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LINEAR DENSITY RESPONSE IN THE RANDOM PHASE APPROXIMATION FOR CONFINED BOSE VAPOURS AT FINITE TEMPERATURE

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ABSTRACT

A linear response framework is set up for the evaluation of collective excitations in a confined vapour of interacting Bose atoms at finite temperature. Focusing on the currently relevant case of contact interactions between the atoms, the theory is developed within a random phase approximation with exchange. This approach is naturally introduced in a two-fluid description by expressing the density response of both the condensate and the non-condensate in terms of the response of a Hartree-Fock reference gas to the selfconsistent Hartree-Fock potentials. Such an approximate account of correlations (i) preserves an interplay between the condensate and the non-condensate through off-diagonal components of the response, which instead vanish in the Hartree-Fock-Bogolubov approximation; and (ii) yields a common resonant structure for the four partial response functions. The theory reduces to the temperature-dependent Hartree-Fock-Bogolubov-Popov approximation for the fluctuations of the condensate when its coupling with the density fluctuations of the non-condensate is neglected. Analytic results are presented which are amenable to numerical calculations and to inclusion of damping rates.

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1. Introduction

The achievement of Bose-Einstein condensation in trapped vapours of alkali atoms [1, 2, 3] is allowing one to probe properties of an inhomogeneuos dilute Bose gas which were not accessible earlier. In particular, the excitation of shape deformation modes in a regime for which there is no detectable non-condensate fraction [4, 5] has allowed tests of theoretical studies of the collective excitations based on a mean-field description of the condensate at zero-temperature [6]-[12]. An extension of the theory to finite temperature has also been given within the Hartree-Fock-Bogolubov approximation (HFBA), with an explicit calculation being performed for the case of isotropic harmonic confinement [13].

Very recently Jin *et al.* [14] have extended the experimental study of low-lying collective excitations to finite temperature. Their measurements were carried out on two modes with different angular momenta and show very striking dependences on temperature for both the mode frequencies and the damping rates. These authors stress the importance of an interplay between condensate and non-condensate as a potentially dissipative process which is not included in the usual mean-field theoretical models.

In this work we present what may be regarded as the first step in transcending a mean-field treatment at finite temperature. This is taken through inclusion of correlations via a random phase approximation with exchange (RPAE). Our approach is inspired to RPA theories of the linear density response in homogeneous quantal fluids [15, 16, 17], which construct the response of the interacting system to weak external perturbations via the response of an ideal reference gas to selfconsistent Hartree potentials. However, in the experimentally relevant situation for the confined Bosecondensed systems we need to include exchange in the selfconsistent potentials set up by density fluctuations in both the condensate and the non-condensate. The requirement of consistency between the equilibrium state and the fluctuations around it then leads us to choose a Hartree-Fock gas as a reference system. This choice also permits us to regain the HFBA limit at finite temperature when the non-condensate fluctuations are neglected.

The layout of the paper is briefly as follows. Section 2 sets out some general aspects of linear density response theory for a two-component system representing an inhomogeneous Bose system in the presence of a condensate. After an evaluation in Section 3 of the density response functions in the HFBA, Section 4 introduces the finite-temperature RPAE for the case of contact interactions between the particles and discusses a general method of solution of the RPAE integral equations in order to display the resonant structure of the partial density response functions. Section 5 derives the RPAE equations by an equation-of-motion approach and elaborates the choice of the reference gas, leaving the comparison with the HFBA theory to an appendix. Finally, Section 6 contains a summary of the results and a discussion of further developments.

2. Linear density response functions

We consider a confined system of Bose particles described by the Hamiltonian H_0 , which is subjected to an external perturbation represented by a scalar potential $U_p(\mathbf{r}, t)$. The perturbation Hamiltonian is

$$H(t) = \int d^3r \,\hat{n}(\mathbf{r}) \, U_p(\mathbf{r}, t) \tag{1}$$

where $\hat{n}(\mathbf{r}) = \hat{\Psi}^{\dagger}(\mathbf{r})\hat{\Psi}(\mathbf{r})$ is the particle density operator and $\hat{\Psi}(\mathbf{r})$ is the field operator. The density change to first order in the perturbation is given by

$$\delta n(\mathbf{r},t) = i \int_{-\infty}^{t} dt' \int d^{3}r' \langle [\hat{n}(\mathbf{r}',t'), \hat{n}(\mathbf{r},t)] \rangle_{eq} U_{p}(\mathbf{r}',t')$$

$$\equiv \int_{-\infty}^{\infty} dt' \int d^{3}r' \chi_{nn}(\mathbf{r},\mathbf{r}';t-t') U_{p}(\mathbf{r}',t') \quad , \qquad (2)$$

defining the linear density response function $\chi_{nn}(\mathbf{r}, \mathbf{r}'; t - t')$. In equation (2) we have set $\hat{n}(\mathbf{r}, t) = \exp(iH_0 t) \hat{n}(\mathbf{r}) \exp(-iH_0 t)$ ($\hbar = 1$) and have assumed that the system was initially at equilibrium. $\langle \hat{O} \rangle_{eq}$ denotes the statistical expectation value of the operator \hat{O} in the equilibrium ensemble.

