Photonic band gaps and defect states induced by excitations of Bose-Einstein condensates in optical lattices

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We study the interaction of a Bose-Einstein condensate in an optical lattice with an additional largely detuned light field propagating through it. If the condensate is in its ground state it acts as a periodic dielectric, and gives rise to photonic band gaps at optical frequencies. The band structure of the combined system of condensed lattice atoms and photons is studied by using the concept of polaritons. If elementary excitations of the condensate are present, they will produce defect states inside the photonic band gaps. The frequency of localized defect states is calculated using the Koster-Slater model. [S1050-2947(99)06704-9]

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I. INTRODUCTION

The achievement of Bose-Einstein condensation in magnetic traps [1] has induced a great interest in the properties of quantum atomic gases and their manipulation by atom optic techniques. Although the latter are usually used for laser cooling in the formation process of a Bose-Einstein condensate (BEC), confinement in an optical dipole trap has been demonstrated only recently [2]. The all-optical confinement of a BEC provides a great potential for the manipulation and application of BEC's. In particular, it opens the new opportunity to study atomic BEC's in optical lattices. In recent years experimentalists have made great efforts to create a BEC in optical lattices. Although there are presently still some technical problems in achieving this goal, the rich physics of uncondensed ultracold atoms in optical lattices [3] and quasicrystals [4] has attracted great interest for both experimentalists and theorists. Recently, several theoretical papers dealing with condensates in optical potentials have been published [5,6].

In this paper we focus on another aspect of this subject: light propagation through a coherent condensate that is placed in an optical lattice. Since the ground state of the condensate in a lattice potential is periodic, it will act as a periodic dielectric for laser light propagating through it. Thus it will give rise to photonic band gaps at optical frequencies.

The phenomenon of photonic band gaps is a natural consequence of the periodicity of the condensate. In fact, it should also occur for uncondensed ultracold atoms in optical lattices. However, in the case of a condensed atomic lattice what is interesting is that, because of the macroscopic occupation of the ground state, a proper description of photonic band gaps is given in terms of polaritons (an entangled coherent system composed of superpositions of photons and excited atoms). Furthermore, elementary excitations may be present in the lattice BEC. In general these excitations are no longer periodic, and will cause distortions of the perfect periodic structure of the condensed atomic lattice. An excitation-induced defect in the atomic lattice in turn causes the occurence of defect states inside photonic band gaps of light propagating through the BEC. In this sense, elementary excitations have a close analogy to lattice defects in solid-state physics which cause defect states in the electronic band structure.

The paper is organized as follows. In Sec. II we will derive the equations of motion. In Sec. III we consider the case where only the lattice laser beams are present, and seek for a periodic solution to the coupled equations of motion describing the ground-state BEC and the lattice laser beams. This solution shows that the optical potential experiences no back-reaction from the condensate if the latter has settled down into its ground state. In this sense, the lattice laser beams just effectively act as a constant periodic potential for the BEC. In Sec. IV we consider the propagation of a weak probe laser beam through the ground-state BEC, and derive the form of the lowest photonic band gap for this beam by using polariton modes. To examine the behavior of a probe laser beam propagating through a weakly nonperiodic BEC, a theory of defect states for photonic band gaps is developed in Sec. V, which is applied in Sec. VI to the Koster-Slater model for a localized elementary excitation. Section VII concludes the paper.

II. EQUATIONS OF MOTION

The system under consideration consists of interacting two-level atoms which are coupled to the electromagnetic field. This coupling is described by using the electric-dipole and rotating-wave approximations so that the corresponding second quantized Hamiltonian is given by

$$H = H_A + H_{\mathrm{NL}} + H_{\mathrm{E.M.}} + H_{\mathrm{int}}, \tag{1}$$

where

$$H_A := \int d^3x \sum_{i=e,g} \Psi_i^\dagger \left\{ \frac{\vec{p}^2}{2M} + V(\vec{x}) + E_i \right\} \Psi_i \tag{2}$$

describes the atomic center-of-mass motion. $V(\vec{x})$ denotes an external potential. M represents the atomic mass, and E_i, $i=e,g$, are the internal energy levels for ground-state and excited atoms, respectively. The corresponding field operators Ψ_g and Ψ_e fulfill the commutation relations $[\Psi_i(\vec{x})^\dagger, \Psi_j(\vec{y})] = \delta_{ij}\delta(\vec{x}-\vec{y})$. H_{NL} is the nonlinear part

of the atomic Hamiltonian which describes two-body collisions. For a dilute Bose gas it can be approximated by

$$H_{\mathrm{NL}} := \tfrac{1}{2}\int d^3x \sum_{i,j=e,g} g_{ij}\Psi_i^\dagger \Psi_j^\dagger \Psi_j \Psi_i , \tag{3}$$

where $g_{ij} := 4\pi\hbar^2 a_{\mathrm{sc}}^{(ij)}/M$ are coupling constants, and $a_{\mathrm{sc}}^{(ij)}$ denote the scattering lengths for scattering between atoms in the internal state i and j.

