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► **To cite this version:**

Mauro Antezza, Yvan Castin. Atom-Light Elementary Excitations in a Periodic Ensemble of Ultracold Atoms. 2009. hal-00365761v1

**HAL Id: hal-00365761**

**<https://hal.science/hal-00365761v1>**

Preprint submitted on 4 Mar 2009 (v1), last revised 16 Sep 2009 (v2)

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# Atom-Light Elementary Excitations in a Periodic Ensemble of Ultracold Atoms

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(Dated: March 4, 2009)

We derive the excitation spectrum for light coupled to atoms in an optical lattice, close to a  $0 \rightarrow 1$  atomic transition, for the branches that are mainly of atomic nature. We explicitly include the quantum atomic motion, which leads to remarkable features such as a finite lifetime of the elementary excitations and their energy dependence with the lattice depth, that will show up in a real experiment as we discuss. It also makes the theory naturally divergence-free and resolves a controversy for the occurrence of a spectral gap.

PACS numbers: 42.50.Ct, 67.85.-d, 71.36.+c

Light propagation in 3D periodic structures is currently the subject of intense studies in various domains of physics, e.g. in photonic crystals where possible opening of a spectral gap is crucial for applications [1]. Since the observation of a Mott phase with atoms in an optical lattice [2], this problem can now be addressed experimentally also with atomic gases [3, 4]. Light propagation in such systems however widely differs from the one in photonic crystals, since atoms act as resonant point-like scatterers with a very high quality factor, rather than as a macroscopically modulated refractive index.

If one includes the vectorial nature of light, this raises non-trivial questions such as the existence of a spectral gap, first investigated in [5, 6]. These works consider point-like atomic dipoles rigidly fixed at periodic positions and reach opposite conclusions for the presence of a gap. In particular, [6] points out the necessity of correctly handling the high frequency divergences appearing for an infinite size system, but still relies on a heuristic regularizing procedure, subtracting an atomic self-energy term which surprisingly depends on the presence of the lattice. None of the works includes the quantum motion of the atoms around their periodic equilibrium positions, which is unavoidable in experiments. Here we provide a well defined answer to all these issues by including this quantum motion, as already done for  $\gamma$  ray nuclear scattering in a crystal [7]. First, we show that this eliminates all needs for regularizing recipes and directly provides a divergence-free theory allowing to decide between [5] and [6]. Second, we predict remarkable features, such as the existence of an imaginary part in the atom-light excitation spectrum, and the dependence of the spectrum on the confinement strength of the atoms in the lattice. Finally, we suggest how to prepare and probe the system in a real experiment.

*Model:* We consider  $N$  atoms with a dipolar coupling to the electromagnetic field, on an electronic transition between the ground state  $g$  of spin  $J_g = 0$  and an excited state  $e$  of spin  $J_e = 1$ . The atoms are trapped at the nodes of an optical lattice with nowhere more than one atom per site [2]. In the deep-lattice limit, tunneling of atoms among sites is negligible, and the  $i^{\text{th}}$  atom is as-

sumed to be harmonically trapped around lattice site  $\mathbf{R}_i$ , with the potential  $U_i(\hat{\mathbf{r}}_i) = m\omega_{\text{ho}}^2(\hat{\mathbf{r}}_i - \mathbf{R}_i)^2/2$ . Here  $m$  is the atomic mass,  $\hat{\mathbf{r}}_i$  is the position operator of atom  $i$ , and  $\omega_{\text{ho}}$  is the atomic oscillation frequency. The Hamiltonian [8] may be split in the non-interacting term  $H_0$  and the atom-field coupling  $V$ ,  $H = H_0 + V$ , with

$$H_0 = \sum_{i=1}^N \left[ \frac{\hat{\mathbf{p}}_i^2}{2m} + U_i(\hat{\mathbf{r}}_i) + \sum_{\alpha} \hbar\omega_0 |i : e_{\alpha}\rangle \langle i : e_{\alpha}| \right] + \int_{\mathcal{D}} d^3k \sum_{\epsilon \perp \mathbf{k}} \hbar ck \hat{a}_{\mathbf{k}\epsilon}^{\dagger} \hat{a}_{\mathbf{k}\epsilon}. \quad (1)$$