In the presence of a condensate, the field operator $\hat{\Psi}(\mathbf{r},t)$ is split into the sum of the condensate wavefunction $\Phi(\mathbf{r},t) = \langle \hat{\Psi}(\mathbf{r},t) \rangle$ and of the field operator $\tilde{\Psi}(\mathbf{r},t)$ for the non-condensate. The density response function is then given as the sum of four components,

$$\chi_{nn}(\mathbf{r},\mathbf{r}';t) = \chi_{cc}(\mathbf{r},\mathbf{r}';t) + \chi_{c\bar{n}}(\mathbf{r},\mathbf{r}';t) + \chi_{\bar{n}c}(\mathbf{r},\mathbf{r}';t) + \chi_{\bar{n}\bar{n}}(\mathbf{r},\mathbf{r}';t)$$
(3)

where

$$\chi_{cc}(\mathbf{r}, \mathbf{r}'; t) = i\theta(t) \left(\Phi_{eq}^{*}(\mathbf{r}') \Phi_{eq}(\mathbf{r}, t) \langle \left[\tilde{\Psi}(\mathbf{r}'), \tilde{\Psi}^{\dagger}(\mathbf{r}, t) \right] \rangle_{eq} + H.c. \right) + i\theta(t) \left(\Phi_{eq}(\mathbf{r}') \Phi_{eq}(\mathbf{r}, t) \langle \left[\tilde{\Psi}^{\dagger}(\mathbf{r}'), \tilde{\Psi}^{\dagger}(\mathbf{r}, t) \right] \rangle_{eq} + H.c. \right) , \qquad (4)$$

$$\chi_{c\tilde{n}}(\mathbf{r},\mathbf{r}';t) = i\theta(t) \left(\Phi_{eq}^{*}(\mathbf{r},t) \langle \left[\tilde{\Psi}^{\dagger}(\mathbf{r}')\tilde{\Psi}(\mathbf{r}'),\tilde{\Psi}(\mathbf{r},t)\right] \rangle_{eq}\right) - H.c. , \qquad (5)$$

$$\chi_{\tilde{n}c}(\mathbf{r},\mathbf{r}';t) = i\theta(t) \left(\Phi_{eq}^{*}(\mathbf{r}')\langle \left[\tilde{\Psi}(\mathbf{r}'),\tilde{\Psi}^{\dagger}(\mathbf{r},t)\tilde{\Psi}(\mathbf{r},t)\right]\rangle_{eq}\right) - H.c , \qquad (6)$$

and

$$\chi_{\tilde{n}\tilde{n}}(\mathbf{r},\mathbf{r}';t) = i\theta(t) \langle \left[\tilde{\Psi}^{\dagger}(\mathbf{r}')\tilde{\Psi}(\mathbf{r}'), \tilde{\Psi}^{\dagger}(\mathbf{r},t)\tilde{\Psi}(\mathbf{r},t) \right] \rangle_{eq} \quad .$$
(7)

Here, *H.c.* denotes the Hermitian conjugate. These equations define a two-by-two matrix of response functions for the inhomogeneous two-component fluid. Within the linear response regime the condensate wavefunction in (4)-(7) is the equilibrium one, with $\Phi_{eq}(\mathbf{r}, t) = \Phi_{eq}(\mathbf{r}) \exp(-i\mu t)$ and μ being the chemical potential.

A more standard approach in linear response theory for a Bose fluid in the presence of a condensate would actually consider applying an external scalar potential $U_p(\mathbf{r}, t)$ coupled to the total density and a gauge-breaking field $\eta_p(\mathbf{r}, t)$ coupled to the field operator $\hat{\Psi}(\mathbf{r})$ through the perturbation Hamiltonian

$$H(t) = \int d^3r \left[U_p(\mathbf{r}, t) \hat{\Psi}^{\dagger}(\mathbf{r}) \hat{\Psi}(\mathbf{r}) + \eta_p(\mathbf{r}, t) \hat{\Psi}^{\dagger}(\mathbf{r}) + \eta_p^*(\mathbf{r}, t) \hat{\Psi}(\mathbf{r}) \right]$$
(8)

(for the case of a homogeneous fluid see Griffin [16]). The change in total density is in this case given by

$$\delta n(\mathbf{r},t) = \Phi_{eq}(\mathbf{r},t)\delta\langle\hat{\Psi}^{\dagger}(\mathbf{r},t)\rangle + \Phi_{eq}^{*}(\mathbf{r},t)\delta\langle\hat{\Psi}(\mathbf{r},t)\rangle + \delta\tilde{n}(\mathbf{r},t)$$
(9)

Explicit evaluation of the first-order changes induced in the field operator and in the non-condensate density in equation (9) shows that this formalism yields the same results as in equations (2)-(7), provided that

$$\eta_p(\mathbf{r},t) = U_p(\mathbf{r},t)\Phi_{eq}(\mathbf{r},t) \quad . \tag{10}$$

We shall in the following adopt the two-fluids framework set out in equations (1)-(7), which will allow us to treat the condensate and the non-condensate on the same basis. However, at some later stage it will be convenient to adopt the expedient of considering the application of different external scalar potentials to the two components of the fluid, for the purpose of separately determining the four partial density response functions in equation (3).