For the description of the electromagnetic field we use the representation in terms of positive end negative frequency parts of the vector potential, $\vec{A}(\vec{x}) = \vec{A}^{(+)}(\vec{x}) + \vec{A}^{(-)}(\vec{x})$. This representation will turn out to be convenient for the adiabatic elimination of excited atoms. The Hamiltonian for the free electromagnetic field then takes the simple form

$$H_{\mathrm{E.M.}} = 2\varepsilon_0 \int d^3x \sum_{a,b=1}^{3} A_a^{(-)}(\hat{\omega}^2)_{ab} A_b^{(+)} . \tag{4}$$

The positive and negative frequency parts are related by $(\vec{A}^{(+)})^\dagger = \vec{A}^{(-)}$ and fulfill the commutation relation $[A_a^{(+)}(\vec{x}), A_b^{(-)}(\vec{y})] = (\hbar/2\varepsilon_0)\hat{\omega}^{-1}\delta_{ab}^T(\vec{x}-\vec{y})$, where $\delta_{ab}^T(\vec{x}-\vec{y})$ is the transverse delta function. The *frequency operator* $\hat{\omega}$ is a pseudodifferential operator [7] whose action is defined in momentum space by

$$[\hat{\omega}\vec{A}](\vec{x}) = (2\pi)^{-3/2}\int d^3k\, e^{i\vec{k}\cdot\vec{x}} c|\vec{k}|\vec{A}(\vec{k}) . \tag{5}$$

The physical interpretation of the frequency operator is simple. It just multiplies a photon mode with its frequency $\omega(\vec{k}) = c|\vec{k}|$. A more compact representation of $\hat{\omega}$ in position space is given by $\hat{\omega} = c\sqrt{-\hat{\Delta}} = c|-i\nabla|$, where $\hat{\Delta}$ denotes the Laplace operator. The usage of the frequency operator $\hat{\omega}$ has advantages, though it is quite uncommon. It allows for a closed representation of the equations of motion in position space which makes it easier to display the essential steps in our derivations. Physically, it just corresponds to the Fourier transformation of the well-known equations for photon momentum eigenmodes $a_\lambda(\vec{k})$ coupled to two-level atoms.

Using the positive and negative frequency parts of the vector potential, the electric-dipole coupling between the atoms and the electromagnetic field in the rotating-wave approximation can be written as

$$H_{\mathrm{int}} = i\int d^3x \{\Psi_g^\dagger \Psi_e(\vec{d}^{\,*}\cdot\hat{\omega}\vec{A}^{(-)}) - \Psi_e^\dagger\Psi_g(\vec{d}\cdot\hat{\omega}\vec{A}^{(+)})\} . \tag{6}$$

The Heisenberg equations of motion derived from the Hamiltonian (1) are given by

$$i\hbar\dot{\Psi}_e = \left\{\frac{\vec{p}^2}{2M} + V + E_e + \sum_{j=e,g} g_{ej}\Psi_j^\dagger\Psi_j\right\}\Psi_e - i\Psi_g(\vec{d}\cdot\hat{\omega}\vec{A}^{(+)}) \tag{7}$$

$$i\hbar\dot{\Psi}_g = \left\{\frac{\vec{p}^2}{2M} + V + E_g + \sum_{j=e,g} g_{gj}\Psi_j^\dagger\Psi_j\right\}\Psi_g + i\Psi_e(\vec{d}^{\,*}\cdot\hat{\omega}\vec{A}^{(-)}) \tag{8}$$

$$i\dot{A}_a^{(+)}(\vec{x}) = \hat{\omega}A_a^{(+)}(\vec{x}) + \frac{i}{2\varepsilon_0}\int d^3y \Psi_g^\dagger(\vec{y})\Psi_e(\vec{y}) \times \sum_{b=1}^{3} d_b^*\,\delta_{ab}^T(\vec{x}-\vec{y}) . \tag{9}$$

III. LATTICE LASER BEAMS AND BEC IN GROUND STATE: DECOUPLING OF THE FIELDS

To analyze the interaction between the atoms and the lattice laser beams in the absence of an external potential $[V(\vec{x}) = 0]$, we restrict ourselves to the particular case where the atomic field is composed of condensed atoms, i.e., a Bose-Einstein condensate. This allows us to make further substantial simplifications. As is well known, a condensate can be described by assuming that all atoms are in the same quantum state ψ_g. This amounts to replacing the field operator Ψ_g in Eq. (8) by the c-number field ψ_g, which then fulfills a nonlinear Schrödinger equation. In addition, we assume that the photon fluctuations of the lattice laser beams are small, and therefore not important for our case. This allows us to replace the operator $\vec{A}^{(+)}$ by a corresponding classical field vector $\vec{A}_L^{(+)}$ of the lattice laser beams.

We consider the regime of coherent interaction where the electromagnetic field is detuned far away from the atomic resonance frequency $\omega_{\mathrm{res}} := (E_e - E_g)/\hbar$. Specifically, we assume that the detuning $\Delta_L := \omega_L - \omega_{\mathrm{res}}$ (with $\omega_L := c|\vec{k}_L|$) of the lattice laser beams is negative (red detuning), and its absolute value is much larger than any other characteristic frequency of our system, so that we can adiabatically eliminate the excited atoms [8–11]. This amounts to replacing the field operator for excited atoms by

$$\Psi_e \approx \frac{-i}{\hbar\Delta_L}\psi_g(\vec{d}\cdot\hat{\omega}\vec{A}_L^{(+)}) . \tag{10}$$

