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Line shapes for light scattered from Bose-Einstein condensates

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We study the coherent scattering of weak near-resonant light off a Bose-Einstein condensate formed by a system of cooled atoms in a trap. Scattering occurs primarily in the forward direction, and exhibits a very narrow feature on top of a broad non-Lorentzian background.

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Several experimental groups have been working toward the realization of a Bose-Einstein condensate (BEC) [1–3] in systems of trapped and cooled atoms [4]. If this goal is achieved, reliable methods must be developed to detect and diagnose the BEC.

The subject of this Rapid Communication is the weak coherent light scattering off a BEC at zero temperature, which is also discussed in Refs. [5–7]. The study of this problem was initiated by Shlyapnikov and Svistunov, and Politzer. They considered the limit of a very large trap, in which atomic and photonic degrees of freedom mix, giving rise to a gap in the excitation spectrum, i.e., the region of frequencies that do not support any propagating modes. Because of this gap the resonant light will be strongly reflected back from the sharp boundary of the condensate. The analysis of Refs. [5,6] applies to the situation when $N\lambda\!\!\!^{-}{}^3/a^3 \gg 1$ and $a/\lambda\!\!\!^{-} \gg 1$, where N denotes the number of atoms, $\lambda\!\!\!^{-}$ is the resonant wavelength $\lambda/2\pi$, and a is the size of the trap's ground state. Javanainen [7] studied a small trap limit ($N\lambda\!\!\!^{-}{}^3/a^3 \gg 1$ and $a/\lambda\!\!\!^{-} \ll 1$), and described the atomic field by just one harmonic oscillator, corresponding to a collective excitation that approximately conserves momentum in the absorption-emission processes. As a result, in the steady state, a small number of atoms remain in the excited state, and the number of scattered photons has a Lorentzian line shape centered at the bare atomic resonant transition frequency.

As shown below, the results are significantly modified in the intermediate regime of parameters, $N\lambda\!\!\!^{-}{}^3/a^3 \sim 1$ and $a/\lambda\!\!\!^{-} \sim 1$. We find that the scattering cross section is non-Lorentzian, and exhibits very narrow resonance structures close to the electronic transition. The narrow feature at line center results from a process akin to Dicke narrowing [8] for scattering from confined particles. Within the scope of the model considered (which neglects spontaneous emission into noncondensate states), the width is related to the geometric mean of the trap frequency and photon recoil energy. We expect such spontaneous emission to lead to a further increase in the width of the central component. The scattering angle is limited by the effective size of the trap. The properties of the scattered light do not significantly depend on details of the excited-state potentials, provided the exciting pulse has a duration less than the typical period of the center-of-mass motion. We also discuss the role played by the contact part of the dipole-dipole interaction, which has been ignored in most of the second quantized theories developed so far.

We consider a range of parameters describing the magneto-optical trap [1,9]. The potential for the atomic center-of-mass motion for a single atom in the ground electronic state can be described by a harmonic oscillator potential of frequency $\omega_t \sim (2\pi)10$ Hz. Although the potential forms a finite barrier, several thousands of energy levels exist within the trap. By exploiting an evaporative cooling technique, the trap will store about 10^8 cesium atoms, which will interact with the resonant light of frequency $\sim(2\pi)4.0\times10^{14}$ Hz. A typical photon recoil energy will then be $\sim(2\pi)2$ kHz, whereas the natural linewidth (half width at half maximum) $\gamma \sim (2\pi)2.5$ MHz. The size of the ground-state wave function in the condensate (assumed to be of harmonic oscillator form) is $a \sim 10$ μm, whereas the resonant wavelength, $\lambda \sim 800$ nm. We note that a for the ground state of the condensate is several times bigger than $1/\sqrt{2M\omega_t}$, with M being the mass of Cs and $\hbar = 1$. The a we use takes into account the (expected) repulsive ground-state interactions, which are believed to increase the size of the condensate [10,11]. In general, atoms in excited electronic states move in a different potential from that characterizing the ground state. Here, we consider the case of zero potential in the excited state (but other potentials should give qualitatively similar results).