3. Density response in the Hartree-Fock-Bogolubov approximation

In the HFBA [18] the field operator for the non-condensate is expanded in terms of normal modes,

$$\tilde{\Psi}(\mathbf{r},t) = \sum_{j} \left[u_{j}(\mathbf{r})e^{-iE_{j}t}\hat{\alpha}_{j} - v_{j}^{*}(\mathbf{r})e^{iE_{j}t}\hat{\alpha}_{j}^{\dagger} \right]$$
(11)

where $\hat{\alpha}_j$ and $\hat{\alpha}_j^{\dagger}$ are the quasiparticle annihilation and creation operators, u_j and v_j are the quasiparticle amplitudes and E_j are the excited state energies. These operators satisfy the canonical commutation relations and their average on the system at equilibrium is given by the Bose factor $f(E_j)$,

$$\langle \hat{\alpha}_j^{\dagger} \hat{\alpha}_k \rangle_{eq} = \delta_{j,k} \left(e^{\beta(E_j - \mu)} - 1 \right)^{-1} \equiv f(E_j) \delta_{j,k}$$
(12)

with $\beta = (k_B T)^{-1}$.

The partial density response functions are easily evaluated by using quasiparticle amplitudes given by the HFBA, with the following results:

$$\chi_{cc}(\mathbf{r}, \mathbf{r}'; t) = i\theta(t) \left\{ \Phi_{eq}^*(\mathbf{r}') \Phi_{eq}(\mathbf{r}, t) \sum_j \left(u_j(\mathbf{r}') u_j^*(\mathbf{r}) e^{iE_j t} - v_j^*(\mathbf{r}') v_j(\mathbf{r}) e^{-iE_j t} \right) - H.c. + \Phi_{eq}(\mathbf{r}') \Phi_{eq}(\mathbf{r}, t) \sum_j \left(u_j^*(\mathbf{r}') v_j(\mathbf{r}) e^{-iE_j t} - v_j(\mathbf{r}') u_j^*(\mathbf{r}) e^{iE_j t} \right) - H.c. \right\}, \quad (13)$$

$$\chi_{\hat{n}\hat{n}}(\mathbf{r},\mathbf{r}';t) = i\theta(t) \left\{ \sum_{j,k} h_{jk} \left[e^{-i(E_j - E_k)t} u_j^*(\mathbf{r}') u_k(\mathbf{r}') (u_k^*(\mathbf{r}) u_j(\mathbf{r}) + v_j(\mathbf{r}) v_k^*(\mathbf{r})) - e^{i(E_j - E_k)t} v_j(\mathbf{r}') v_k^*(\mathbf{r}') (u_j^*(\mathbf{r}) u_k(\mathbf{r}) + v_k(\mathbf{r}) v_j^*(\mathbf{r})) \right] + \sum_{j,k} f_{jk} \left[e^{-i(E_j + E_k)t} v_j(\mathbf{r}') u_k(\mathbf{r}') (u_k^*(\mathbf{r}) v_j^*(\mathbf{r}) + u_j^*(\mathbf{r}) v_k^*(\mathbf{r})] - H.c. \right\}$$
(14)

and

$$\chi_{\bar{n}c}(\mathbf{r},\mathbf{r}';t) = 0 , \qquad (15)$$

$$\chi_{c\tilde{n}}(\mathbf{r},\mathbf{r}';t) = 0.$$
⁽¹⁶⁾

Here, $h_{jk} = f(E_j) - f(E_k)$ and $f_{jk} = 1 + f(E_j) + f(E_k)$. These expressions are fully determined since $\Phi_{eq}(\mathbf{r}, t)$ satisfies the Gross-Pitaevskii equation with eigenvalue μ , while $u_j(\mathbf{r})$ and $v_j(\mathbf{r})$ at energy E_j satisfy the Bogolubov equations in the Popov approximation [18].

As is evident from the structure of equations (13)-(16), the HFBA treats the excitations of the condensate independently of those of the non-condensate. We briefly point out below, for the sake of completeness, how results already known for the condensate can be recovered from equation (13). We then discuss the predictions made by the HFBA in equation (14) for the excitations of the non-condensate.

3.1. Oscillations of the condensate

The density change of the condensate is given in the HFBA by the response function χ_{cc} and consists of two terms describing the excitation of particles out of the condensate (first term in equation (13)) and their de-excitation (second term in equation (13)).

With the notation

$$\langle \langle u_j | U_p | \Phi_{eq} \rangle \rangle \equiv i \int_{-\infty}^t dt' \int d^3 r' \ e^{iE_j t'} u_j^*(\mathbf{r}') U_p(\mathbf{r}', t') \Phi_{eq}(\mathbf{r}')$$
(17)

etcetera, we have for the excitation term the expression

$$\delta n_c^{exc}(\mathbf{r},t) = -\Phi_{eq}^*(\mathbf{r},t) \sum_j \left[u_j(\mathbf{r}) e^{-iE_j t} \langle \langle u_j | U_p | \Phi_{eq} \rangle \rangle - v_j^*(\mathbf{r}) e^{iE_j t} \langle \langle v_j^* | U_p | \Phi_{eq} \rangle \rangle \right].$$
(18)

