Dielectric formalism and damping of collective modes in trapped Bose-Einstein condensed gases

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We present the general dielectric formalism for Bose-Einstein condensed systems in external potential at finite temperatures. On the basis of a model arising within this framework as a first approximation in an intermediate temperature region for large condensate we calculate the damping of low-energy excitations in the collisionless regime.

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The recent experimental observation of Bose-Einstein condensation in alkali metal vapours [1], [2] , [3] gave a new impetus to the research of degenerate Bose systems. Much of the theoretical apparatus developed in the sixties for the study of superfluid helium can be well applied in this case also. The present situation is even a bit simpler, as, due to the low density, interatomic collisions play a much less important role than in case of the helium II. There is, however, an additional complication due to the presence of the external trapping potential.

The Bose-Einstein condensation is also a prime example of continuous phase transitions and spontaneous symmetry breaking. Indeed, the presence of the condensate implies that the phase invariance of the Hamiltonian is absent in the ground state of the system. One of the most spectacular consequences of a broken continuous symmetry is the strong and direct coupling among different correlation (response) functions. Its consequences have been most fully exploited by the dielectric formalism first introduced at zero temperature [4], [5] and later generalized to finite temperature [6], [7] (for an enlightening discussion of features and further references see [8]). A most useful scheme for calculation has been developed by Gould and Wong [9]. Note that the formalism proved to be useful in interpreting neutron scttering experiments in liquid helium (see papers by H.R.Glyde and by A.Griffin in [10] and for a recent experiment [11]).

Our purpose is to generalize the dielectric formalism to inhomogeneous systems and apply it to trapped Bose condensed gases. The emphasis in this paper besides general considerations is put on a simple model emerging from the general theory and the calculation of the damping of the lowest lying excitations in the collisionless regime. This is motivated by the fact that at present the measured damping rates of low frequency collective excitations [12]- [15] are in the focus of interest, partly, because they are more characteristic of the Bose-Einstein condensation than the excitation frequencies. Recently a number of papers have been devoted to the calculation of the damping in the collisionless regime in case of homogeneous systems and of trapped gases as well [16]- [22]. In particular the results in [18] are directly relevant to the experimental situation [14].

Let us start by summarizing the extension of the dielectric formalism to the inhomogeneous system. This formalism emphasizes the importance of quantities which are proper and irreducible simultaneously. Having in mind perturbation theory and the corresponding Feynman graphs, we shall call the proper part of a quantity a part which cannot be cut into two by splitting a single interaction line. In contrast, an irreducible part will be a graph which cannot be cut into two by splitting a single line corresponding to a bare propagator (i.e., unperturbed Green's function).

As usually, we start from the Hamiltonian

$$\hat{H} = \int d^3\vec{r}\hat{\psi}^\dagger(\vec{r})\left(-\frac{\nabla^2}{2m} + U(\vec{r})\right)\hat{\psi}(\vec{r}) + \frac{1}{2}\int d^3\vec{r_1}\int d^3\vec{r_2}\hat{\psi}^\dagger(\vec{r_1})\hat{\psi}^\dagger(\vec{r_2})v(\vec{r_1},\vec{r_2})\hat{\psi}(\vec{r_1})\hat{\psi}(\vec{r_2}) \quad (1)$$