Here  $\omega_0$  is the bare atomic resonance frequency, the sum  $\sum_{\alpha}$  over the three directions of space  $x, y, z$  accounts for the three-fold degeneracy of  $e$ ,  $\mathcal{D}$  is the three-dimensional Fourier space truncated by a cut-off  $k < k_M$ , and the annihilation and creation operators obey usual bosonic commutation relations such as  $[\hat{a}_{\mathbf{k}\epsilon}, \hat{a}_{\mathbf{k}'\epsilon'}^{\dagger}] = \delta_{\epsilon,\epsilon'} \delta(\mathbf{k}-\mathbf{k}')$ , where  $\epsilon$  and  $\mathbf{k}$  are the photon polarization and wavevector. The dipolar coupling operator is [9]

$$V = - \sum_{i=1}^N \hat{\mathbf{D}}_i \cdot \hat{\mathbf{E}}_{\perp}(\hat{\mathbf{r}}_i) \quad (2)$$

where  $\hat{D}_{i,\alpha} = d|i : e_{\alpha}\rangle \langle i : g| + \text{h.c.}$  is the component along direction  $\alpha$  of the dipole operator  $\hat{\mathbf{D}}_i$  of the  $i^{\text{th}}$  atom, proportional to the atomic dipole moment  $d$ ,  $\hat{\mathbf{E}}_{\perp}(\mathbf{r}) = \int_{\mathcal{D}} d^3k \sum_{\epsilon \perp \mathbf{k}} [\mathcal{E}_k \epsilon \hat{a}_{\mathbf{k}\epsilon} e^{i\mathbf{k}\cdot\mathbf{r}} + \text{h.c.}]$  is the transverse electric field operator, and  $\mathcal{E}_k = i(2\pi)^{-3/2} [\hbar kc / (2\epsilon_0)]^{1/2}$ .

*Method:* We treat the coupling  $V$  to second order of perturbation theory, to calculate atom-field elementary excitations mainly of atomic nature. In practice for a lattice spacing  $\sim 1/k_0$ , where  $k_0 = \omega_0/c$  is the resonant wavevector, this requires  $\Gamma \ll \omega_{\text{ho}}$ , where  $\Gamma = d^2 k_0^3 / (3\pi\epsilon_0 \hbar)$  is the free space atomic spontaneous emission rate. The energies of the system up to second order in  $V$  are eigenvalues of the effective Hamiltonian

$$H_{\text{eff}} = PHP + PVQ \frac{Q}{E^{(0)}Q - QH_0Q} QVP, \quad (3)$$

where  $E^{(0)}$  is an eigenenergy of  $H_0$ ,  $P$  projects orthogonally onto the corresponding eigenspace of  $H_0$ , and

$Q = I - P$ . We now obtain the excitation energies of the system as the difference between excited states energies and the ground state energy.

For the perturbative calculation of the ground state energy  $E_g$ , we take for  $P$  the projector over the state with all the atoms in the electronic and motional ground states, and the field in vacuum, so that  $E_g^{(0)} = N\frac{3}{2}\hbar\omega_{\text{ho}}$ . We obtain  $E_g = N\epsilon_g$ , with [10]

$$\epsilon_g = \frac{3}{2}\hbar\omega_{\text{ho}} - \frac{d^2}{\epsilon_0} \int_{\mathcal{D}} \frac{d^3k}{(2\pi)^3} \frac{\hbar ck}{\hbar\omega_0 + \hbar ck}. \quad (4)$$