The Hamiltonian governing the evolution of the atoms in the trap takes the following second quantized form in the rotating-wave approximation (RWA):

$$\begin{aligned}\mathscr{H} = &\sum_{\mathbf{n}} E^g_{\mathbf{n}} g^\dagger_{\mathbf{n}} g_{\mathbf{n}} + \sum_{\mathbf{m}} (E^e_{\mathbf{m}} + \omega_0) \mathbf{e}^\dagger_{\mathbf{m}} \mathbf{e}_{\mathbf{m}} \\ &+ \sum_{\mathbf{n},\mathbf{m}} \sum_{\mu} \int d\mathbf{k} \rho(k) [\eta_{\mathbf{nm}}(\mathbf{k}) g^\dagger_{\mathbf{n}} a^\dagger_{\mathbf{k}\mu} \mathbf{e}_{\mathbf{m}} \cdot \boldsymbol{\epsilon}_{\mathbf{k}\mu} + \text{H.c.}] \\ &+ \sum_{\mu} \int d\mathbf{k} \; cka^\dagger_{\mathbf{k}\mu} a_{\mathbf{k}\mu} + \mathscr{H}_c , \end{aligned} \tag{1}$$

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where $g_{\mathbf{n}}$, $g_{\mathbf{n}}^{\dagger}$ denote atomic annihilation and creation operators for the **n**th state of the ground-state potential. For a rotationally invariant potential, n is actually a triple index (n_x, n_y, n_z). The corresponding energy is $E_{\mathbf{n}}^{g}=\omega_t(n_x+n_y+n_z)$. $\mathbf{e}_{\mathbf{m}}$, $\mathbf{e}_{\mathbf{m}}^{\dagger}$ denote atomic annihilation and creation operators in the excited-state potential. In the case of zero potential they annihilate and create plane waves of momentum $\mathbf{m}$. The corresponding energies are $E_{\mathbf{m}}^{e}+\omega_0=\mathbf{m}^2/2M+\omega_0$. We consider here the transition from an s state to a p state and therefore $\mathbf{e}_{\mathbf{m}}$'s and $\mathbf{e}_{\mathbf{m}}^{\dagger}$'s have a corresponding vector character. This is not the case for the transition in cesium ($6S_{1/2}F=4$ to $6P_{3/2}F=5$), but the character of the transition is not essential for our conclusions. $a_{\mathbf{k}\mu}$ and $a_{\mathbf{k}\mu}^{\dagger}$ denote annihilation and creation operators for photons of momentum $\mathbf{k}$ and linear polarization $\boldsymbol{\epsilon}_{\mathbf{k}\mu}$ ($\mu=1,2$). All operators fulfill standard bosonic commutation relations. $\rho(k)$ is a slowly varying function of k related to the natural linewidth $\gamma=(8\pi^2k_0^2/3c)|\rho(k_0)|^2$, with $k_0=\omega_0/c$. $\eta_{\mathbf{nm}}(\mathbf{k})$ describe the transition from the **n**th state of the ground-state potential to the **m**th state of the excited-state potential,

$$\eta_{\mathbf{nm}}(\mathbf{k})=\langle\mathbf{n}|e^{-i\mathbf{k}\cdot\mathbf{R}}|\mathbf{m}\rangle. \tag{2}$$

The last part of the Hamiltonian has to be included when the dipole approximation is used [12] and is usually neglected. It is the contact interaction between atoms in the excited and ground states. For atoms moving (or even condensing) inside the trap, such a neglect cannot be justified *a priori*, since atomic wave functions may well overlap. Only when the contact term is taken into account does the total Hamiltonian include fully the strong resonant atomic interactions due to electronic dipole-dipole forces and exchange of transverse photons [13,14].

In the first quantization picture the contact term has the form

$$\mathcal{H}_c^{1}=4\pi e^2\sum_{i>j}\mathbf{r}_i\cdot\mathbf{r}_j\delta(\mathbf{R}_i-\mathbf{R}_j), \tag{3}$$

where $\mathbf{r}_i$ and $\mathbf{R}_i$ are electronic and atomic positions, respectively. The sum extends over $i>j$, since the diagonal term contributes to renormalization of the electronic transition frequency. In the second quantized form the contact term can be conveniently written in the coordinate representation, when we introduce atomic fields:

$$\psi_g(\mathbf{R})=\sum_{\mathbf{n}}\langle\mathbf{R}|\mathbf{n}\rangle g_{\mathbf{n}}, \tag{4}$$

$$\boldsymbol{\psi}_e(\mathbf{R})=\sum_{\mathbf{m}}\langle\mathbf{R}|\mathbf{m}\rangle\mathbf{e}_{\mathbf{m}}, \tag{5}$$

and their Hermitian conjugates. In terms of these fields it is

$$\mathcal{H}_c=4\pi d^2\int d\mathbf{R}\psi_g^{\dagger}(\mathbf{R})\boldsymbol{\psi}_e^{\dagger}(\mathbf{R})\cdot\boldsymbol{\psi}_e(\mathbf{R})\psi_g(\mathbf{R}), \tag{6}$$

where $d=|\langle e\mathbf{r}\rangle|$ is the absolute value of the dipole moment.