Inserting Eq. (10) into Eqs. (8) and (9), one easily finds (to first order in $1/\Delta_L$)

$$i\hbar\dot{\psi}_g = \left\{\frac{\vec{p}^2}{2M} + V + E_g + g_{gg}\psi_g^\dagger\psi_g + \frac{1}{\hbar\Delta_L}(\vec{d}\cdot\hat{\omega}\vec{A}_L^{(-)})(\vec{d}\cdot\hat{\omega}\vec{A}_L^{(+)})\right\}\psi_g \tag{11}$$

$$i(\dot{A}_L^{(+)}(\vec{x}))_a = \hat{\omega}(A_L^{(+)}(\vec{x}))_a + \frac{1}{2\varepsilon_0\hbar\Delta_L}\int d^3y |\psi_g(\vec{y})|^2(\vec{d}\cdot\hat{\omega}\vec{A}_L^{(+)}(\vec{y}))\sum_{b=1}^{3} d_b^*\,\delta_{ab}^T(\vec{x}-\vec{y}) . \tag{12}$$

Equations (11) and (12) describe the coherent coupling of a ground-state atomic field to the lattice laser beams. The physics implicit in these equations is straightforward. The laser beams induce an optical potential for ground-state atoms which is proportional to the light intensity $[\propto(\hat{\omega}\vec{A}_L)^2]$. The atoms, in turn, act on the electromagnetic field like a dielectric, where the index of refraction is determined by the density $|\psi_g|^2$ of ground-state atoms.

We are interested in how the condensate affects the lattice laser beams and the corresponding back-reaction in the optical potential. For simplicity, we take the laser beam to be parallel to the x axis. Further, we assume that the BEC has settled to its ground state which, because of the periodicity of the optical potential provided by the lattice laser beams, is periodic. It is then convenient to decompose the fields into a discrete Fourier series

$$\psi_g(x)=\sum_{l\in\mathbf{Z}}\psi_l\exp[il\vec{k}_L\cdot\vec{x}],$$

$$\Omega^{(L)}(x):=\frac{1}{\hbar}\vec{d}\cdot\hat{\omega}\vec{A}_L^{(+)}(x)=\sum_{l\in\mathbf{Z}}\Omega_l^{(L)}\exp[il\vec{k}_L\cdot\vec{x}].$$

We remark that $\vec{k}_L$ does *not* denote the wave vector of the laser beams. It is defined by its relation to the spatial period x_L of the optical lattice by $\vec{k}_L=\vec{e}_x 2\pi/x_L$. This period x_L differs in general slightly from the wavelength of the laser beams outside the atomic medium [12]. Transforming Eqs. (11) and (12) to momentum space we arrive at the following one-dimensional set of equations:

$$i\hbar\dot{\psi}_l=\frac{\hbar^2k_L^2}{2M}l^2\psi_l+\frac{g_{gg}}{(2\pi)^2}\sum_{m,n\in\mathbf{Z}}\psi^*_{m+n-l}\psi_m\psi_n+\frac{\hbar}{(2\pi)^3\hbar\Delta_L}\sum_{m,n\in\mathbf{Z}}\psi_{l+m-n}\Omega_m^{(L)*}\Omega_n^{(L)},\quad(13)$$

$$i\hbar\dot{\Omega}_l^{(L)}=\hbar\omega_L|l|\Omega_l^{(L)}+\frac{\omega_L|l|\vec{d}_\perp^{\,2}}{2(2\pi)^3\varepsilon_0\Delta_L}\sum_{m,n\in\mathbf{Z}}\Omega_m^{(L)}\psi^*_{m+n-l}\psi_n,\quad(14)$$

where we have defined the transversal dipole moment of the atoms $\vec{d}_\perp:=\vec{d}-\vec{k}_L(\vec{d}\cdot\vec{k}_L)/\vec{k}_L^2$. We can now exploit the fact that the optical frequency ω_L is typically (very) much larger than any other frequency scale involved in the system. This allows us to perform a rotating-wave approximation by inserting $\tilde{\Omega}_l^{(L)}:=\exp\{i\omega_L t|l|\}\Omega_l^{(L)}$ into Eqs. (13) and (14) and neglecting all terms which rotate at multiples of the frequency ω_L. This procedure results in the simplified equations

$$i\hbar\dot{\psi}_l=\left\{\frac{\hbar^2k_L^2}{2M}l^2+\frac{\hbar}{(2\pi)^3\Delta_L}\sum_{m\in\mathbf{Z}}|\Omega_m^{(L)}|^2\right\}\psi_l+\frac{g_{gg}}{(2\pi)^2}\sum_{m,n\in\mathbf{Z}}\psi^*_{m+n-l}\psi_m\psi_n+\frac{\hbar}{(2\pi)^3\Delta_L}\sum_{m\in\mathbf{Z}}\psi_{l+2m}\Omega_m^{(L)*}\Omega_{-m}^{(L)},\quad(15)$$

$$i\hbar\dot{\Omega}_l^{(L)}=\hbar\omega_L|l|\left\{1+\frac{\vec{d}_\perp^{\,2}}{2(2\pi)^3\varepsilon_0\Delta_L}\sum_{n\in\mathbf{Z}}|\psi_n|^2\right\}\Omega_l^{(L)}+\frac{\vec{d}_\perp^{\,2}}{2(2\pi)^3\varepsilon_0\Delta_L}\omega_L|l|\Omega_{-l}^{(L)}\sum_{n\in\mathbf{Z}}\psi^*_{n-2l}\psi_n.\quad(16)$$