In equation (18) we recognize the typical structure $\delta n_c^{exc} \propto \Phi_{eq}^*(u_j - v_j)$ [19] and the existence of selection rules such as used by Dodd *et al.* [20] to evaluate the excitations of the condensate in the presence of vortices. With the same notation the de-excitation part is given by

$$\delta n_c^{de-exc}(\mathbf{r},t) = -\Phi_{eq}^*(\mathbf{r},t) \sum_j \left[v_j^*(\mathbf{r}) e^{iE_j t} \langle \langle \Phi_{eq} | U_p | u_j \rangle \rangle - u_j(\mathbf{r}) e^{-iE_j t} \langle \langle \Phi_{eq} | U_p | v_j^* \rangle \rangle \right].$$
(19)

The excitation energies $E_j - \mu$ correspond to resonances in $\chi_{cc}(\mathbf{r}, \mathbf{r}'; \omega)$. In relation to experiments [4, 5, 14], the HFBA results account for the observed eigenfrequencies of harmonically confined condensates at zero temperature [6]-[11], but do not seem to account for their observed temperature dependence [13]. Of course, as a mean field theory the HFBA does not include damping of the modes.

3.2. Oscillations of the non-condensate

The oscillations of the non-condensate are described by the $\tilde{n}-\tilde{n}$ response function given in the HFBA by equation (14). It is seen from that equation that these oscillations are of two types, corresponding to the excitation of single quasiparticles (first and second term in equation (14)) and of pairs of quasiparticles (third term in equation (14)). The density change of the non-condensate associated with the former type of excitations is

$$\delta \tilde{n}^{(1)}(\mathbf{r},t) = \sum_{j,k} (f(E_j) - f(E_k)) \left((u_k^*(\mathbf{r})u_j(\mathbf{r}) + v_j(\mathbf{r})v_k^*(\mathbf{r})) \left\langle \left\langle u_j | U_p | u_k \right\rangle \right\rangle e^{-i(E_j - E_k)t} - \left(u_j^*(\mathbf{r})u_k(\mathbf{r}) + v_k(\mathbf{r})v_j^*(\mathbf{r}) \right) \left\langle \left\langle v_j^* | U_p | v_k^* \right\rangle \right\rangle e^{i(E_j - E_k)t} \right)$$
(20)

For the two-quasiparticle excitation process we have

$$\delta \tilde{n}^{(2)}(\mathbf{r},t) = \sum_{j,k} (1 + f(E_j) + f(E_k)) \left((u_k^*(\mathbf{r})v_j^*(\mathbf{r}) + u_j^*(\mathbf{r})v_k^*(\mathbf{r})) \left\langle \left\langle v_j^* | U_p | u_k \right\rangle \right\rangle e^{i(E_j + E_k)t} - \left(v_k(\mathbf{r})u_j(\mathbf{r}) + v_j(\mathbf{r})u_k(\mathbf{r}) \right) \left\langle \left\langle u_j | U_p | v_k^* \right\rangle \right\rangle e^{-i(E_j + E_k)t} \right)$$
(21)

From equation (21) we remark that the two-particle process in the HFBA vanishes in the dilute-gas limit at zero temperature.

In the recent experiments of Jin *et al.* [14] two discrete eigenfrequencies of the noncondensate have been observed. For temperatures higher than T_c these excitations are to a good approximation described by equation (20) evaluated in the ideal-gas limit. This is perhaps not surprising, since the non-condensate is in a very dilute regime. The same approximation seems to hold for the eigenfrequencies of the non-condensate even in a limited range of temperatures below T_c , in which the HFBA fails to account for the eigenfrequencies of the condensate.

4. Random phase approximation

Here and in the following sections we develop an approach invoking a random phase approximation with inclusion of exchange (RPAE). Its main feature is that it treats the dynamics of condensate and non-condensate fluctuations on the same footing.

The need to include the dynamics of non-condensate fluctuations into the theory comes from the aforementioned experimental observations of Jin *et al.* [14] of *both* condensate *and* non-condensate normal modes. In this spirit, Zaremba *et al.* [21] have recently pioneered an approach which develops hydrodynamic equations including a time-dependent non-condensate density. By allowing the non-condensate to fluctuate, it is possible to satisfy the generalized Kohn theorem [22] and to obtain the analogue of "second sound" as an out-of-phase fluctuation of condensate and non-condensate densities.

The RPAE works in the linear response regime and does not include the damping mechanism due to nonlinear interactions between the condensate modes (these large amplitude effects are instead contained in the time-dependent Gross-Pitaevskii equation [23, 24]). However, the RPAE keeps into account the coupling between the dynamics of the condensate and that of the non-condensate. This mechanism is thought to be important for an explanation of the behaviour of the observed frequency shifts with temperature. We support this by noticing that these shifts become significant when the temperature of the system becomes of the order of the chemical potential, that is when the non-condensate cloud starts being significantly populated.