For the excited state energies, we take for  $P$  the projector  $P_e$  over all the states  $||i : e_\alpha\rangle$ , where  $||i : e_\alpha\rangle$  represents the atom  $i$  in the electronic state  $e_\alpha$ , the  $N - 1$  other atoms in the ground electronic state, all the atoms in the motional ground state, and the field in vacuum. Then  $P$  projects over a subspace of dimension  $3N$ . Since this excited subspace is coupled by  $V$  to the continuous part of the spectrum of  $H_0$ , one has to replace  $E^{(0)}$  by  $E_e^{(0)} + i0^+$  in (3), with  $E_e^{(0)} = E_g^{(0)} + \hbar\omega_0$ , which gives rise to a complex excited state energy  $E_e$ , eigenvalue of

$$H_{\text{eff}}^e = [(N - 1)\epsilon_g + \epsilon_e]P_e + \sum_{i \neq j} \sum_{\alpha, \beta} \bar{g}_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j) ||i : e_\alpha\rangle \langle j : e_\beta|. \quad (5)$$

Here  $\epsilon_e$  is the complex energy of a single atom [10]

$$\epsilon_e = \hbar\omega_0 + \frac{3}{2}\hbar\omega_{\text{ho}} + \frac{d^2}{3\epsilon_0} \int_{\mathcal{D}} \frac{d^3k}{(2\pi)^3} \frac{\hbar ck}{\hbar\omega_0 + i0^+ - \hbar ck}. \quad (6)$$

To obtain the excitation energies of the system we subtract the ground state energy  $E_g$  from (5). In this subtraction, the dangerous terms proportional to the number of atoms  $N$  disappear and the interatomic distance independent term gives the excitation energy for a single atom, that we split in a real part and an imaginary part:

$$\epsilon_e - \epsilon_g \equiv \hbar\omega_A - i\frac{\hbar\Gamma}{2}. \quad (7)$$

As expected,  $\Gamma$  is the free space spontaneous emission rate, and the effective atomic resonance frequency  $\omega_A$  deviates from  $\omega_0$  by Lamb shift type terms.

Most interesting are the position dependent terms in (5), which contain the effective coupling amplitude  $\bar{g}_{\alpha\beta}(\mathbf{r})$  for the transfer of the atomic excitation in between two different sites separated by  $\mathbf{r}$ . This coupling amplitude appears as the inverse Fourier transform  $\bar{g}_{\alpha\beta}(\mathbf{r}) = \int_{\mathcal{D}} [d^3k/(2\pi)^3] e^{i\mathbf{k}\cdot\mathbf{r}} \check{g}_{\alpha\beta}(\mathbf{k})$  of the function

$$\check{g}_{\alpha\beta}(\mathbf{k}) = \frac{3\pi\hbar\Gamma}{k_0^3} \frac{k^2\delta_{\alpha\beta} - k_\alpha k_\beta}{k_0^2 - k^2 + i0^+} e^{-k^2 a_{\text{ho}}^2}. \quad (8)$$

The effect of the quantum motion on the intersite coupling here enters through the size of the harmonic oscillator ground state  $a_{\text{ho}} = [\hbar/(2m\omega_{\text{ho}})]^{1/2}$ .

The integral defining  $\bar{g}_{\alpha\beta}(\mathbf{r})$  is cut at large  $k$  by the Gaussian factor of momentum width  $1/a_{\text{ho}} \ll k_M$ . Hence we can evaluate the coupling amplitude  $\bar{g}_{\alpha\beta}(\mathbf{R}_i - \mathbf{R}_j)$  by extending the integral over  $\mathbf{k}$  to the whole space. In this limit, the coupling amplitude is the average over the harmonic oscillator ground state probability distributions of  $\mathbf{r}_i$  and  $\mathbf{r}_j$  of the function  $g_{\alpha\beta}(\mathbf{r}_i - \mathbf{r}_j)$ , where [9]

$$g_{\alpha\beta}(\mathbf{r}) = -\frac{3\hbar\Gamma}{4k_0^3} [k_0^2\delta_{\alpha\beta} + \partial_{r_\alpha}\partial_{r_\beta}] \frac{e^{ik_0 r}}{r} \quad (9)$$