These equations have some properties which allow us to decouple the system for some physically interesting cases. The most important one is that the atoms only couple counterpropagating modes, i.e., $\Omega_l^{(L)}$ and $\Omega_{-l}^{(L)}$. This is a direct consequence of energy conservation, since a transition to any other mode would require an amount of energy on the order of $\hbar\omega_L$, which cannot be provided by the interaction with the condensate. In addition, it is not difficult to see that both the mean density $\overline{\rho}:=\Sigma_n|\psi_n|^2$ and the mean light intensity per mode, $\overline{I_l}:=|\Omega_l^{(L)}|^2+|\Omega_{-l}^{(L)}|^2$, are conserved quantities, reflecting the conservation of the total number of atoms and the number of photons with energy $\hbar\omega_L|l|$, respectively. Therefore, the first sums on the right-hand sides of Eqs. (15) and (16) just produce a constant shift of the energy levels.

We now consider a solution of the system of equations (15) and (16) which corresponds to a standing-wave lattice laser beam interacting with a BEC in its ground state in the coherent regime. For a standing-wave lattice, we can make the ansatz $\Omega_l^{(L)}=\Omega_{-l}^{(L)}$. In addition, in the ground state of the BEC the time dependence of all coefficients ψ_l is given by $\psi_l(t)=\exp[-i\mu t/\hbar]\psi_l(0)$, where μ denotes the chemical potential and $\psi_l(0)$ can be chosen to be real. It is then not difficult to show that $\Omega_l^{(L)}=\Omega_{-l}^{(L)}$ holds for all times (by differentiating both sides and comparing the results). In addition, the expression $\Omega_l^{(L)}\Omega_{-l}^{(L)*}$, which describes the optical potential in Eq. (15), is time independent, too.

An immediate consequence of this fact is that in the coherent regime the optical potential is decoupled and the condensate behaves as if it were moving in a given external periodic potential. However, this conclusion is only valid if we consider an infinite BEC. In practice, the BEC is finite, and the frequency of the light field is fixed by the laser source. As a consequence, the lattice wave vector k_L *inside* the BEC is in general different from ω_L/c [12]. Thus, even if the equations of motion decouple for a *given* wave vector k_L, the optical potential is altered because k_L is changed as compared to the vacuum. Nevertheless, once this has been taken into consideration the influence of the lattice laser beams on the BEC can be replaced by an external potential

$V(\vec{x})$ with periodicity π/k_L. In this sense, the condensate and the lattice laser beam self-consistently settle into a stationary state.

IV. POLARITON BAND THEORY FOR LIGHT INTERACTING WITH A CONDENSATE

In Sec. III we have shown how the combined system of a BEC and lattice laser beams behaves in its ground state. We are now interested in a different situation where a running probe laser beam propagates through the ''lattice condensate'' (condensate plus lattice laser beams). The behavior of the probe laser can be intuitively understood by considering the BEC as a kind of dielectric for the probe laser beam. Since the BEC is periodic, the probe laser beam will effectively propagate through a periodic dielectric. We thus expect it to show the phenomenon of photonic band gaps [13].

To describe the interaction of the probe laser beam with the condensate, we will assume that the ground-state BEC changes little, so that ψ_g enters as a given external field into the equations of motion for excited atoms (7) and for the probe laser beam (9). The validity of this assumption is a consequence of the macroscopic population of the ground state: a small change in the number of ground state atoms has little effect on the macroscopic wave function of the BEC, so that for a weak probe laser beam the change in ψ_g can be neglected. For uncondensed atoms this approximation is not valid, since no state is macroscopically occupied, and one has to employ a density-matrix approach to describe the dynamics of the fields.

As a consequence of the elimination of the ground-state atoms, the coupled equations of motion describe polariton modes, i.e., entangled superpositions of excited matter and photons [14,15]. Thus it is really ''polaritonic'' band gaps rather than photonic band gaps that we are studying. However, for sufficiently large detunings of the lattice laser beams the entanglement is very small, so that the result indeed can be considered to be photonic band gaps.

To find a suitable expression for the ground-state wave function ψ_g, we use the results of Sec. III, i.e., consider the case where the BEC moves in a periodic potential of the form

$$V(\vec{x}) = -V_0 \cos(2k_L x) \tag{17}$$

(we choose the factor of $2k_L$ since the potential created by an optical lattice of wave vector k_L would create such a potential [11]). In addition, we consider a very weak probe beam and neglect the four-wave mixing effect due to the interference between the probe laser and the lattice lasers [12]. As a result, the ground state of the BEC can effectively be described by the Gross-Pitaevskii equation

$$\mu \psi_g = \left\{ \frac{\vec{p}^2}{2M} + V(\vec{x}) \right\} \psi_g + g_{gg} |\psi_g|^2 \psi_g , \tag{18}$$

where μ is the chemical potential. In the experimentally realized dilute Bose condensates the interaction energy of the two-body collisions between atoms is usually large, so that one can perform the Thomas-Fermi approximation by neglecting the kinetic energy. This transforms Eq. (18) into a simple algebraic equation whose solution is of the form $|\psi_g(x)|^2 = \rho_0 + \rho_1 \cos(2k_L x)$. This solution is valid for all x if the optical potential is not too strong, so that ρ_1 is smaller than ρ_0. If ρ_1 is not too close to ρ_0 we can furthermore simplify the wave function to

$$\psi_g(x) \approx \sqrt{\rho_0} + \frac{\rho_1}{2\sqrt{\rho_0}} \cos(2k_L x) \tag{19}$$