For weak light scattering at $T=0$, when all the atoms are in the BEC, we linearize the atomic amplitudes around the ground state, and substitute the operators $g_{\mathbf{n}}$ by their appropriate mean values [5,7],

$$\langle g_{\mathbf{n}}\rangle\rightarrow\delta_{\mathbf{n}0}\sqrt{N}. \tag{7}$$

This linearization reduces the Hamiltonian to a quadratic form in the operators for photons and excited-state amplitudes. The contact Hamiltonian after the linearization (7) is

$$\mathcal{H}_c=N\delta\int d\mathbf{R}\boldsymbol{\psi}_e^{\dagger}(\mathbf{R})\cdot\boldsymbol{\psi}_e(\mathbf{R})e^{-R^2/2a^2}, \tag{8}$$

where $\delta=6\pi\gamma/(\sqrt{2\pi}ka)^3$. It is an inhomogeneous collective shift which depends locally on the density of the atoms in the ground state. Numerically, $N\delta$ is about $62\times N/10^7$ MHz. Upon eliminating the atomic excited-state operators, a scattering equation for the field operator takes the following general form:

$$\dot{a}_{\mathbf{k}\mu}=-icka_{\mathbf{k}\mu}-\sum_{\mu'}\int d\mathbf{k}'\int_0^t dt'\times\mathcal{K}(t-t';\mathbf{k},\mu,\mathbf{k}',\mu')a_{\mathbf{k}'\mu'}(t'). \tag{9}$$

The kernel $\mathcal{K}(t-t';\mathbf{k},\mu,\mathbf{k}',\mu')$ can be evaluated analytically in the case of a zero potential or an harmonic potential in the excited state (for details see Ref. [15]). Here we stress only that the kernel in Eq. (9) has a simple physical meaning. Namely, it describes the amplitude for the process of absorption of a photon with momentum $\mathbf{k}'$ at time t', accompanied by the formation of a wave packet in the excited-state potential. This wave packet then undergoes evolution until it recombines to the ground state at time t, emitting a photon of momentum $\mathbf{k}$. The evolution includes the free part and the effects of the contact potential. Note that the free evolution of the wave packet in the time interval $\tau=t-t'$ consists primarily in quantum diffusion and drift caused by the momentum of the absorbed photon [16]. When the wave packet drifts away from the center of the trap and diffuses sufficiently strongly, recombination accompanied by emission becomes impossible. Thus the kernel $\mathcal{K}(t-t';\mathbf{k},\mu,\mathbf{k}',\mu')$ decays on a characteristic time scale $1/\Gamma$. It is easy to verify that Γ must be of the order of $\sqrt{\omega_t k^2/2M}$. $1/\Gamma$ is simply the time needed for the excited-state wave packet to move a distance $\sim a$ with the recoil velocity. We estimate that $\Gamma\sim800$ Hz, although its effective value can be larger due to spontaneous emission into noncondensed states, which we neglect in this Rapid Communication.

When the limit $a\rightarrow\infty$ is taken in Eq. (9) we recover the results of Refs. [5,6]. Momentum becomes then a proper quantum number and the dispersion relation exhibits a "gap." Such a solution decays, however, on a time scale $1/\Gamma$ and is not the one we are interested in. For $t\rightarrow\infty$ [or practically, $t\gg1/\Gamma\sim1/(800\text{ Hz})$] the incident field has enough time to penetrate the system and *a long-time coherent response* will build up [17]. In this limit the solution for the scattering, Eq. (9), becomes

$$\langle a_{\mathbf{k}\mu}(t)\rangle \sim \alpha\delta(\mathbf{k}-\mathbf{k}_L)\delta_{\mu\mu_L}e^{-i\omega_L t} + B(\mathbf{k},\mu)\delta(ck-\omega_L)e^{-i\omega_L t}, \tag{10}$$

where α is the amplitude of the incident coherent field, ω_L and $\mathbf{k}_L$ its frequency and wave vector, and $B(\mathbf{k},\mu)$ is the scattering amplitude. Thus, as $t\to\infty$ only coherent elastic scattering is possible.