assuming two-body interactions. Here $\hat{\psi}(\vec{r})$ is the Bose field operator and $U(\vec{r})$ denotes the external potential. Separating out the condensate part we have $\hat{\psi}(\vec{r}) = \Phi_0(\vec{r}) + \hat{\phi}(\vec{r})$, where $\Phi_0(\vec{r}) =< \hat{\psi}(\vec{r}) >$ stands for the condensate wave function. The angular bracket here and hereafter denotes ensemble averaging with the grand canonical statistical operator $e^{-\beta(\hat{H}-\mu\hat{N})}/\mathrm{Tr}e^{-\beta(\hat{H}-\mu\hat{N})}$. The density autocorrelation function is defined by $\chi(\vec{r_1},\tau,\vec{r_2},\tau') = -\left\langle T_\tau\left[\tilde{n}(\vec{r},\tau)\tilde{n}(\vec{r'},\tau')\right]\right\rangle$, where $\tilde{n}(\vec{r}) = \hat{n}(\vec{r}) - \langle\hat{n}(\vec{r})\rangle = \Phi_0(\vec{r})\hat{\phi}^\dagger(\vec{r}) + \Phi_0(\vec{r})\hat{\phi}(\vec{r}) + \hat{\phi}^\dagger(\vec{r})\hat{\phi}(\vec{r}) - \left\langle\hat{\phi}^\dagger(\vec{r})\hat{\phi}(\vec{r})\right\rangle$ is the density deviation operator. The field operators here are given in Matsubara representation, τ playing the role of imaginary time. We shall also need the temperature Green's functions defined by $G_{1,1}(\vec{r},\tau,\vec{r'},\tau') = G_{2,2}(\vec{r'},\tau',\vec{r},\tau) = -\left\langle T_\tau\left[\hat{\phi}(\vec{r},\tau)\hat{\phi}^\dagger(\vec{r'},\tau')\right]\right\rangle$,
$G_{1,2}(\vec{r},\tau,\vec{r'},\tau') = -\left\langle T_\tau\left[\hat{\phi}(\vec{r},\tau)\hat{\phi}(\vec{r'},\tau')\right]\right\rangle$
and $G_{2,1}(\vec{r},\tau,\vec{r'},\tau')$ is obtained by replacing $\hat{\phi}$ by $\hat{\phi}^\dagger$ in $G_{1,2}(\vec{r},\tau,\vec{r'},\tau')$. In the Fourier transforms $G_{\alpha,\beta}(\vec{r},\vec{r'},\omega)$

and $\chi(\vec{r_1},\vec{r_2},\omega)$ the frequency ω takes on only the discrete values $\omega_n = 2n\pi/(\hbar\beta)$ where n is an integer. The physically meaningful retarded correlation function and Green's function can be constructed by a suitable analytic continuation [23]. We shall denote both the temperature and the retarded functions by the same symbol.

The proper part of a quantity (correlation function, Green's function etc.) will be denoted by a tilde over the corresponding symbol. The definition of the proper part directly implies that

$$\chi(\vec{r_1},\vec{r_2},\omega) = \tilde{\chi}(\vec{r_1},\vec{r_2},\omega) + \frac{1}{\hbar}\int d^3\vec{r_3}\int d^3\vec{r_4}\,\tilde{\chi}(\vec{r_1},\vec{r_4},\omega)v(\vec{r_4},\vec{r_3})\,\chi(\vec{r_3},\vec{r_2},\omega)\,, \quad (2)$$

Eq.(2) remains valid also for the corresponding retarded correlation functions (i.e., after analytic continuation). When $\chi(\vec{r_3},\vec{r_2},\omega)$ has a pole in ω (and $\tilde{\chi}(\vec{r_3},\vec{r_2},\omega)$ is nonsingular at that ω value),

$$\int d^3\vec{r_3}\left(\delta(\vec{r_1}-\vec{r_3}) - \frac{1}{\hbar}\int d^3\vec{r_4}\tilde{\chi}(\vec{r_1},\vec{r_4},\omega)v(\vec{r_4},\vec{r_3})\right) \times\xi(\vec{r_3}) = 0 \quad (3)$$

should hold, where $\xi(\vec{r_3})$ is an eigenfunction.

A remarkable feature of the Bose condensed system is the 'mixing' of correlation functions of different order, that is a consequence of the related symmetry breaking [4]- [8]. This is the basis of the dielectric formalism and can be expressed by the generalization of one of its basic relationships to inhomogeneous systems as

$$\tilde{\chi}(\vec{r_1},\vec{r_2},\omega) = \tilde{\chi}^{(r)}(\vec{r_1},\vec{r_2},\omega) + \int d^3\vec{r_3}\int d^3\vec{r_4}\tilde{\Lambda}_\alpha(\vec{r_1},\vec{r_3},\omega)\,\tilde{G}_{\alpha,\beta}(\vec{r_3},\vec{r_4},\omega) \times\Lambda_\beta(\vec{r_4},\vec{r_2},\omega)\,. \quad (4)$$

Here $\tilde{\chi}^{(r)}$ is the proper and irreducible regular part of the density correlation function, $\tilde{\Lambda}_\alpha$ stands for the proper part of the anomalous vertex Λ_α which is due to the presence of the condensate and represents the contribution of graphs with one outer particle line and one outer interaction line. $\tilde{G}_{\alpha,\beta}$ is the proper part of the Green's function. For repeated 'spinor' indices a summation is understood.