(this time-independent expression is valid in a frame rotating at frequency $E_g/\hbar$). We remark that this expression produces qualitatively correct results for the lowest photonic band even if the kinetic energy is not negligible or $\rho_1 \approx \rho_0$. The reason for this is that the corresponding corrections essentially introduce higher coefficients in the Fourier series of Eq. (19). Since for a weak interaction these higher coefficients only couple higher bands, they do not affect the results for the lowest band. Furthermore, for a wide range of parameters the change in ρ_1 is not very large, so that Eq. (19) will still produce good estimations, even if the underlying assumptions are not well fulfilled.

Since ψ_g does not depend on y and z, it is advantageous to rescale the wave functions as $\psi \to L_\perp \psi$, where $L_\perp$ is the typical extension of the BEC in the y and z direction. This guarantees that the one-dimensional integral $\int dx |\psi|^2$ is dimensionless, and can be interpreted as a particle number. In the actual calculations this rescaling leads to the appearance of various factors of $L_\perp$. $L_\perp$ will not enter the final results, however.

Introducing the (classical) field $\Omega^{(P)}(x) := \vec{d} \cdot \hat{\omega} \vec{A}_P^{(+)}(x)$ for the probe laser's Rabi frequency, Eqs. (7) and (9) can be reduced to the polariton equations of motions [15]

$$i\hbar \dot{\psi}_e = \left\{ \frac{\vec{p}^2}{2M} + \hbar \omega_{\rm res} + \frac{g_{eg}}{L_\perp^2} |\psi_g|^2 \right\} \psi_e - i\hbar \psi_g \Omega^{(P)}, \tag{20}$$

$$i\hbar \dot{\Omega}^{(P)} = \hbar \hat{\omega} \Omega^{(P)} + \frac{i|\vec{d}_\perp|^2}{2\varepsilon_0 L_\perp^2} \hat{\omega} (\psi_g^* \psi_e), \tag{21}$$

where ψ_g (divided by $L_\perp$) is given by Eq. (19). Since the density of excited atoms should be very small, we have neglected two-body collisions between excited atoms [$g_{ee} = 0$ in Eq. (7)]. Because ψ_g depends only on x, and since we consider the case that ψ_e and $\Omega^{(P)}$ also do not depend on y and z, the transverse δ function of Eq. (9) can be reduced to an ordinary δ function [to prove this, one can transform Eq. (9) to momentum space].

For later use it will be convenient to consider the solutions $\langle x|\phi\rangle := (\psi_e(x), \Omega^{(P)}(x))$ of Eqs. (20) and (21) as elements of a polariton Hilbert space with the conserved scalar product

$$\langle \phi' | \phi \rangle := \int dx \left\{ \psi_e'^* \psi_e + \frac{2\varepsilon_0 \hbar L_\perp^2}{|\vec{d}_\perp|^2} \Omega^{(P)\prime *} \hat{\omega}^{-1} \Omega^{(P)} \right\}. \tag{22}$$

Physically the quantity $\langle \phi | \phi \rangle$ is related to the number of excitations (number of excited atoms plus number of photons) in our system. It is a conserved quantity because of the

rotating-wave approximation made in Sec. II. Equations (20) and (21) can be rewritten in the form $i\hbar\partial_t|\phi\rangle = H_{\rm pol}|\phi\rangle$ with the polariton Hamiltonian

$$H_{\rm pol} := \frac{1}{2}(\mathbf{1}+\sigma_3)\left\{\frac{\vec{p}^2}{2M}+\hbar\omega_{\rm res}+\frac{g_{eg}}{L_\perp^2}|\psi_g|^2\right\}+\frac{1}{2}(\mathbf{1}-\sigma_3)\hbar\hat{\omega} - i\hbar\psi_g\sigma_+ + \frac{i|\vec{d}_\perp|^2}{2\varepsilon_0 L_\perp^2}\hat{\omega}\psi_g^*\sigma_-, \tag{23}$$

where σ_i are the Pauli matrices. We remark that $H_{\rm pol}$ is Hermitian with respect to the scalar product (22), i.e., $\langle\phi'|H_{\rm pol}\phi\rangle = \langle H_{\rm pol}\phi'|\phi\rangle$.

To derive the polariton band structure we have to find the eigenvalues of the operator $H_{\rm pol}$. Since ψ_g is periodic, $H_{\rm pol}$ commutes with the operator of discrete translations of amount π/k_L, and thus has a common set of eigenvectors with this operator. The eigenvectors $|\phi_{n,q}\rangle$ therefore can be characterized by two quantum numbers $n\in\{0,1,2,\cdots\}$ and $q\in[-k_L,k_L]$ which denote the band index and the quasimomentum, respectively. The eigenvalues of the discrete translation operator are given by $\exp[iq\pi/k_L]$, and belong to eigenvectors which are simply given by momentum eigenstates with momentum $\hbar k_m := \hbar(q+2mk_L)$ for integer m. The eigenvalues $\hbar\omega_{n,q}$ of the Hamiltonian can be found by expanding Eqs. (20) and (21) in this basis and searching for stationary solutions. The corresponding equations

