Classical rotons in cold atomic traps

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We predict the emergence of a roton minimum in the dispersion relation of elementary excitations in cold atomic gases in the presence of diffusive light. In large magneto-optical traps, multiple scattering of light is responsible for the collective behavior of the system, which is associated to an effective Coulomb-like interaction between the atoms. In optically thick clouds, the rescattered light undergoes diffusive propagation, which is responsible for a stochastic short-range force acting on the atoms. We show that the dynamical competition between these two forces is by the appearance of a roton minimum in the dispersion relation. Making use of the fluctuation-dissipation theorem, we show that the roton minimum is related to classical long-range order in the system.

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Since the first ideas advanced by Landau [1,2], the concept of “roton minimum” in the dispersion of the collective modes of a certain physical system has played a central role in the description of superfluidity. After the success of the theory in the context of superfluid phases of 4He, rotons have received considerable attention since then and have been identified in many different quantum interacting systems. Recently Cormack et al. [3] suggest that rotons may appear in already moderately interacting ultracold Bose gases, and Kalman et al. [4] have numerically observed their emergence in two-dimensional dipolar bosonic gases. In fact, the emergence of a roton minimum in the excitation spectrum strongly depends upon the shape of the interacting potential or, equivalently, on how particles are correlated. The correlational origin of the roton minimum has been firstly suggested by Feynman, where the static structure factor $S(k)$ is expressed in terms of the dispersion relation $\omega(k)$ as

$$\omega(k) = \frac{\hbar k^2}{2mS(k)} \quad (1)$$

This has an enormous implication on the interpretation of the physical properties of the system in terms of the dispersion relation: The presence of a roton minimum is the signature of strong correlations in the system. In the limit of large mode softening, i.e., for rotons with zero frequency, the system can develop mechanical instabilities, which can lead to interesting physics. In Ref. [5] Henkel et al. have suggested that the presence of a “roton zero” is at the origin of crystallization in ultracold Rydberg gases. In this paper we describe the classical origin of a roton minimum in the excitation spectrum of cold atomic clouds confined in magneto-optical traps (MOTs). Due to the competition between long-range interactions between the atoms and the stochastic forces associated with the diffusion of light, atoms in MOTs experience a complex effective interaction. We suggest that a new dispersion mode may result from the dynamical coupling of the density waves with the fluctuations of the light intensity inside the trap. Finally, by applying an hydrodynamic version of the fluctuation-dissipation theorem, and thus generalizing the relation between $S(k)$ and $\omega(k)$ of Eq. (1), we show the emergence of (classical) long-range order, extending the concept of rotons to the classical regime. The remainder of the paper is devoted to the understanding the physical origin of such a classical roton minimum.

A route for the most intriguing complex behavior in large magneto-optical traps relies exactly on the multiple scattering of light [6,7]. Due to the consecutive scattering and reabsorption of photons, the atoms experience a mediated long-range interaction potential similar to Coulomb system $\sim 1/r$ [8,9], and the system can therefore be regarded as a one-component trapped plasma. In a series of previous works, we have put in evidence the important consequences of such a plasma description of a cold atomic gas [10,14], whereas the formal analogy and the application of plasma physics techniques reveal themselves to be appropriate to the description of driven mechanical instabilities [15–19] or even more exotic phenomena, like phonon lasing [20]. Moreover, in such optically thick traps, it is known that light does not propagate ballistically, rather exhibiting a diffusive behavior [21]. In this situation, the energy transport velocity $v_E$, i.e., the velocity that accounts for the propagation of energy by the scattered wave, is smaller than $c$ [22,23]. Labeyrie et al. [24] have experimentally observed that $v_E$ can, indeed, be several orders of magnitude smaller than $c$ in the case of resonant light propagating in traps, already with a moderate optical thickness. More recently, the diffusive behavior of light has been identified as a source of dynamical instabilities leading to the formation of photon bubbles in magneto-optical traps [25].

In what follows, we consider the dynamics of cold atoms in MOTs to be described by the Vlasov equation

$$\left( \frac{\partial}{\partial t} + v \cdot \nabla + \frac{1}{m} \sum_i F_i \cdot \nabla_v \right) f(r,v,t) = 0, \quad (2)$$

where the distribution function $f(r,v,t)$ is the normalized to the total number of particles

$$N = \int d\mathbf{r} \int d\mathbf{v} f(r,v,t). \quad (3)$$

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The total force $\sum F_i = F_r + F_c$ accounts for both the trapping and cooling forces. Evidence [26,27] suggests that the density profile is approximately constant for large traps (typically with $N \sim 10^9$–$10^{10}$ atoms), which allows us to consider the system to be homogeneous and thus to neglect the effects of the trap. The collective force can be described by a Poisson equation [9,10]

$$\nabla \cdot F_c(r,t) = Q \int dv f(r,v,t). \tag{4}$$

The prefactor in Eq. (4) represents an effective charge $Q = \sigma_L (\sigma_R - \sigma_L) / c$ of the atoms induced by light, where $\sigma_R$ and $\sigma_L$ are the scattering and absorption cross sections [6–9], and $I$ is the light intensity. For most of the experimental conditions, the scattering cross section is larger than the absorption cross section, i.e., $\sigma_R > \sigma_L$, enforcing the effective charge to be a positive quantity. We have showed that the positiveness of $Q$ is an essential condition for the existence of stable oscillations in the system (see, e.g., Ref. [10]).