is proportional to the component along  $\alpha$  of the classical electric field radiated by a point-like dipole of frequency  $\omega_0$  oriented along direction  $\beta$  [8]. A crucial consequence of the average is that, whereas  $g_{\alpha\beta}(\mathbf{r})$  has the electrostatic  $1/r^3$  divergence at the origin, the function  $\bar{g}_{\alpha\beta}(\mathbf{r})$  is regular even in  $\mathbf{r} = \mathbf{0}$ , with a value

$$\bar{g}_{\alpha\beta}(\mathbf{0}) = \frac{\hbar\Gamma}{2}\delta_{\alpha\beta} \left[ \frac{\text{Erfi}(k_0 a_{\text{ho}}) - i}{e^{(k_0 a_{\text{ho}})^2}} - \frac{1 + 2(k_0 a_{\text{ho}})^2}{2\pi^{1/2}(k_0 a_{\text{ho}})^3} \right] \quad (10)$$

where  $\text{Erfi}(x) = 2\pi^{-1/2} \int_0^x dy \exp(y^2)$  is the imaginary error function. For large  $r$ , the average over the atomic motion does not suppress the long range nature of the radiated dipolar field  $\propto \exp(ik_0 r)/r$ . From (17) one has indeed  $\bar{g}_{\alpha\beta}(\mathbf{r}) \simeq g_{\alpha\beta}(\mathbf{r}) \exp(-k_0^2 a_{\text{ho}}^2)$  as soon as  $r \gg a_{\text{ho}}$ . *Periodic case:* We now take the limit  $N \rightarrow +\infty$  with one atom per lattice site, realizing for the light field a periodic potential, here an arbitrary Bravais lattice. To diagonalize  $H_{\text{eff}}^e$  we rely on Bloch theorem: The eigenvectors  $|\psi_{\mathbf{q}}\rangle$  depend on the lattice site position  $\mathbf{R}_i$  as

$$\langle i : e_\alpha | |\psi_{\mathbf{q}}\rangle = d_\alpha e^{i\mathbf{q}\cdot\mathbf{R}_i}, \quad (11)$$

where the Bloch vector  $\mathbf{q}$  is chosen in the first Brillouin zone of the lattice. I.e. the ‘‘dipole’’ carried by atom  $i$  differs from the one  $\mathbf{d}$  carried by the atom in  $\mathbf{R} = \mathbf{0}$  by a global phase factor. Thus the infinite dimension eigenvalue problem on the excitation spectrum  $\varepsilon_{\mathbf{q}}$ ,

$$[H_{\text{eff}}^e - E_g P_e] |\psi_{\mathbf{q}}\rangle = \varepsilon_{\mathbf{q}} |\psi_{\mathbf{q}}\rangle, \quad (12)$$

reduces to the diagonalization of the  $3 \times 3$  matrix  $M$ ,  $M\mathbf{d} = \varepsilon_{\mathbf{q}}\mathbf{d}$ , with matrix elements

$$M_{\alpha\beta} = \left( \hbar\omega_A - i\frac{\hbar\Gamma}{2} \right) \delta_{\alpha\beta} + \sum_{\mathbf{R} \in L^*} \bar{g}_{\alpha\beta}(\mathbf{R}) e^{i\mathbf{q}\cdot\mathbf{R}}, \quad (13)$$

where the sum runs over the lattice  $L$  excluding the origin. By adding and subtracting  $\bar{g}_{\alpha\beta}(\mathbf{0})$  and using Poisson’s summation formula we convert this sum into a sum over the reciprocal lattice  $RL$ :

$$M_{\alpha\beta} = \left( \hbar\omega_A - i\frac{\hbar\Gamma}{2} \right) \delta_{\alpha\beta} - \bar{g}_{\alpha\beta}(\mathbf{0}) + \frac{1}{\mathcal{V}_L} \sum_{\mathbf{K} \in RL} \check{g}_{\alpha\beta}(\mathbf{K} - \mathbf{q}) \quad (14)$$

where  $\mathcal{V}_L$  is the primitive unit cell volume of the lattice.