In order to define the RPAE for the specific system of an inhomogeneous Bosecondensed gas, we introduce at this point a matrix of "proper susceptibilities" $\bar{\chi}$, by analogy with a well known approach to homogeneous fluids [15, 17]. This matrix relates the density changes of the condensate and the non-condensate to the selfconsistent Hartree-Fock potentials. We write the latter in the form

$$U_{HF}^{c}(\mathbf{r},t) = U_{p}^{c}(\mathbf{r},t) + \alpha \,\delta n_{c}(\mathbf{r},t) + 2\alpha \,\delta \tilde{n}(\mathbf{r},t)$$
⁽²²⁾

and

$$U_{HF}^{\tilde{n}}(\mathbf{r},t) = U_{p}^{\tilde{n}}(\mathbf{r},t) + 2\alpha \,\delta n_{c}(\mathbf{r},t) + 2\alpha \,\delta \tilde{n}(\mathbf{r},t) \quad .$$
⁽²³⁾

We are using different external scalar potentials for the two components of the fluid, as a device to determine the four partial density response functions. Furthermore, we are considering the special case of contact interactions between the particles, with $\alpha = 4\pi\hbar^2 a/m$ where a is the scattering length and m is the particle mass.

The RPAE follows naturally by evaluating the diagonal elements of $\bar{\chi}$ from a suitably chosen "reference" gas and by setting its off-diagonal elements equal to zero. As we shall see explicitly below, the latter approximation on $\bar{\chi}$ still preserves the off-diagonal elements of the response matrix of the fluid.

After Fourier transform with respect to the time variable the RPAE equations thus read

$$\delta n_c(\mathbf{r},\omega) = \int d^3 r' \,\chi_c^0(\mathbf{r},\mathbf{r}';\omega) \left(U_p^c(\mathbf{r}',\omega) + \alpha \delta n_c(\mathbf{r}',\omega) + 2\alpha \delta \tilde{n}(\mathbf{r}',\omega) \right) \tag{24}$$

and

$$\delta \tilde{n}(\mathbf{r},\omega) = \int d^3 r' \,\chi_{\tilde{n}}^0(\mathbf{r},\mathbf{r}';\omega) \left(U_p^{\tilde{n}}(\mathbf{r}',\omega) + 2\alpha \delta n_c(\mathbf{r}',\omega) + 2\alpha \delta \tilde{n}(\mathbf{r}',\omega) \right). \tag{25}$$

In these equations χ_c^0 and $\chi_{\bar{n}}^0$ are the density response functions of the condensate and non-condensate components of the reference gas.

The choice of the reference gas will be discussed in the next section. Here, instead, we want to display the general structure of the solution of equations (24) and (25). A formal solution can be obtained by expansion into a complete orthonormal set of basis functions, so as to convert the problem into one of matrix inversion, and by comparison of the results with equations (2) and (3) (extended to the case of two different scalar

potentials). The results for the density response functions in matrix notation are as follows:

$$\chi_{cc} = \left(1 - 2\alpha\chi_{\tilde{n}}^{0}\right) \left[\left(1 - \alpha\chi_{c}^{0}\right) \left(1 - 2\alpha\chi_{\tilde{n}}^{0}\right) - 4\alpha^{2}\chi_{c}^{0}\chi_{\tilde{n}}^{0} \right]^{-1}\chi_{c}^{0}$$

$$(26)$$

$$\chi_{c\tilde{n}} = 2\alpha \chi_c^0 \left[\left(1 - \alpha \chi_c^0 \right) \left(1 - 2\alpha \chi_{\tilde{n}}^0 \right) - 4\alpha^2 \chi_c^0 \chi_{\tilde{n}}^0 \right]^{-1} \chi_{\tilde{n}}^0$$

$$\tag{27}$$

$$\chi_{\tilde{n}c} = 2\alpha \chi_{\tilde{n}}^{0} \left[\left(1 - \alpha \chi_{c}^{0} \right) \left(1 - 2\alpha \chi_{\tilde{n}}^{0} \right) - 4\alpha^{2} \chi_{c}^{0} \chi_{\tilde{n}}^{0} \right]^{-1} \chi_{c}^{0}$$

$$\tag{28}$$

and

$$\chi_{\tilde{n}\tilde{n}} = \left(1 - \alpha \chi_c^0\right) \left[\left(1 - \alpha \chi_c^0\right) \left(1 - 2\alpha \chi_{\tilde{n}}^0\right) - 4\alpha^2 \chi_c^0 \chi_{\tilde{n}}^0 \right]^{-1} \chi_{\tilde{n}}^0 \tag{29}$$

The appearance of a common "denominator" in the expressions (26)-(29) reflects the fact that the RPA is in general leading to collective excitations of the system as a whole.

5. Equation-of-motion approach to the random phase approximation with exchange

At this point we need to specify the reference gas to be adopted in the RPAE for the inhomogeneous Bose fluid. The reference system is to be described by a set of single-particle orbitals and energy levels. In the case of a homogeneous Bose fluid, translational symmetry forces the choice of a plane-wave set of orbitals. Furthermore, contact interactions in k-space merely add a constant term to the energy. As we shall elaborate in the discussion below, we believe that an optimal choice of the reference system for the inhomogeneous fluid in the RPAE is provided by the Hartree-Fock theory (HFA). This choice (i) allows consistency between the treatment of the equilibrium state and that of the fluctuations around it, and (ii) yields results which in the appropriate limit reduce to the HFBA treatment for the condensate at finite temperature in the Popov approximation (see Appendix A).