The scattering amplitude in this on-shell approximation [Eq. (10)], see Ref. [18], satisfies

$$B(\mathbf{k},\mu) = -2\pi\tilde{\mathcal{K}}(-i\omega_L;\mathbf{k},\mu,\mathbf{k}_L,\mu_L) - 2\pi\frac{k_L^2}{c}\sum_{\mu'}\int d\Omega_{\mathbf{k}'} \times \tilde{\mathcal{K}}(-i\omega_L;\mathbf{k},\mu,\mathbf{k}',\mu')B(\mathbf{k}',\mu'), \tag{11}$$

where $|\mathbf{k}|=|\mathbf{k}'|=|\mathbf{k}_L|=\omega_L/c$, while $\tilde{\mathcal{K}}(z;\mathbf{k},\mu,\mathbf{k}',\mu')$ denotes the Laplace transform of $\mathcal{K}(\tau;\mathbf{k},\mu,\mathbf{k}',\mu')$. The integration is over the solid angle $d\Omega_{\mathbf{k}'}$.

The quantity of interest is the total number of scattered photons of frequency ω_L per unit time and normalized to the total number of photons incident upon the area πa^2 (normalized cross section), given by

$$\sigma(\omega_L) = \frac{k_L^2}{c^2a^2}\sum_{\mu}\int d\Omega_{\mathbf{k}}|B(\mathbf{k},\mu)|^2. \tag{12}$$

One might try to solve Eq. (11) using the Born approximation, i.e., neglecting the second, self-energy term on the right-hand side. Such attempts fail miserably, partially due to the large optical thickness of the condensate. Self-energy terms are extremely important close to resonance and one must fully account for them. We have solved Eq. (11) numerically. To accomplish this we discretized the solid angle and solved the resulting finite set of linear equations. One can also construct an approximate analytic solution for Eq. (11), if one neglects the dependence of $\tilde{\mathcal{K}}$ on the polarization product $\boldsymbol{\epsilon}_{\mathbf{k}\mu}\cdot\boldsymbol{\epsilon}_{\mathbf{k}'\mu'}$. This is a good approximation, since the scattering occurs mainly in the forward direction and the scattered photons have polarizations that are approximately perpendicular to $\mathbf{k}_L$ and do not couple to each other.

After neglecting the polarization dependence of $\tilde{\mathcal{K}}$, $B(\mathbf{k},\mu)$ can be expanded in spherical harmonics. For $\mathbf{k}=k_L(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, $\mathbf{k}_L=k_L(0,0,1)$, and $\boldsymbol{\epsilon}_{\mu_L}=(1,0,0)$, the expansion is

$$B(\mathbf{k},\mu) = \sum_{l=0}^{\infty} B_l(k_L)P_l(\cos(\theta))\sqrt{(2l+1)/4\pi}, \tag{13}$$

where $P_l(x)$ are Legendre polynomials. The $B_l(k_L)$ are

$$B_l = \frac{-2\pi N|\rho(k_L)|^2(4\pi)^2\mathcal{Q}_l/(\sqrt{2\pi})^3}{1+2\pi N|\rho(k_L)|^2(4\pi)^2\mathcal{Q}_l k_L^2/(\sqrt{2\pi})^3 c}, \tag{14}$$

where

$$\mathcal{Q}_l = \int_0^\infty \zeta^2 d\zeta\, \frac{e^{-\zeta^2/2}j_l^2(k_L a\zeta)}{\Gamma + i(\omega_0-\omega_L+N\delta\exp[-\zeta^2/2])}. \tag{15}$$

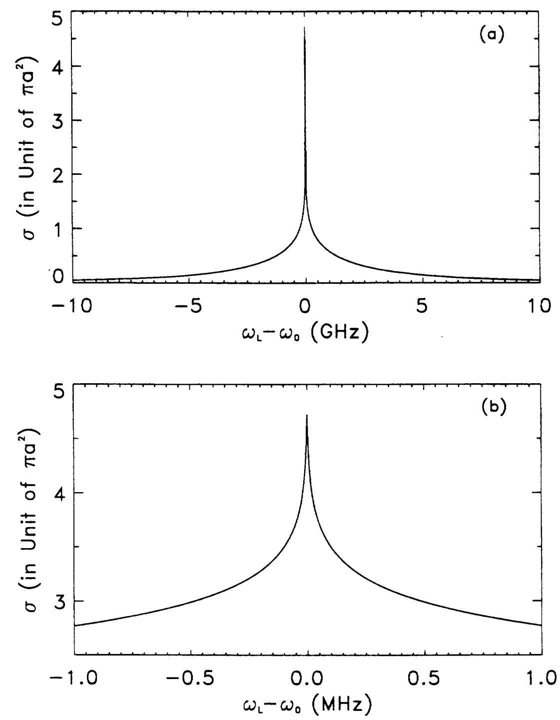

FIG. 1. Scattering cross section of the BEC for $N=10^7$ (the rest of the parameters as given in the text). (a) shows the overall shape; (b) is an enlargement of the central region.