Since the imaginary part of the symmetric matrix  $M$  is scalar, see (14), the imaginary part of the excitation spectrum can be calculated explicitly:

$$\text{Im} \varepsilon_{\mathbf{q}} = -\frac{\hbar\Gamma}{2} \left(1 - e^{-k_0^2 a_{\text{ho}}^2}\right). \quad (15)$$

Such a non-zero value seems to contradict the classical result of [11], also obtained in [5, 6], that light has a real spectrum in a periodic atomic structure. This is due to the lack of the atomic motion in [5, 6], that, if included, adds new degrees of freedom similar to the phonons in a crystal. These phonons, invoked as a possible source of dissipation in [11], lead to a residual linewidth in the  $\gamma$  ray nuclear scattering in a crystal where an expression analogous to Eq.(15) was derived [7].

The non-zero imaginary part of  $\varepsilon_{\mathbf{q}}$  is indeed due to the decay of the system out of the subspace where all the atoms are in their motional ground state. When an excited atom  $e_{\alpha}$  in its motional ground state  $|\mathbf{0}\rangle_{\text{ho}}$  spontaneously emits a photon of polarization  $\epsilon$  and momentum  $k_0\mathbf{n}$ ,  $|\mathbf{n}| = 1$ , its probability density to fall in  $g$  with an excited motional state is [12]  $(3\Gamma/2)|\epsilon_{\alpha}|^2[1 - |_{\text{ho}}\langle\mathbf{0}|\exp(-ik_0\mathbf{n}\cdot\hat{\mathbf{r}})|\mathbf{0}\rangle_{\text{ho}}|^2]$ , which after sum over  $\epsilon \perp \mathbf{n}$  and average over the direction  $\mathbf{n}$ , exactly gives the decay rate  $-2\text{Im} \varepsilon_{\mathbf{q}}/\hbar$ . This process conserves the quasi-momentum  $\mathbf{q}$ . If the emitted photon carries away the quasi-momentum  $\mathbf{q}_{\text{ph}}$ , the resulting  $g$  atom in the motional excited state is coherently delocalized over the whole lattice, with a probability amplitude  $\propto e^{i\mathbf{q}_{\text{at}}\cdot\mathbf{R}}$  of being in site  $\mathbf{R}$ , and a quasi-momentum  $\mathbf{q}_{\text{at}} = \mathbf{q} - \mathbf{q}_{\text{ph}}$ . Since  $\mathbf{q}_{\text{ph}}$  belongs to a continuum, this spontaneous emission process opens up a continuum of final states, hence the possibility to have for a fixed  $\mathbf{q}$  a continuous spectrum for  $H$  and a complex  $\varepsilon_{\mathbf{q}}$ . Experimentally, to obtain long lived elementary excitations, one may operate in the so-called Lamb-Dicke regime,  $k_0 a_{\text{ho}} \ll 1$ , where the loss rate  $-2\text{Im} \varepsilon_{\mathbf{q}}/\hbar \simeq \Gamma(k_0 a_{\text{ho}})^2$  is much smaller than  $\Gamma$ .

We now turn to the real part of the excitation spectrum. In (14) we replace  $\check{g}_{\alpha\beta}(\mathbf{0})$  and  $\check{g}_{\alpha\beta}$  by their explicit expressions (10) and (8). Then  $\text{Re} \varepsilon_{\mathbf{q}} - \hbar\omega_A$  is an eigenvalue of the  $3 \times 3$  real symmetric matrix