The phase-space dynamics of light can be described a transport equation for the luminescence $g_{\omega}(r,u,t)$ accounting for several processes like absorption, gain, elastic, and inelastic diffusion, which may be written as [11]

$$\left( \frac{\partial}{\partial t} + u \cdot \nabla \right) g_{\omega}(r,u,t) = -\gamma_{\text{ext}} g_{\omega}(r,u,t) + \frac{\gamma_c}{4\pi} \int g_{\omega}(r,u',t) \times p(u,u') d\Gamma' + \eta(r,t), \tag{5}$$

where $\gamma_{\text{ext}}$ and $\gamma_c$, respectively, represent the extinction (resulting from the sum of pure absorption) and elastic scattering coefficients (see Ref. [12] for a detailed derivation of the coefficients in the presence of Doppler broadening), $\eta$ is the power emission function, and $\Gamma'$ is the solid angle defined around the direction of $u$ (in this version, the inelastic processes are input in the absorption and emission terms). Taking moments from equation (5), we can derive recursive equations for the intensity $I(r,t) = \int g_{\omega}(r,u,t) du$. Assuming Markovian processes only, and using the fact that $p(u,u')$ (generally dependent on the internal structures of the scatters) is a isotropic function, we can make use of Fick’s law $j_\omega = -D \nabla I$ as a closure condition, where the photon current is defined as $j_\omega = \int u g_{\omega} du$. Under this approximation, the light intensity can be described by the diffusion equation

$$\frac{\partial I}{\partial t} - \nabla \cdot D \nabla I = -\gamma_{\text{ext}} I. \tag{6}$$

In the case of isotropic diffusion, the diffusion coefficient is determined by $D = \ell^2 / \tau$ [13], where the photon mean-free path is $\ell = 1 / n \sigma_L$, with $n = \int f dv$ standing for the atomic density. According to experimental results [24], the diffusion time $\tau$ can be considered as independent from the atom density, so the diffusion coefficient explicitly reads

$$D(r,t) = \frac{1}{\sigma_L n^2} = \frac{1}{\sigma_L^2} \left[ \int f(r,v,t) dv \right]^{-2}. \tag{7}$$

In practice, the Markovian approximation remains valid as long as the optical thickness $b = a \gamma_{\text{ext}} / v_E$ is much larger than unit ($b \sim 40$ already for traps of moderate sizes $a \sim 2$–3 mm [24]). Such a condition is verified provided that $\ell \ll a$ [11,12]. The equilibrium solution to the diffusion equation (6) is $I_0(r) \sim \sin(k_{\text{ext}} r) / k_{\text{ext}}$, where $k_{\text{ext}} = \sqrt{\gamma_{\text{ext}} / D_0}$. The vanishing condition at the edge of the trap determines the value of the absorption constant as $\gamma_{\text{ext}} = \pi \lambda^2 / D_0^2$. In what follows, we consider fluctuations of very small scale in respect to the variation of the light intensity, in the wave vector range $k \gg k_{\text{ext}}$. In that case, we can safely neglect the right-hand side of Eq. (6) in first order. Therefore, linearization of Eqs. (2), (4), and (7) with $f = f_0 + \delta f$, $I = I_0 + \delta I$, and $D = D_0 + \delta D$ yields

$$\left( \frac{\partial}{\partial t} + u \cdot \nabla \right) \delta f + \frac{1}{m} \delta F_c \cdot \nabla f_0 = 0, \tag{8}$$

$$\frac{\partial}{\partial t} \delta I - D_0 \nabla^2 \delta I - \delta D \nabla^2 I_0 = 0, \tag{9}$$

$$\nabla \cdot \delta F_c = Q_0 \int \delta f dv + Q_0 n_0 \frac{\delta I_0}{I_0}, \tag{10}$$

where $Q_0 = \sigma_L (\sigma_R - \sigma_L) I_0 / c$. By Fourier transforming the perturbed equations, we obtain the following kinetic dispersion relation:

$$1 = \frac{\omega_p^2}{k^2} \left( 1 + \frac{\omega_d}{i \Omega - D_0 k^2} \right) \int \frac{1}{v_z} \frac{\partial F_0}{\partial v_z} dv_z, \tag{11}$$