Eq.(4) allows us to derive the relation

$$\int d^3\vec{r_2}\int d^3\vec{r_3}\tilde{\Lambda}_\gamma(\vec{r_1},\vec{r_2},\omega)\tilde{G}_{\gamma,\beta}(\vec{r_2},\vec{r_3},\omega)G^{-1}_{\beta,\alpha}(\vec{r_3},\vec{r_4},\omega) = \int d^3\vec{r_2}\int d^3\vec{r_3}\tilde{\chi}(\vec{r_1},\vec{r_2},\omega)\chi^{-1}(\vec{r_2},\vec{r_3},\omega)\Lambda_\alpha(\vec{r_3},\vec{r_4},\omega) \quad (5)$$

Here the inverses are understood in the integral operator sense. This equation implies the coincidence of the eigenvalues of the density correlation functions and the Green's functions. The eigenvalue equation in case of the Green's functions is

$$\frac{1}{\hbar}\int d^3\vec{r_4}\tilde{G}_{\alpha,\beta}(\vec{r_1},\vec{r_4},\omega) \times\left(\Sigma_{\beta,\gamma}(\vec{r_4},\vec{r_3},\omega) - \tilde{\Sigma}_{\beta,\gamma}(\vec{r_4},\vec{r_3},\omega)\right)\varphi_\gamma(\vec{r_3}) = \varphi_\alpha(\vec{r_1})\,. \quad (6)$$

Here $\Sigma_{\beta,\gamma}$ stands for the (irreducible) self-energy, and $\tilde{\Sigma}_{\beta,\gamma}$ for its proper part. The eigenvectors ξ and φ_α belonging to the same eigenvalue ω are related by $\xi(\vec{r_1}) = \int d^3\vec{r_2}\Lambda_\alpha(\vec{r_1},\vec{r_2},\omega)\varphi_\alpha(\vec{r_2})$, or, the other way round,

$$\varphi_\alpha(\vec{r_1}) = \int d^3\vec{r_2}\int d^3\vec{r_3}\int d^3\vec{r_4}\tilde{G}_{\alpha,\beta}(\vec{r_1},\vec{r_2},\omega) \times\tilde{\Lambda}_\beta(\vec{r_2},\vec{r_3},\omega)v(\vec{r_3},\vec{r_4})\xi(\vec{r_4})\,. \quad (7)$$

Up to now we have given expressions that are valid in all order of the perturbation theory. Note that in the Bogolyubov approximation Eq.(6) can be transformed into the familiar Bogolyubov equations for u and $-v$, the components of φ_α. The same remains true in the finite temperature generalization of the Bogolyubov theory by Popov [24], [8].

We turn now to present a model based upon the general formalism introduced above and to work out the damping of the low energy excitations in this framework in the weak-coupling regime $< \hat{n} > g << k_BT$. Here $g = 4\,\pi\,\hbar^2\,a/m$, where a is the s-wave scattering length assumed to be positive and to describe the interaction between atoms at the relevant energies. The model arising is the generalization to nonzero external potential that of treated in detail for homogeneous system in [6].

The anomalous vertex Λ_α will be approximated by

$$\Lambda_\alpha(\vec{r_1},\vec{r_2},\omega) = \Phi_0(\vec{r_1})\delta(\vec{r_1}-\vec{r_2})\,, \quad (8)$$

where the condensate wave function $\Phi_0(\vec{r_1})$ is assumed to be real.

As for the proper Green's functions, we shall consider the approximation when

$$\tilde{G}_{1,2} = \tilde{G}_{2,1} = 0 \quad (9)$$

$$\left(\hbar\omega - \tilde{H}\right)\tilde{G}_{1,1}(\vec{r_1},\vec{r_2},\omega) = \hbar\delta(\vec{r_1}-\vec{r_2})\,. \quad (10)$$

Here $\tilde{H} = \hat{T} + U(\vec{r_1}) - \mu + g\Phi_0^2(\vec{r_1}) + 2\,g\,n_T(\vec{r_1})$ with $\hat{T} = -\frac{\hbar^2}{2\,m}\Delta$ standing for the operator of the kinetic energy and μ for the chemical potential. Further, $n_T(\vec{r}) = \left\langle\hat{\phi}^\dagger(\vec{r})\hat{\phi}(\vec{r})\right\rangle$ is the density of the noncondensate part. Note that $\tilde{G}_{2,2}(\vec{r_1},\vec{r_2},\omega) = \tilde{G}_{1,1}(\vec{r_2},\vec{r_1},-\omega)$. Eq.(10) can be derived when the Hartree-Fock terms are retained in the self-energy graphs for the contribution of thermally excited particles, which corresponds to the Popov approximation [24], [8].