$$\begin{aligned} \delta M_{\alpha\beta} = & \frac{\hbar\Gamma}{2} \delta_{\alpha\beta} \left[ \frac{1 + 2(k_0 a_{\text{ho}})^2}{2\pi^{1/2}(k_0 a_{\text{ho}})^3} - \text{Erfi}(k_0 a_{\text{ho}}) e^{-k_0^2 a_{\text{ho}}^2} \right] \\ & + \frac{3\pi\hbar\Gamma}{k_0^3 \mathcal{V}_L} \sum_{\mathbf{K} \in RL} \frac{\delta_{\alpha\beta} K'^2 - K'_{\alpha} K'_{\beta}}{k_0^2 - K'^2} e^{-K'^2 a_{\text{ho}}^2} \quad (16) \end{aligned}$$

where  $\mathbf{K}' \equiv \mathbf{K} - \mathbf{q}$ . Clearly, divergences appear in the spectrum when  $\mathbf{q}$  is at a distance  $k_0$  from a vector  $\mathbf{K}$  of the reciprocal lattice. E.g. if  $\mathbf{q}$  approaches  $k_0\mathbf{n}$  where  $|\mathbf{n}| = 1$ , a divergent contribution appears in  $\delta M_{\alpha\beta}$ , proportional to the projector  $\delta_{\alpha\beta} - n_{\alpha} n_{\beta}$  on the plane orthogonal to  $\mathbf{n}$ . Since this projector is of rank two, generically two eigenvalues of  $\delta M$  diverge, to  $+\infty$  for  $q < k_0$  and to  $-\infty$  for  $q > k_0$ , the third eigenvalue remaining finite.

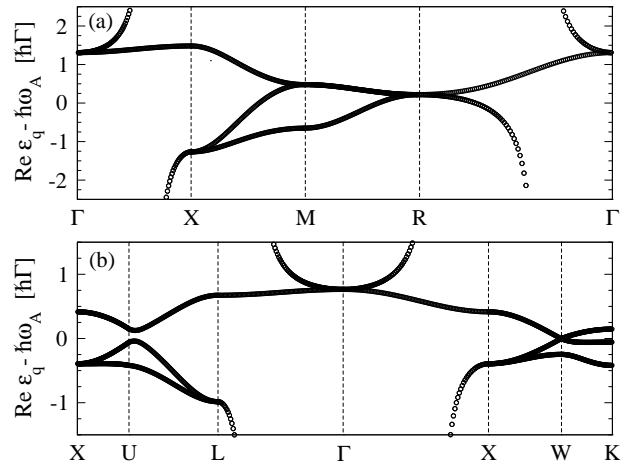


FIG. 1: Atom-light elementary excitation spectrum in a periodic atomic structure, as a function of the Bloch vector along the standard irreducible path in the first Brillouin zone. (a) Simple cubic lattice, with a lattice constant  $a$  ( $\mathcal{V}_L = a^3$ ). (b) Face-centered cubic lattice, with a lattice constant  $2a$  ( $\mathcal{V}_L = 2a^3$ ). Here  $k_0 a = 2$  and  $k_0 a_{\text{ho}} = 1/\sqrt{30}$ , which leads to  $a_{\text{ho}}/a \simeq 0.09$ . In both cases the band structure is gapless.

This gives rise to five continuous energy bands, as expected from the coupling of the three atomic states  $|e_{\alpha}\rangle$  to the two polarizations of light. The present order of perturbation theory is actually meaningful in the interval  $|\text{Re} \varepsilon_{\mathbf{q}} - \hbar\omega_A| \ll \hbar\omega_{\text{ho}}$ . In non-perturbative theories (for fixed atomic positions) [5, 6], the vertical asymptotes are replaced by the oblique ones of the free light dispersion relation  $\varepsilon_{\mathbf{q}} = \hbar c q$ . The slope  $\hbar c$  is in practice infinite as compared to the typical slope  $\hbar\Gamma a$  that one obtains for  $|\varepsilon_{\mathbf{q}} - \hbar\omega_A| \sim \hbar\Gamma$  and for  $1/k_0 \sim$  the lattice period  $a$ .