with $\Omega = \omega + i \gamma$. Here we have defined $f_0(v,r) = n_0 F_0(v)$, such that $\int F_0(v) dv = 1$ and considered perturbations parallel to the wave vector $k = k_{\text{ext}}$. One observes that the dynamics of the system is described by two different frequencies. The first is associated with the oscillations of the atoms due to the long-range force, corresponding to an effective plasma frequency [10]

$$\omega_p = \sqrt{Q_0 n_0 / m}. \tag{12}$$

The second important quantity is the rate at which the photons scatter inside the trap, or simply the diffusion frequency

$$\omega_d = \frac{2 \nabla^2 I_0}{I_0} D_0. \tag{13}$$

We notice that the latter changes with the scale at which the diffusive processes occur (micro-, meso-, or macroscopic), as it depends upon the length scale $L = \sqrt{2 \nabla^2 I_0 / \Omega_0} \approx \sqrt{2} / k_{\text{ext}}$ at which the light intensity varies. We will discuss the macroscopic case below, but we again stress that our analysis remains valid as long as the light intensity varies much slower than the typical excitation wavelength, which means that the $\omega_d$ can be treated as a constant quantity. The integral in Eq. (11) can be evaluated using the Landau prescription, according to which the full information about the initial conditions is cast if the integration path is set to pass below the pole $\Omega = v_z k$. We split the integral into two parts

$$\int \frac{1}{v_z} \frac{\partial F_0}{\partial v_z} dv_z = \text{Pr} \int \frac{1}{v_z - \Omega / k} \frac{\partial F_0}{\partial v_z} dv_z + i \pi \int \frac{\partial F_0}{\partial v_z} \left. \right|_{v_z = \Omega / k} dv_z, \tag{14}$$

where Pr stands for the Cauchy principal value. Assuming a phase speed $v_{\text{ph}} = \omega / k$ much greater than the width of the
distribution, such that $F_0$ and its derivatives get small as $v_z$ gets large, we may expand the denominator in (14), which simply yields
\[
Pr \int \frac{1}{v_z - \Omega/k} \frac{\partial F_0}{\partial v_z} \, dv_z \simeq \frac{k^2}{\omega^2} \int F_0 \left( 1 + \frac{3}{\Omega^2} \right) \, dv_x \, dv_y \, dv_z.
\]

Assuming the atomic equilibrium to be described by a Maxwell distribution
\[
F_0(v) = \frac{1}{(2\pi v_{th}^2)^{3/2}} e^{-v^2/2v_{th}^2},
\]
with $v_{th} = \sqrt{k_B T/m}$ standing for the thermal speed, we may finally write
\[
1 = \frac{\omega_p^2}{\Omega^2} \left[ \left( 1 + \frac{u^2 k^2}{\Omega^2} \right) \left( 1 + \frac{\omega_d}{\Omega - D_0 k^2} \right) \right]
+ i \frac{\omega_p^2 \Omega^2}{k^2} \frac{\partial f_0}{\partial v_z} \bigg|_{v_z = \Omega/k},
\]
where we have defined the sound speed $u_s = \sqrt{3} v_{th}$. Assuming small damping, $\gamma \ll \omega$, we may explicitly separate the real and imaginary parts of the modes,
\[
\omega^2 = \left( \omega_p^2 + u_s^2 k^2 \right) \left( 1 - \frac{\omega_d D_0 k^2}{\omega_p^2 + D_0 k^4} \right)
\]
and
\[
\gamma = \frac{\omega_d \omega_p^2 + u_s^2 k^2}{2 \omega_p^2 + 3 D_0 k^4} - \frac{2 \omega_p^2}{3 \sqrt{8\pi} k^3 \lambda_D^3} e^{-3/(2\lambda_D^2)},
\]
where $\lambda_D = u_s/\omega_p$ is the effective Debye length. We now discuss some of features of the dispersion and show, in particular, that contains a roton minimum in some range of parameters.