Inserting Eqs.(4), (8) into Eq.(3) we get

$$\xi(\vec{r_1}) - \frac{g}{\hbar}\int d^3\vec{r_2}\tilde{\chi}^{(r)}(\vec{r_1},\vec{r_2},\omega)\xi(\vec{r_2}) - \frac{g}{\hbar}\phi_0(\vec{r_1})\int d^3\vec{r_2}\left[\tilde{G}_{1,1}(\vec{r_1},\vec{r_2},\omega) + \tilde{G}_{1,1}(\vec{r_2},\vec{r_1},-\omega)\right]\phi_0(\vec{r_2})\xi(\vec{r_2}) = 0\,. \quad (11)$$

Let us divide this equation by $\phi_0(\vec{r_1})$ and apply to it the operator $\left(\hbar\omega - \tilde{H}\right)\left(-\hbar\omega - \tilde{H}\right)$.

We get

$$2\,g\tilde{H}\Phi_0(\vec{r_1})\xi(\vec{r_1}) = \left(\hbar^2\omega^2 - \tilde{H}^2\right) \times \left(\frac{\xi(\vec{r_1})}{\Phi_0(\vec{r_1})} - \frac{g}{\hbar}\frac{1}{\Phi_0(\vec{r_1})}\int d^3\vec{r_2}\tilde{\chi}^{(r)}(\vec{r_1},\vec{r_2},\omega)\xi(\vec{r_2})\right) \quad (12)$$

The condensate wave function $\Phi_0(\vec{r})$ can be determined from the Gross-Pitaevskii equation [23]

$$\tilde{H}\Phi_0(\vec{r}) = 0 \quad (13)$$

Keeping only the term containing ω^2 on the r.h.s. of Eq.(12), neglecting $\tilde{\chi}^{(r)}$ and using Eq.(13), we arrive at

$$\omega_0^2\,\xi_0(\vec{r}) = -\frac{g}{m}\vec{\nabla}\left(\left(\Phi_0(\vec{r})\right)^2\,\vec{\nabla}\xi_0(\vec{r})\right)\,. \quad (14)$$

This amounts to the hydrodynamic approximation known to yield accurate values for the excitation frequences when $\hbar\omega << \mu$ [25], [26], [27]. Hereafter we shall be interested in this regime, and our aim is the calculation of the decay rate. This is determined in leading order by the term containing $\tilde{\chi}^{(r)}$ in Eq.(12). Therefore, we consider this term a perturbation and solve Eq.(12) perturbatively (still omitting the small term containing $\tilde{H}^2$ which does not influence the decay to this order).

We write the frequency as $\omega = \omega_0 + \omega_1$ where the correction ω_1 is supposed to be small compared to the leading term ω_0. Similarly, the eigenfunction is decomposed as $\xi(\vec{r}) = \xi_0(\vec{r}) + \xi_1(\vec{r})$.

Collecting the corrections we get in first order

$$2\,\omega_0\,\omega_1\xi_0(\vec{r_1}) - \omega_0^2\frac{g}{\hbar}\int d^3\vec{r_2}\tilde{\chi}^{(r)}(\vec{r_1},\vec{r_2},\omega_0)\xi_0(\vec{r_2}) = -\omega_0^2\,\xi_1(\vec{r}) - \frac{g}{m}\vec{\nabla}\left(\left(\Phi_0(\vec{r_1})\right)^2\,\vec{\nabla}\xi_1(\vec{r_1})\right)\,. \quad (15)$$