**Band structures:** We illustrate (16) by calculating the band structure in the two lattice geometries of [5, 6]: In Fig.1 we show  $\text{Re} \varepsilon_{\mathbf{q}} - \hbar\omega_A$  as a function of the Bloch vector along the standard irreducible path in the first Brillouin zone, for the simple cubic (Fig.1a) and for the face-centered cubic (fcc) (Fig.1b) lattices [13]. The figure reveals the lack of an omnidirectional gap. In the simple cubic case, for  $k_0 a < \pi\sqrt{3}$ , this may be understood by considering the segment between the center  $\Gamma$  and the corner  $R$  of the first Brillouin zone: The cubic symmetry leads to a three-fold degeneracy of  $\varepsilon_{\mathbf{q}}$  in  $R$  and in  $\Gamma$ ; the band which continuously crosses the sphere of radius  $k_0$  thus closes the energy gap between the (here twofold degenerate) diverging bands. In the fcc case, an important element for the absence of a gap is the crossing of two energy bands at the  $W$  point. This crossing is related to the existence of a dimension two irreducible representation of the  $W$  point symmetry group [14]. This essential degeneracy is also present in Fig.2 of [6]. We also explored the bcc and several generic less symmetric Bravais lattices without finding an omnidirectional gap.

**Dependence with  $a_{\text{ho}}$ :** We now determine the dependence

of the real part of the spectrum with the size of the harmonic oscillator ground state, starting from (13). The idea is to multiply  $\bar{g}_{\alpha\beta}(\mathbf{R})$  by  $e^{k_0^2 a_{\text{ho}}^2}$  and then to take the derivative with respect to  $a_{\text{ho}}^2$ . In the Fourier representation (8), this pulls out a factor  $k_0^2 - k^2$  which exactly cancels the denominator. The resulting Fourier integral is now essentially Gaussian and can be directly calculated:

$$u_{\alpha\beta}(\mathbf{r}) \equiv \partial_{a_{\text{ho}}^2} \left[ e^{k_0^2 a_{\text{ho}}^2} \bar{g}_{\alpha\beta}(\mathbf{r}) \right] = \frac{3\hbar\Gamma e^{k_0^2 a_{\text{ho}}^2}}{8\pi^{1/2} (k_0 a_{\text{ho}})^3} \times (-\delta_{\alpha\beta} \Delta_{\mathbf{r}} + \partial_{r_\alpha} \partial_{r_\beta}) e^{-r^2/(4a_{\text{ho}}^2)}. \quad (17)$$

From (13) one then obtains a sum excluding the origin:

$$\partial_{a_{\text{ho}}^2} \left[ e^{k_0^2 a_{\text{ho}}^2} \delta M_{\alpha\beta} \right] = \sum_{\mathbf{R} \in L^*} u_{\alpha\beta}(\mathbf{R}) e^{i\mathbf{q} \cdot \mathbf{R}}. \quad (18)$$

It is apparent that each term of the sum is exponentially small since, in the deep lattice limit, the harmonic length  $a_{\text{ho}}$  is much smaller than the lattice spacing. Keeping these terms is actually beyond accuracy of our Hamiltonian (see [9]). We can thus set the right-hand side of (18) to zero, which leads to  $\delta M_{\alpha\beta} = e^{-k_0^2 a_{\text{ho}}^2} \delta M_{\alpha\beta}^0$ , where  $\delta M_{\alpha\beta}^0$  is independent of  $a_{\text{ho}}$  and is simply the limit of  $\delta M_{\alpha\beta}$  when  $a_{\text{ho}} \rightarrow 0$ . This shows that the real part of the excitation spectrum is a Gaussian function of  $a_{\text{ho}}$ :

$$\text{Re } \varepsilon_{\mathbf{q}} - \hbar\omega_A = e^{-k_0^2 a_{\text{ho}}^2} (\varepsilon_{\mathbf{q}}^0 - \hbar\omega_A), \quad (19)$$

where  $\varepsilon_{\mathbf{q}}^0$  is the limit of the excitation energy for  $a_{\text{ho}} \rightarrow 0$ . Eq.(19) allows an extremely efficient evaluation of  $\varepsilon_{\mathbf{q}}^0$  which, when applied to the self-consistent Eq.(6) of [5], allowed us to reproduce the numerical results of [6] and hence to disprove the ones of [5]. Eq.(19) shows that changing  $a_{\text{ho}}$  amounts to a mere rescaling of the vertical axis of Fig.1 and cannot open or close an energy gap. The situation may be different for anisotropic microtraps.