According to typical experimental conditions [24], the mean-free path is found to value $\ell \sim 300 \mu m$ and the diffusion coefficient $D_0 \simeq 0.66 m^2 s^{-1}$. Based on our previous estimates [10], the effective plasma frequency and Debye length, respectively, value $\omega_p \sim 2\pi \times 100$ Hz and $\lambda_D \sim 100 \mu m$. Therefore, for a system of size $a \sim 1$ cm, the diffusive approximation is valid provided that the diffusion and plasma frequencies are of the same order, $\omega_d \sim \omega_p$. This is achieved if $k_d = \sqrt{D_0/\omega_p} \sim 1$ cm is of the same order of $L$, which may be possibly achieved for typical experimental parameters. Moreover, the values of $\omega_p$ and $\omega_d$ can be varied by changing the detuning of the cooling lasers and the optical thickness of the system. In Fig. 1, it is depicted the emergence of a roton minimum in the dispersion relation (18). As the values of $\omega_d$ increase (i.e., for stronger diffusion), the frequency decreases (mode softening). At the critical value $\omega_d^{(c)} = 2 \omega_p$, the mode softens towards zero, which is a clear manifestation of a roton instability mechanism. For $\omega_d > \omega_d^{(c)}$, the system enters a crystalized phase. The mechanism of crystallization via mode softening was recently investigated in the quantum framework of supersolidity [5]. An important remark is related to the Landau damping at short wavelengths. Modes in the region $k \lambda_D \gg 1$ undergo a kinematic damping. Fortunately, rotons are possible to be excited at longer wavelengths ($k \omega_p \lambda_D < 1$), thus avoiding the Landau damping mechanism. We observe that the onset of diffusion tends to decrease the damping rate (see Fig. 1). This encourages hope for rotons to be experimentally observable.

Another important property of the classical rotons described above is that they carry useful information about the long-range correlation of the system. From the dissipation-fluctuation theorem [28], the dynamic structure factor is given by $S(k,\omega) = (k_B T/k^2/\pi\omega) \text{Im} \left( \epsilon(k,\omega) \right)^{-1}$, where $\epsilon(k,\omega) \equiv 1 + \chi(k,\omega)$ and $\chi(k,\omega)$ is the susceptibility. As a result, the dispersion relation (17) is defined as the root of the function $\epsilon(k,\omega) \equiv 1 + \chi(k,\omega)$. In the absence of hydrodynamic damping, the static structure factor $S(k) = \pi^{-1} S(k,\omega) \text{Re} \left( \epsilon(k,\omega) \right)^{-1}/\Omega^2$ is finally given by the classical expression [29]
\[
S(k) = \frac{\omega_p^2 k^2}{\omega(k)^2}.
\]

In Fig. 2 we illustrate the behavior of $S(k)$ for the same parameters of Fig. 1.
The static two-point correlation function \( g(r) = \langle n(r)n(0) \rangle / \langle n(0) \rangle^2 \) can then be easily calculated provided the relation \( g(r) = 1 + \mathcal{F}^{-1}[S(k) - 1] \) [30] (\( \mathcal{F} \) represents the Fourier transform), which after the integrating out the angular variables simply reads

\[
g(r) = 1 + \frac{1}{\pi^2} \int_0^\infty \frac{k \sin(kr)}{r} [S(k) - 1]dk.
\]  

Computing the integral in the complex plane, we can immediately reconstruct the correlation function. It is observed that the appearance of a minimum in the excitation spectrum (18) is associated with the occurrence of long-range correlation (at the scale of \( \lambda_D \)) in the system. By inspection, one founds that the roton minimum occurs at \( k_{\text{rot}} \approx \lambda_D/\ell_d^2 \), which is exactly the period at which the correlation function oscillates (see Fig. 3). This feature can be qualitatively understood in the context of Percus-Yevick (PY) theory [31,32], where the correlation function is approximated by \( g(r)^{PY} \approx 1 + \arctan(\omega_d r + \delta_0) e^{-\omega_d r} \), with \( \delta_0 \) being a constant and \( \omega_d = \omega_0 + ik_0 \) the pole of the function \( S(k) - 1 \). We remark, however, that the PY theory was originally developed for hard-sphere potentials and therefore does not describe systems with long-range interactions. For that reason, we have not used it to compute \( g(r) \) in (21).

In conclusion, we have derived the excitation spectrum of large (optically thick) magneto-optical traps in the presence of diffusive light. We have explicitly established the dispersion relation for the particular case of a thermal atomic distribution, revealing the emergence of a roton minimum for a set of parameters compatible with current experimental conditions. We have also shown that an increase of the light diffusivity is associated to the softening of the roton minimum, which may eventually lead to roton instability. Using the relation between the static structure factor and the dispersion relation, we have explicitly demonstrated that the roton minimum is related to the emergence of classical long-range correlations in the system. The experimental observation of the effect can be made possible by measuring the fluorescence spectrum of the modulated system (e.g., modulating the intensity of the cooling laser). The expected smoking gun of the roton effect is thus the appearance of a turning point of the most pronounced peak around the frequency \( \sim \omega_d \).

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\begin{thebibliography}{9}
\bibitem{InelasticProcesses} In the presence of inelastic processes, the diffusion coefficient should be more precisely defined as \( D = \ell^2 \tau^{-1}[\gamma_{\text{ext}}/\gamma_{\text{tot}} + 1 - g] \), where \( g \) is the anisotropy coefficient [11], which is to vanish in the present discussion.
\end{thebibliography}