We begin by examining the equations of motion for the condensate wavefunction $\Phi(\mathbf{r}, t)$ and for the non-condensate field operator $\tilde{\Psi}(\mathbf{r}, t)$ within the Hartree-Fock approximation. These are [25]:

$$i\frac{\partial}{\partial t}\Phi = \left(-\frac{\nabla^2}{2m} + V_e + \alpha |\Phi|^2 + 2\alpha \tilde{n}\right)\Phi + U_p^c \Phi$$
(30)

and

$$i\frac{\partial}{\partial t}\tilde{\Psi} = \left(-\frac{\nabla^2}{2m} + V_e + 2\alpha|\Phi|^2 + 2\alpha\tilde{n}\right)\tilde{\Psi} + U_p^{\tilde{n}}\tilde{\Psi} .$$
(31)

In the above equations we have defined the non-condensate density as $\tilde{n} = \langle \Psi^{\dagger} \Psi \rangle$. In the case of weak external perturbations the equations can be linearized to read

$$\left(i\frac{\partial}{\partial t} + \frac{\nabla^2}{2m} - V_e - \alpha |\Phi_{eq}|^2 - 2\alpha \tilde{n}_0\right)\delta\Phi = \left(U_p^c + \alpha\delta n_c + 2\alpha\delta\tilde{n}\right)\Phi_{eq} \quad (32)$$

and

$$\left(i\frac{\partial}{\partial t} + \frac{\nabla^2}{2m} - V_e - 2\alpha|\Phi_{eq}|^2 - 2\alpha\tilde{n}_0\right)\delta\tilde{\Psi} = \left(U_p^{\tilde{n}} + 2\alpha\delta n_c + 2\alpha\delta\tilde{n}\right)\tilde{\Psi}_{eq}$$
(33)

where we have set $\delta n_c = \delta |\Phi|^2$. By operator inversion we find

$$\delta \Phi = G_0^{GP} \left(U_p^c + \alpha \delta n_c + 2\alpha \delta \tilde{n} \right) \Phi_{eq}$$
(34)

and

$$\delta \tilde{\Psi} = G_0^{HF} \left(U_p^c + 2\alpha \delta n_c + 2\alpha \delta \tilde{n} \right) \tilde{\Psi}_{eq} \,. \tag{35}$$

With G_0 we have indicated the Green's functions in the Gross-Pitaevskii (GP) or Hartree-Fock (HF) approximations and have left implicit the convolution integral required in the inversion.

The structure of equations (34) and (35) can now be compared with that of equations (24) and (25). It is evident that, in order to obtain a consistent treatment, we need to construct the reference gas susceptibilities χ_c^0 and χ_n^0 with single particle orbitals which are eigenvectors of the Gross-Pitaevskii operator and of the Hartree-Fock operator, respectively. Although both the condensate and the non-condensate are thereby being consistently treated in the Hartree-Fock theory, this will necessarily lead to the use of different single-particle orbitals and energy levels in the evaluation of the two reference-gas susceptibilities. This is a peculiarity of the Bose-condensed system, which comes from the fact that there is no exchange in the condensate.

We come now to a more detailed derivation of the RPAE equations, using the equation of motion for the density matrix as in the treatment of the Fermi fluid given by Singwi *et al.* [26]. In a Bose-condensed system the density matrix of the non-condensate is defined as

$$\tilde{\rho}(\mathbf{r},\mathbf{r}',t) = \langle \Psi^{\dagger}(\mathbf{r},t)\Psi(\mathbf{r}',t)\rangle - \Phi^{*}(\mathbf{r},t)\Phi(\mathbf{r}',t) = \langle \tilde{\Psi}^{\dagger}(\mathbf{r},t)\tilde{\Psi}(\mathbf{r}',t)\rangle .$$
(36)

We also introduce a parallel quantity for the condensate as

$$\rho_c(\mathbf{r}, \mathbf{r}', t) = \Phi^*(\mathbf{r}, t)\Phi(\mathbf{r}', t) . \qquad (37)$$

Of course, the factorized form of ρ_c shows that this is not a true density matrix, but merely a convenient device allowing a "two-fluid" visualization.

In the occupation-number basis [25] we express the non-condensate field operator as

$$\tilde{\Psi}(\mathbf{r},t) = \sum_{j} \langle \mathbf{r} | j \rangle \hat{c}_{j}(t)$$
(38)

and the condensate wavefunction as

$$\Phi(\mathbf{r},t) = \sum_{j} \langle \mathbf{r} | j \rangle z_j(t) .$$
(39)

The functions introduced in (36) and (37) become

$$\rho_{ij} \equiv \langle i | \tilde{\rho} | j \rangle = \langle \hat{c}_j^{\dagger} \hat{c}_i \rangle \tag{40}$$

and

$$\langle i|\rho_{\rm c}|j\rangle = z_j^* z_j \ . \tag{41}$$

5.1. RPAE equation for the non-condensate

The equation of motion for the non-condensate density matrix in the HFA is [25]

$$i\frac{\partial}{\partial t}\tilde{\rho}_{ij} = \sum_{r} h_{ir}^{HF}\tilde{\rho}_{rj} - \tilde{\rho}_{ir}h_{rj}^{HF} + U_{ir}^{\tilde{n}}\tilde{\rho}_{rj} - \tilde{\rho}_{ir}U_{rj}^{\tilde{n}}$$
(42)