*Experimental issues:* The perturbative regime  $\Gamma \ll \omega_{\text{ho}}$  may be reached with alkaline-earth atoms: e.g.  $^{88}\text{Sr}$  was recently trapped in a deep 3D lattice, with  $a_{\text{ho}} \sim 0.05a \sim 20\text{nm}$  [4], and it has a narrow line  $5s^2 \ ^1S_0 \rightarrow 5s5p \ ^3P_1$  realizing the needed  $J_g = 0 \rightarrow J_e = 1$  transition, with  $\Gamma \sim 0.05\omega_{\text{ho}}$ . To produce and spectroscopically probe elementary excitations with  $q \neq k_0$ , one cannot use the direct  $g \rightarrow e$  coupling with resonant light, but one can use an indirect Raman coupling [15].

In Wigner ion crystals [16],  $e$  and  $g$  experience the same Coulomb shift. On the contrary, for neutral atoms, the lattice potential is a lightshift, that may deviate from one of the two assumptions of (1), (i)  $e$  experiences a *scalar* lightshift, and (ii) the lightshifts of  $e$  and  $g$  are equal. For a lattice obtained by incoherent superposition of laser standing waves along  $x$ ,  $y$ ,  $z$  linearly polarized along  $y$ ,  $z$  and  $x$  respectively, violation of (i) breaks the harmonic oscillator isotropy: the sublevel  $e_x$  (resp.  $e_y, e_z$ ) has an oscillator length  $\eta_e a_{\text{ho}}$  along  $z$  (resp.  $x, y$ ) different from the one  $a_{\text{ho}}$  along the other two directions. This

does not break the three-fold degeneracy of the motional ground state in  $e$  but it reduces the overlap between the motional ground state of  $e_\alpha$  and that of  $g$ . Hence after spontaneous emission, even if one neglects the atom recoil ( $k_0 a_{\text{ho}} \rightarrow 0$ ), the atom in  $g$  can populate an excited motional state, giving a non-zero decay rate to the elementary excitations. Similarly, violation of condition (ii) leads to an oscillator length in  $g$  equal to  $\eta_g a_{\text{ho}}$ ,  $\eta_g \neq 1$ , which also increases the decay rate. For  $k_0 a_{\text{ho}} \rightarrow 0$ , combining both violations gives

$$\text{Im } \varepsilon_{\mathbf{q}} = -\frac{\hbar\Gamma}{2} \left( 1 - \frac{8}{[\eta_e \eta_g + (\eta_e \eta_g)^{-1}](\eta_g + \eta_g^{-1})^2} \right). \quad (20)$$

E.g. if one has achieved  $\eta_e \simeq 1$  at the expense of having an optical lattice depth in  $g$  twice as small/large as in  $e$ , one still finds a small decay rate  $\simeq 0.04\Gamma$ .

In conclusion, the quantum nature of the atomic motion leads to several key features for light propagation in a periodic atomic ensemble: the excitation spectrum has a non-zero imaginary part and its real part significantly depends on the harmonic oscillator length  $a_{\text{ho}}$ , as may be observed with alkaline-earth atoms such as strontium. It also naturally provides a divergence-free theory in the limit  $a_{\text{ho}} \rightarrow 0$ , which confirms the results of [6] against the ones of [5] for fixed atomic positions.

We acknowledge insightful discussions with I. Carusotto, D. Wilkowski, E. Arimondo, D. Basko, and financial support from IFRAF and ANR Gascor.

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