Multiplying Eq.(15) with $\xi_0(\vec{r_1})$ and integrating over $\vec{r_1}$ the r.h.s. of the equation identically vanishes (as the operator appearing in the hydrodynamic equation is a self-adjoint one), and we are left with an equation not containing $\xi_1(\vec{r})$ any longer, i.e., with an equation for ω_1 alone. It gives

$$\omega_1 = \frac{g\,\omega_0}{2\,\hbar}\frac{\int d^3\vec{r_1}\int d^3\vec{r_2}\xi_0^*(\vec{r_1})\tilde{\chi}^{(r)}(\vec{r_1},\vec{r_2},\omega_0)\xi_0(\vec{r_2})}{\int d^3\vec{r_1}|\xi_0(\vec{r_1})|^2}\,. \quad (16)$$

The damping is determined by the imaginary part of this expression. When evaluating Eq.(16) we apply the Thomas-Fermi approximation for the determination of $\Phi_0(\vec{r})$, as a relevant approximation in the regime where experiments are done. This means that in Eq.(13) we may neglect the kinetic energy term compared to the others. Moreover, when solving (14), the finiteness of the temperature will be taken into account only in the normalization condition of the condensate wave function. For a justification of this procedure see Ref. [28]. Thus we use $\left(\Phi_0(\vec{r})\right)^2 = \left(\mu_0 - U(\vec{r})\right)/g$ with $N_0/N = 1 - (T/T_c)^3$ where N and N_0 are the total and the condensate number of particles, respectively.

By inserting $\Phi_0(\vec{r})$ into Eq.(14) the zeroth order eigenfunction $\xi_0(\vec{r})$ is determined [26], [27] by separating Eq.(14) in oblate spherical coordinates and using a polynomial Ansatz.

The quantity $\tilde{\chi}^{(r)}(\vec{r_1},\vec{r_2},\omega)$ is approximated by the (dressed) loop $= \sum_n \tilde{G}_{\alpha,\beta}(\vec{r_1},\vec{r_2},\omega_n)\tilde{G}_{\beta,\alpha}(\vec{r_2},\vec{r_1},\omega_n-\omega)$ where the proper Green's function $\tilde{G}_{\alpha,\beta}(\vec{r_1},\vec{r_2},\omega_n)$ satisfies Eqs.(9) and (10). Note that according to (16) we need $\tilde{\chi}^{(r)}$ only inside the condensate. In the Thomas-Fermi approximation applied to $\tilde{G}$ one obtains for large condensate

$$\tilde{\chi}^{(r)}(\vec{r_1},\vec{r_2},\omega) = \frac{1}{(2\pi)^3}\int d^3\vec{k}e^{i\vec{k}(\vec{r_1}-\vec{r_2})}\tilde{\chi}^{(r)}(\vec{k},\omega)\,. \quad (17)$$

where $\tilde{\chi}^{(r)}(\vec{k},\omega)$ stands for the bubble graph with free propagators investigated in [6] in detail. This means that the spectrum related to $\tilde{G}$ is quasicontinuous in our approximation. For the damping we need only the imaginary part of $\tilde{\chi}^{(r)}(\vec{k},\omega)$, which can be calculated analytically [6].

The expression (16) for the damping was evaluated (using the above listed approximations) by Monte-Carlo integration, using 10^8 points for the numerator. The Fourier transform has previously been evaluated numerically. The error of the evaluation of the expression (16) was less than 1%. The weak coupling condition is satisfied if $T/T_c > 0.6$ taking the parameters of the JILA experiment [14]. At temperatures close to T_c the Thomas-Fermi approximation loses its validity. Choosing as an intermediate temperature $T/T_c = 0.7$ our result is $118\,s^{-1}$ $(115\,s^{-1})$ for the damping rate at $m = 0$ $(m = 2)$, where m is the value of the L_z angular momentum component, according to which the solutions of Eq.(14) can be classified due to the cylindrical symmetry. This agrees within experimental error with the measured value [14] and also with the result of [18] which was derived using approximations different from ours.

We have applied Eq.(3) with Eq.(4) in our calculation, i.e., treated the density fluctuations, which are directly measured. The Eqs.(5)-(7) of the dielectric formalism make possible to determine the corresponding parameters (not presented here) of the Green's functions $G_{\alpha,\beta}$ and the eigenfunctions φ_α when the temperature is below the critical one. A basic advantage of the dielectric formalism is that the decoupling of the density and one-particle fluctuation spectra can be followed when the temperature increases across T_c [6], a fact which has been exploited in case of liquid helium [10], [11]. In case of trapped Bose gases further experiments along these lines would help further developing the theory.

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