where h_{ij}^{HF} is the HF single particle Hamiltonian expressed in the occupation number basis,

$$h_{ij}^{HF} = \langle i| - \frac{\nabla^2}{2m} + V_e|j\rangle + 2\sum_{k,l} \langle ik|v|lj\rangle (z_k^* z_l + \tilde{\rho}_{kl}) .$$

$$\tag{43}$$

By linearizing the time-Fourier transform of equation (42) in the HF single particle basis (eigenfunctions $\psi_j(\mathbf{r})$ with eigenvalues ϵ_j) we obtain

$$(\omega - (\epsilon_i - \epsilon_j) + i\eta)\delta\tilde{\rho}_{ij} = (f(\epsilon_i) - f(\epsilon_j))\left(U_{ij}^{\tilde{n}} + 2\sum_{k,l}\langle ik|v|lj\rangle(\delta(z_k^*z_l) + \delta\tilde{\rho}_{kl})\right)$$
(44)

where we have set $\tilde{\rho}_{ij}^0 = f(\epsilon_j)\delta_{i,j}$ for the equilibrium density matrix, with *i* and *j* different from zero since it describes the excited states, and we have introduced a factor $\eta = 0^+$ to allow for an adiabatic turning on of the external potential.

In order to come back to the real space description we recall that the non-condensate density has been expanded as

$$\delta \tilde{n}(\mathbf{r},\omega) = \sum_{ij} \psi_i(\mathbf{r}) \psi_j^*(\mathbf{r}) \delta \tilde{\rho}_{ij} , \qquad (45)$$

while the condensate density is given by

$$\delta n_c = \sum_{ij} \psi_i(\mathbf{r}) \psi_j^*(\mathbf{r}) \delta(z_j^* z_i) ; \qquad (46)$$

moreover for contact interactions we find

$$\sum_{kl} \langle ik | v | lj \rangle (\delta(z_k^* z_l) + \delta \tilde{\rho}_{kl}) = \alpha \sum_{kl} \int d^3 r' \psi_i^* \psi_k^* \psi_j \psi_l (\delta(z_k^* z_l) + \delta \tilde{\rho}_{kl})$$
$$= \alpha \int d^3 r' \psi_i^* \psi_j (\delta n_c + \delta \tilde{n}) .$$
(47)

If we now express the reference response function for the non-condensate as

$$\chi_{\tilde{n}}^{0}(\mathbf{r},\mathbf{r}',\omega) = \sum_{j\neq 0,k\neq 0} \frac{f(\epsilon_{k}) - f(\epsilon_{j})}{\omega - (\epsilon_{j} - \epsilon_{k}) + i\eta} \psi_{j}^{*}(\mathbf{r}')\psi_{j}(\mathbf{r})\psi_{k}^{*}(\mathbf{r})\psi_{k}(\mathbf{r}') , \qquad (48)$$

by using the relations (45-48) in the sum over all the modes of (44) we obtain

$$\sum_{i,j} \psi_j^*(\mathbf{r}) \psi_i(\mathbf{r}) \delta \tilde{\rho}_{ij} = \int d^3 r' \chi_{\tilde{n}}^0(\mathbf{r}, \mathbf{r}', \omega) \left(U_p^{\tilde{n}} + 2\alpha (\delta n_c + \delta \tilde{n}) \right) .$$
(49)

This is equation (25), with $\chi_{\tilde{n}}^0$ given by equation (48).

5.2. RPAE equation for the condensate

The derivation of the RPAE equation for the condensate follows the same lines as that for the non-condensate, with some differences that we wish to remark. The HFA equation of motion for ρ_c in the occupation number basis is

$$i\frac{\partial}{\partial t}\rho_{ij}^c = \sum_r h_{ir}^{GP}\rho_{rj}^c - \rho_{ir}^c h_{rj}^{GP} + U_{ir}^c \rho_{rj}^c - \rho_{ir}^c U_{rj}^c$$
(50)

where h_{ij}^{GP} is the Gross-Pitaevskii single particle Hamiltonian

$$h_{ij}^{GP} = \langle i| -\frac{\nabla^2}{2m} + V_e|j\rangle + \sum_{k,l} \langle ik|v|lj\rangle (z_k^* z_l + 2\tilde{\rho}_{kl}) .$$
(51)

One must choose the eigenstates of the Gross-Pitaevskii operator ($\phi_i(\mathbf{r})$, say, with e_i denoting the corresponding energy levels) in order to diagonalize the equation of motion for the condensate.