$$\hbar\omega\psi_e(k_m) = \left\{\frac{\hbar^2k_m^2}{2M}+\hbar\omega_{\rm res}\right\}\psi_e(k_m)+\frac{g_{eg}}{L_\perp^2}\left\{\rho_0\psi_e(k_m)+\frac{\rho_1}{2}[\psi_e(k_{m+1})+\psi_e(k_{m-1})]\right\}-i\hbar L_\perp\sqrt{\rho_0}\Omega^{(P)}(k_m) - i\hbar L_\perp\frac{\rho_1}{4\sqrt{\rho_0}}[\Omega^{(P)}(k_{m+1})+\Omega^{(P)}(k_{m-1})], \tag{24}$$

$$\hbar\omega\Omega^{(P)}(k_m) = \hbar c|k_m|\Omega^{(P)}(k_m)+i\frac{|\vec{d}_\perp|^2c|k_m|}{2\varepsilon_0 L_\perp}\left\{\sqrt{\rho_0}\psi_e(k_m)+\frac{\rho_1}{4\sqrt{\rho_0}}[\psi_e(k_{m+1})+\psi_e(k_{m-1})]\right\} \tag{25}$$

can easily be solved numerically. Figure 1(c) shows the resulting band structure near the upper band edge of the lowest frequency band for a condensate of density $\rho_0 = 1.1\rho_1 = 10^{14}\ \mathrm{cm}^{-3}$. In order to describe the limit of a photonic instead of a polariton band structure, we have assumed a very large detuning of $\Delta_L = 100$ GHz of the lattice. However, the results given below do not change very much if a smaller detuning is assumed. We have furthermore set $|\vec{d}_\perp| \approx ea_0$, with e being the electron's charge and a_0 denoting Bohr's radius. The wave vector of the lattice was taken to be $k_L = 10^7\ \mathrm{m}^{-1}$.

An excellent analytical approximation for the band structure can be made by assuming that for $q\in(0,k_L)$ only the modes $\Omega^{(P)}(q)$, $\Omega^{(P)}(q-2k_L)$, $\psi_e(q)$, and $\psi_e(q-2k_L)$ are important. The problem is then reduced to finding the eigenvalues of a 4×4 matrix. For $q=k_L$ the eigenvalues have a simple form, and allow one to derive the following expression for the band gap $\Delta\omega$, separating the two lowest energy bands:

$$\Delta\omega = s_+ - s_-, \tag{26}$$

where we have defined the frequencies $\nu_i := |\vec{d}_\perp|^2\rho_i/(2\hbar\varepsilon_0)$ and furthermore have introduced the abbreviations $s_\pm := \sqrt{(\Delta_L/2)^2+\omega_{\rm res}(\sqrt{\nu_0}\pm\sqrt{\nu_1}/4)^2}$. For a large detuning $|\Delta_L|$, i.e., in the limit of a photonic band gap, this expression simplifies to $\Delta\omega = \omega_0\nu_1/|\Delta_L|$. For the numerical values given above, the band gap takes the value $\Delta\omega\approx 40$ GHz.

For $q\neq k_L$ the band structure is given by a rather complicated expression. Therefore, we have further simplified the analytical result by fitting it to a square root [16]. The lowest polariton band then takes the form

$$\omega_{0,q} \approx \omega_{0,\max} + \overline{\nu} - \sqrt{c^2(|q|-k_L)^2+\overline{\nu}^2}, \tag{27}$$

where

$$\omega_{0,\max} = \omega_{\rm res} - \frac{|\Delta_L|}{2} - s_+ \tag{28}$$

denotes the upper edge of the lowest frequency band, and

$$\overline{\nu} := \frac{\Delta\omega}{(\omega_{0,\max}-\omega_{\rm res})^2}s_+(s_++s_-) \tag{29}$$

determines the curvature of the band. In the limit of a large detuning this simplifies to $\overline{\nu}\approx\Delta\omega/2$.

V. THEORY OF LOCALIZED DEFECTS

In Sec. IV we have studied polariton band gaps of light generated by the lattice condensate in its ground state. However, in general the BEC might be in a state corresponding to a (coherent) elementary excitation which usually are not periodic. Thus we expect defects in the lattice condensate. As is well known from solid-state theory, a defect or an impurity in an otherwise periodic potential can lead to defect states, i.e., states whose energy eigenvalue lies inside the gap between two energy bands (see, e.g., Ref. [17]). In the system under consideration this phenomenon could be exploited to acquire knowledge about nonperiodic elementary excitations of the Bose condensate by observing light propagation