Here $\zeta=R/a$ is the radial coordinate scaled to the width of the ground state, and $j_l(x)$ denote spherical Bessel functions. Comparison of the above formula with the numerical solution of Eq. (11) shows that the approximate solution describes very well the line shape, although it underestimates the overall cross section.

When the contact term (6) is neglected, the total cross section,

$$\sigma = 2\sum_{l=0}^{\infty} B_l^2(k_L)k_L^2/(c^2a^2), \tag{16}$$

becomes the sum of Lorentzians, characterized by the width $\gamma_{\mathrm{eff}}^l=\Gamma+\gamma_L^l$, with

$$\gamma_L^l = N3\sqrt{2\pi}\gamma e^{-k_L^2a^2}I_{l+\frac{1}{2}}(k_L^2a^2)/(2k_La), \tag{17}$$

where $I_l(x)$ denote modified Bessel functions.

For $l\ll k_L^2a^2$, all γ_L^l's are roughly equal to $\gamma_{\mathrm{eff}}\approx 3N\gamma/(2k_L^2a^2)$ [7]. One might think that if only low angular momentum harmonics contributed to scattering, the cross section would be a sum of Lorentzians with approximately the same width, i.e., it would itself be Lorentzian. However, the γ_L^l's decrease quite significantly with increasing l. In fact, the contribution from higher l's is also important. As a result, the line shape becomes non-Lorentzian, and exhibits a very narrow spike close to resonance (Fig. 1). The lower bound for the width of this spike is determined by quantum diffusion rate $\Gamma\leq 800$ Hz. Typically, with $N=10^7$, it is a few times broader than Γ. This narrow feature in the spectrum is an analog of the coherent Dicke narrowing [8]. It is worth noticing that even close to resonance the angular distribution of the scattered light has a width of the order $1/(k_L a)$ [15].

The situation changes somewhat when the contact term (6) is taken into account. However, for the parameters considered here, the differences are hardly noticeable. Physically, within our model, we have included all the effects of atom-atom interactions due to exchange of transverse photons. Such interactions are repulsive, and divergent as $1/R^3$ at short distances. Therefore, the singular part of these $1/R^3$ terms can be regarded to be already essentially of the form of a contact potential. Inclusion of the full contact Hamiltonian (3) does not then change the overall picture significantly. The curve in Fig. 1 was calculated for $N\delta \approx 62$ (MHz), and exhibits a slight asymmetry of order of 0.3%, in contrast to the result obtained for $N\delta = 0$ without the contact term. But for other choices of parameters, the effects of contact interactions can be more pronounced. In particular, additional structures in the line shape may be possible between ω_0 and $\omega_0 + N\delta$ [15], since in this region some of the atoms are shifted into resonance with the incident light.

To summarize, we have calculated the line shapes for coherent scattering from a BEC, using a somewhat more accurate theory than previously employed. This line shape has three appealing properties. First, it exhibits a very broad resonance of width of the order of γ_{eff}. To detect even a partial condensation it will be sufficient to shine a strongly detuned light on the system of cooled atoms. Those atoms that are not in the condensate phase will Rayleigh scatter with a cross section of effective linewidth γ ($\ll \gamma_{\text{eff}}$) and will not significantly contribute. Condensed atoms will produce quite a strong signal. Second, the very narrow feature ($\sim\Gamma$) in the spectrum at $\omega_L \simeq \omega_0$ suggests obvious applications of this system for precision spectroscopy. This is one of the comparatively rare examples of a situation in which such a narrow resonance is present. (The Dicke narrowed spectrum [8] is also similar in shape with this sharp spectral feature.) Yet the response of the system at this resonance is strong. This is in contrast to normal narrow resonances associated with weak transitions. From the experimental point of view, the spike at $\omega_L \simeq \omega_0$ is especially interesting, since it will not be smeared out due to fluctuations in the number of condensed atoms. One should stress, however, that other dissipative processes, such as spontaneous emission out of the condensate might lead to some increase of Γ [15]. Third, the line shape is non-Lorentzian, asymmetric, and in some circumstances exhibits additional interesting features.

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