \approx 0$, using the numerical values of section 3. We also have $E_c(0) = E_A + J(0)$, and $\hbar J_1 = 10^{-7}$ eV. In figure 7 the plot is for $\hbar \tilde{J} = 10^{-4}$ eV, where $\hbar |g| = \hbar \tilde{J}$. Figure 8 is for $\hbar \tilde{J} = 5 \times 10^{-4}$ eV, where $\hbar |g| < \hbar \tilde{J}$. Note that the scattering amplitude changes sign at $\theta \approx 54.74$ and we can turn off scattering by using this proper angle. In figure 9, we plot this for $\hbar \tilde{J} = 10^{-3}$ eV. Here two resonances appear. Figure 10 is for $\hbar \tilde{J} = 5 \times 10^{-3}$ eV. Now the resonances tend to the negative–positive crossover angle.
Figure 7. The scattering amplitude versus $\theta$, for $k \approx 0$ polaritons, with $\hbar \tilde{J} = 10^{-4}$ eV.

Figure 8. The scattering amplitude versus $\theta$, for $k \approx 0$ polaritons, with $\hbar \tilde{J} = 5 \times 10^{-4}$ eV.

The negative scattering amplitude corresponds to a repulsive effective potential, and polaritons scatter far off the impurity. Meanwhile the positive scattering amplitude corresponds to an attractive potential. Here even the formation of bound states could be expected, allowing for localized polaritons. The bound state signature appears in the pole of the scattering amplitude of equation (27) but by including the ln term of equation (22) in the denominator. We get a
shallow bound state that falls inside the polariton line width, and which presents as a resonance scattering state inside a continuum.

5. Summary

We demonstrated that defects in an optical lattice in the Mott insulator phase will change the dynamics of resonant excitons and cavity polaritons. For a very low density of defects, the
exciton and polariton pictures still hold and the defect simply acts as a scatterer for such quasi-particles. We calculated the scattering amplitude for excitons and polaritons showing that the defects can be approximated by effective potentials. In the case of one atom per site the vacancy scattering effective potential for excitons is a hard disk of radius equal to the lattice constant $a$, which is quite different for polaritons, where only the excitonic part contributes significantly to the scattering. The scattering effective potential for long wavelength polaritons is just a square barrier of height $2|X_k|^2\Lambda_k$ and width $a$, where $|X_k|^2$ is the exciton weight in the cavity polariton, and which appears here as the scattering is only for the polariton excitonic part. For the case of zero exciton–photon detuning, and in the limit $ka \ll 1$, we have $|X_k|^2 = 1/2$, and $\Lambda_k$ is of the order of the Rabi splitting. Meanwhile for large negative detuning we have $|X_k|^2 \ll 1$, and $\Lambda_k$ is of the order of the exciton–photon detuning. As $|X_k|^2$ and $\Lambda_k$ are functions of the detuning, hence the scattering amplitude can be controlled by changing the detuning, with a scattering resonance at zero detuning.

In the case of a two atoms per site lattice with a defect represented by a single atom site, we found two distinct cases. If the on-site dipole–dipole coupling $J_0$ is larger than the Rabi splitting, we got similar results to the case of one atom per site. But if $J_0$ is smaller than the Rabi splitting, hence the polariton scattering effective potential is identical to the scattering of a square barrier of height $J_0$ and width $a$. The parameter $J_0$ can be easily controlled by changing the photon polarization, as we presented for the case of asymmetric optical lattice sites. Also we showed that at a fixed angle $J_0$ can change sign from positive to negative, and then also the scattering amplitude changes sign.

We conclude that cavity polaritons can be used as a useful tool to observe defects in an optical lattice. As the polariton is partly exciton and partly photon, where the photon part can be controlled externally, the above results suggest that one can recognize the kind of defect in each case. For example in transmission or reflection experiments, for an incident field with a fixed wavevector $k$, in the transmitted or reflected signals we get a scattering ring of radius $k$ with the appropriate intensity which we obtained from the scattering cross-section.

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Appendix A. This calculation of equations (10) integrals

Here we give the calculation details of the two integrals of equations (10).

The oscillating integral is written explicitly as

$$I_{os} = -\frac{2m_{ex}}{\hbar^2} \left( \frac{a}{2\pi} \right)^2 \int_{0}^{+\infty} dk' \int \limits_{-\pi}^{+\pi} d\theta \lim_{\eta \to 0, \ k_{\perp} \to k, \ k'_{\perp} \to 0} \frac{k' e^{ik'r \sin \theta}}{k^2 - k'^2 + i\eta},$$

(A.1)

where $r = |r_i|$ is the distance of the $i$ site from the origin, and $k' = |k'|$. The integral over $k'$ is from zero to infinity, which is possible here due to the oscillating exponents, where the contributions of large wavevectors are negligible. The integral over $\theta$ is calculated by

$$J_0(k'r) = \frac{1}{2\pi} \int_{-\pi}^{+\pi} d\theta \ e^{ik'r \sin \theta},$$

(A.2)
where $J_0(x)$ is the zero-order Bessel function of the first kind. We now have

$$I_{os} = \frac{2m_{ex}}{\hbar^2} \left( \frac{a}{2\pi} \right)^2 2\pi \int_0^{+\infty} dk' \lim_{\eta \to 0} \frac{k'J_0(k'r)}{k'^2 - k^2 - i\eta}. \quad (A.3)$$

We use the result

$$\int_0^{+\infty} dk' \lim_{\eta \to 0} \frac{k'J_0(k'r)}{k'^2 - k^2 - i\eta} = \frac{\pi}{2} H_0^{(1)}(kr), \quad (A.4)$$

where $H_0^{(1)}(x)$ is the zero order of the Hankel function of the first kind, which is defined by

$$H_0^{(1)}(x) = J_0(x) + iN_0(x),$$

where $N_0(x)$ is the zero-order Bessel function of the second kind.

The scattered wave is observed very far from the impurity, that is at $r \to +\infty$. For large $x$, we have the asymptotic expansions

$$J_0(x) \sim \sqrt{\frac{2}{\pi x}} \cos \left( x - \frac{\pi}{4} \right), \quad N_0(x) \sim \sqrt{\frac{2}{\pi x}} \sin \left( x - \frac{\pi}{4} \right), \quad (A.5)$$

which yield

$$H_0^{(1)}(x) \sim \sqrt{\frac{2}{\pi x}} e^{i(x - \pi/4)}. \quad (A.6)$$

The result is

$$I_{os} = -\frac{\pi}{2\Delta_{ex}} \sqrt{\frac{i\pi}{2kr}} e^{ikr}, \quad (A.7)$$

where we defined the effective exciton bandwidth in equation (13).

For the static integral the angle integral gives $2\pi$, we have

$$I_{st} = \frac{2m_{ex}}{\hbar^2} \left( \frac{a}{2\pi} \right)^2 2\pi \int_0^{\pi/a} dk' \lim_{\eta \to 0} \frac{k'}{k'^2 - k^2 - i\eta}. \quad (A.8)$$

Here, due to the fact that no oscillations exist, it is not possible to extend the integral to infinity. We used a cut-off at the Brillouin zone boundary. Such a cut-off is a physical one as the maximum exciton wavevector is for a wavelength that equals the lattice constant. The integration, in the limit of $ka \ll 1$, yields

$$I_{st} = -\frac{\pi}{2\Delta_{ex}} \left[ \ln \left( \frac{ka}{a} \right) + i\frac{\pi}{2} \right]. \quad (A.9)$$

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