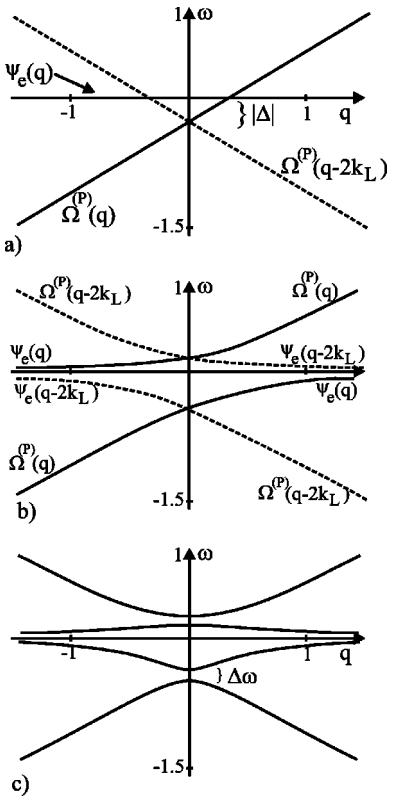

FIG. 1. Band structure of polaritons near the band edge k_L. Displayed is $10^4(\omega-\omega_{\rm res})/\omega_{\rm res}$ vs $10^4(q-k_L)/k_L$. (a) shows the free dispersion relation for the relevant field components in the absence of any interaction. For a homogeneous BEC, $\psi_g=\sqrt{\rho_0}$, a mixing of excited atoms and photons leads to the formation of two separate avoided crossings [solid and dashed lines in (b)]. The labels indicate the asymptotic form of the polariton modes, where they correspond to either excited atoms (ψ_e) or photons ($\Omega^{(P)}$). For a periodic ground-state BEC, the two avoided crossings are combined to form band gaps (c).

through the BEC. In addition, defect theory can also be applied to study the back-reaction of an excited BEC on the optical potential.

The existence of defect states for photonic band gaps has been examined in the microwave regime for ordinary dielectric materials [13,18]. The method of calculation that we adopt is closely related to the Green's-function approach of Ref. [17].

Specifically we consider the situation that the condensate's wave function is given by $\psi_G(x)=\psi_g(x)+\delta\psi_g(x)$, where ψ_g (divided by $L_\perp$) is given by Eq. (19), and $\delta\psi_g$ describes a coherent elementary excitation of the condensate which we assume to be localized in the x direction. This allows us to estimate the resulting energy eigenstates by adapting the Koster-Slater model [19] to the case of polariton band gaps.

Our aim is to find solutions of the equation

$$\hbar\omega_{\rm defect}|\phi\rangle=(H_{\rm pol}+H_{\rm defect})|\phi\rangle, \tag{30}$$

where

$$H_{\rm defect}:=-i\hbar\,\delta\psi_g\sigma_+ +\frac{i|\vec{d}_\perp|^2}{2\varepsilon_0 L_\perp^2}\hat{\omega}\,\delta\psi_g^*\sigma_- \tag{31}$$

describes the influence of the elementary excitation $\delta\psi_g$, and $\omega_{\rm defect}$ is the defect eigenfrequency.

To find the solutions of Eq. (30) we expand $|\phi\rangle$ in terms of Wannier functions,

$$|W_{n,\nu}\rangle:=\frac{1}{\sqrt{2k_L}}\int_{-k_L}^{k_L}dq\,e^{-\pi i\nu q/k_L}|\phi_{n,q}\rangle, \tag{32}$$

where ν is an integer number. The functions $W_{n,\nu}(x)$ are localized around the lattice point $\pi\nu/k_L$ which makes them a convenient tool to study localized defects. Inserting $|\phi\rangle=\Sigma_{n,\nu}\phi_{n,\nu}|W_{n,\nu}\rangle$ into Eq. (30), one easily deduces the equation

$$\omega_{\rm defect}\phi_{n,\nu}=\sum_\mu\omega_{n,\nu-\mu}\phi_{n,\mu} +\sum_{m,\mu}\langle W_{n,\nu}|H_{\rm defect}/\hbar|W_{m,\mu}\rangle\phi_{m,\mu}, \tag{33}$$

with

$$\omega_{n,\nu-\mu}:=\frac{1}{2k_L}\int_{-k_L}^{k_L}dq\,e^{\pi i(\nu-\mu)/k_L}\omega_{n,q}. \tag{34}$$

Since the Wannier basis is countable, Eq. (33) can be interpreted as a matrix equation. In particular, one now can exploit the fact that both the Wannier functions and $H_{\rm defect}$ are localized. This implies that, at least approximately, only a finite number, say an $N\times N$ submatrix, of the matrix elements $\langle W_{n,\nu}|H_{\rm defect}|W_{m,\mu}\rangle$ is nonvanishing.

Introducing the Green's function $G:=(\omega_{\rm defect}\mathbf{1}-H_{\rm pol}/\hbar)^{-1}$, whose matrix elements are given by

$$\langle W_{n,\nu}|G|W_{m,\mu}\rangle=\delta_{n,m}\frac{1}{2k_L}\int_{-k_L}^{k_L}dq\,\frac{e^{\pi i(\nu-\mu)/k_L}}{\omega_{\rm defect}-\omega_{n,q}} =:\delta_{n,m}G_{n,\nu-\mu} \tag{35}$$

the eigenvalue problem can be reduced to

$$\phi_{n,\nu}=\sum_{m,\mu,\lambda}G_{n,\nu-\mu}\langle W_{n,\mu}|H_{\rm defect}/\hbar|W_{m,\lambda}\rangle\phi_{m,\lambda}. \tag{36}$$

As is well known in solid-state theory [17], it is sufficient to consider only the eigenvalue problem of the $N\times N$ subspace, where the matrix elements of $H_{\rm defect}$ are nonzero, to derive the frequencies of the defect states.

VI. KOSTER-SLATER MODEL FOR PHOTONIC BAND GAPS

Having derived the matrix eigenvalue equation (36) for a determination of the defect frequency, it is straightforward to apply the Koster-Slater model [19] to the problem at hand. In this model the assumption is made that both the Wannier functions and the perturbation $U_{\rm np}$ are localized in such a way that only one matrix element of the perturbation is nonzero,

$$\langle W_{n,\nu}|H_{\rm defect}|W_{m,\mu}\rangle=U_0\delta_{n,0}\delta_{m,0}\delta_{\nu,0}\delta_{\mu,0}. \tag{37}$$

This model is not valid if $\delta\psi_g$ is too strongly localized (i.e., on a scale much smaller than the lattice spacing π/k_L) [20], but should produce qualitative estimates of defect frequencies for moderately localized perturbations.

Inserting Eq. (37) into the eigenvalue equation (36) and using Eq. (35) to evaluate the only relevant matrix element of G, $\langle W_{0,0}|G|W_{0,0}\rangle$, we find that the defect frequency ω_{defect} has to fulfill the condition

$$1=\frac{U_0}{\hbar}\frac{1}{2k_L}\int_{-k_L}^{k_L}\frac{dq}{\omega_{\text{defect}}-\omega_{0,q}}. \tag{38}$$

The integral can be calculated exactly for the photonic band of Eq. (27), but, since the resulting expression is somewhat complicated, it is more instructive to use the following approximation which is valid if the defect frequency ω_{defect} is close to the upper edge $\omega_{0,\max}$ of the lowest frequency band:

$$\frac{1}{2k_L}\int_{-k_L}^{k_L}\frac{dq}{\omega_{\text{defect}}-\omega_{0,q}}\approx\frac{\pi}{\omega_L}\sqrt{\frac{\overline{\nu}}{2(\omega_{\text{defect}}-\omega_{0,\max})}}. \tag{39}$$

Inserting this into Eq. (38), for the frequency of the defect state we find the expression

$$\omega_{\text{defect}}-\omega_{0,\max}\approx\frac{\pi^2}{2}\frac{\overline{\nu}}{\omega_L^2}\frac{U_0^2}{\hbar^2}. \tag{40}$$

It is of interest to know how large this frequency difference is for realistic systems. To achieve this we first have to estimate the value of $U_0=\langle W_{0,0}|H_{\text{defect}}|W_{0,0}\rangle = i\hbar\int dx\{W_\Omega^* W_e\delta\psi_g^* - W_e^* W_\Omega\delta\psi_g\}$ with $\langle x|W_{0,0}\rangle = (W_e(x), W_\Omega(x))$. A rough estimate of this integral can be made by setting both $\delta\psi_g$ and the Wannier function to be constant over one wavelength λ_L, and to be zero outside this range. The normalization condition $\langle W_{0,0}|W_{0,0}\rangle=1$ then leads approximately to $1=\lambda_L\{|W_e|^2+|W_\Omega|^2/(\omega_L|d_\perp|^2/2\hbar\varepsilon_0 L_\perp^2)\}$. Using this condition U_0 takes its maximal value for $W_e=1/\sqrt{2\lambda_L}$:

$$U_0\approx 2\hbar\,\delta\psi_g\sqrt{\omega_L\frac{|d_\perp|^2}{2\hbar\varepsilon_0 L_\perp^2}}. \tag{41}$$

Assuming a defect amplitude of $\delta\psi_g=\epsilon\sqrt{\rho_0}L_\perp$ over the extent of $W_{0,0}(x)$, where ϵ is small compared to one, we can derive an estimate of the defect frequency (40) of

$$\omega_{\text{defect}}-\omega_{0,\max}\approx 2\pi^2\epsilon^2\frac{\overline{\nu}}{\omega_L}\nu_0. \tag{42}$$

Using the same numbers as in Sec. IV (that is, $\rho_i=10^{14}$ cm^{-3} and $\Delta_L=10^{11}$ s^{-1}) as well as $\epsilon=0.3$, this frequency difference can be shown to be of the order of 100 Hz. Though this number is too small to be measurable, it should be pointed out that it applies only to a defect corresponding to an elementary excitation over one wavelength. A different type of defect can produce a much different result. For example, if we do not consider a weak elementary excitation but rather a strong localized excitation, we can estimate its effect, by assuming a larger value for ϵ. A threefold increase of the local density ($\epsilon=3$) would lead to a defect frequency $\omega_{\text{defect}}-\omega_{0,\max}$ of about 10 KHz, for instance.

VII. CONCLUSIONS

In this paper we have analyzed the interaction of a lattice (or ''crystallized'') Bose-Einstein condensate with largely detuned laser beams. We have derived a periodic solution of the coupled equations of motion, corresponding to a free BEC and a standing lattice laser beam. We found that, if the condensate is in its ground state, these equations decouple and the effect of the lattice laser beam on the condensate is not affected by the condensate itself (no back-reaction). In this situation it is thus equivalent to consider a condensate in some external periodic potential with the same periodicity.

Building on this result, we then assumed that the condensate moves in an external periodic potential. Since the condensate's ground state is then periodic, too, it forms a kind of periodic dielectric. A probe laser beam propagating through this dielectric will then experience the formation of photonic band gaps. We have analyzed this situation using the concept of polaritons, i.e., entangled superpositions of excited atoms and photons.

If the condensate is not in its ground state but in a state corresponding to a localized elementary excitation the periodicity of the system is perturbed. This leads to the formation of defect states inside a polariton band gap.

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