Within the same scheme the equilibrium density matrix for the condensate is $(z_j^* z_i)_0 = \delta_{i,0} \delta_{j,0} N_0$, where N_0 is the condensate fraction, depending on temperature as determined from a thermodynamic treatment [27, 28]. The linear fluctuation of ρ_c then is $\delta \rho_{ij}^c = \delta \rho_{0j}^c \delta_{i,0} + \delta \rho_{i0}^c \delta_{j,0}$. With these definitions, the linearized Fourier transform of equation (50) is:

$$(\omega - (e_i - \mu) + i\eta)\delta\rho_{i0}^c \,\delta_{j,0} + (\omega + (e_j - \mu))\delta\rho_{0j}^c \,\delta_{i,0} =$$
(52)
= $N_0(\delta_{j,0} - \delta_{i,0}) \left(U_{ij}^c + \sum_{k,l} \langle ik|v|lj \rangle (\delta(z_k^* z_l) + 2\delta\tilde{\rho}_{kl}) \right) .$

It is now easy to go back to the real-space equation (24) by using the expression of the condensate density,

$$\delta n_c = \sum_{i \neq 0} \left(z_i \phi_0^* \phi_i + z_i^* \phi_0 \phi_i^* \right)$$
(53)

and of the condensate reference susceptibility,

$$\chi_c^0(\mathbf{r}, \mathbf{r}', \omega) = \sum_{j \neq 0} \left(\frac{N_0}{\omega - (e_j - \mu) + i\eta} \phi_0(\mathbf{r}') \phi_0^*(\mathbf{r}) \phi_j(\mathbf{r}) \phi_j^*(\mathbf{r}') - \frac{N_0}{\omega + e_j - \mu + i\eta} \phi_0(\mathbf{r}) \phi_0^*(\mathbf{r}') \phi_j(\mathbf{r}') \phi_j^*(\mathbf{r}) \right) .$$
(54)

In summary, equations (48) and (54) give the susceptibilities of the reference gas in the RPAE. They involve the Hartree-Fock and the Gross-Pitaevskii orbitals and energy levels, respectively. It can also be shown that from equations (42) and (50) the HF theory leads to hydrodynamic-like equations for the particle densities and current densities, of a form which ensures that the generalized Kohn theorem [22] is satisfied (Minguzzi and Tosi, to be published).

6. Summary and future directions

We have in this work set up an RPAE formalism for the collective dynamics of an inhomogeneous Bose gas at finite temperature. The system is treated within the linear response theory as a "two-component fluid", the components being the condensate and the non-condensate.

The RPAE assumes that the fluid responds to the self-consistent Hartree-Fock potentials via the response functions of a Hartree-Fock gas. This ensures consistency between the treatment of the equilibrium state and that of its deformations induced by external perturbations. It also ensures that the HFB-Popov theory is regained when the coupling with the fluctuations of the non-condensate is neglected.

In essence, what we have proposed is a practical way to go beyond the HFBA by including the coupling with non-condensate fluctuations into the description of the Bosecondensed system. A microscopic derivation of the RPAE equations by an equation-ofmotion approach has helped to bring more physical insight into the approximations that we have proposed. As we have pointed out, the RPAE gives some account of correlations between condensate and non-condensate by preserving non-zero off-diagonal elements in the susceptibility matrix.

The strategy one would adopt to use the RPAE in actual calculations may be briefly mentioned. One has to (i) determine the single particle orbitals and energy levels of the reference system as functions of temperature, in order to build the susceptibilities given in equations (48) and (54); (ii) solve the integral equations (24) and (25), thus obtaining the four partial response functions by comparison with the definitions (4)-(7); and (iii) search for the resonances of the response in the complex frequency plane. These give the excitation frequencies of the system as a whole.

Some additional simplifications seem possible in treating the experimentally relevant case of dilute Bose-condensed gases: (i) the role of the interactions in the reference gas is presumably minor; and (ii) in view of the resonant structure of the denominators in equations (48) and (54), the search for low-lying collective modes should mainly involve the single-particle levels which lie in the same frequency range.

Let us now comment on the insights on further progress that can be drawn from the development presented in this work. The issue of the mechanisms of damping of the collective excitations is of main interest here. It is relevant to recall that damping of sound waves in a homogeneous Bose fluid was obtained in an RPA treatment by Szépfalusy and Kondor [17]. However, in that case the condensate is coupled to a continuum of levels. Instead, the single particle orbitals for the gas in harmonic confinement have discrete energy eigenvalues, with spacings which are not much smaller than the low-lying collective excitation frequencies. Broadening of the single-particle levels can be understood as due to the interplay between thermal fluctuations and interparticle interactions and could be very simply included in the RPAE equations in a phenomenological fashion by replacing the parameter η in equations (48) and (54) by temperature-dependent relaxation rates. Such an approach was proposed in early work of Mermin [29] to take collisions between particles into account in the RPA dielectric function of the electron gas.

At a more fundamental level, important damping mechanisms for the collective excitations should be associated with those couplings between the condensate and the non-condensate which in a linear response framework are described by the off-diagonal proper susceptibilities. These are neglected in the RPAE, and could be taken into account in a perturbative expansion of the three- and four-point correlation functions entering the equations of motion for $\Phi(\mathbf{r},t)$ and $\Psi(\mathbf{r},t)$ beyond the approximations shown in equations (30) and (31). Their relevance to a microscopic evaluation of relaxation times can be understood from the discussion given by Kadanoff and Baym [30], showing that the analogue of the collision integral for a normal Fermi or Bose fluid in the Born approximation is given by the second-order perturbative expansion of the self-energy. In such a viewpoint one may surmise that the three-point term, i.e. $\Phi^* \langle \tilde{\Psi}^{\dagger} \tilde{\Psi} \tilde{\Psi} \rangle$ and its complex conjugate, should give an important contribution to damping of condensate motions via correlations with the non-condensate fluctuations. This process should exhibit a strong temperature dependence from Bose factors favouring scattering into non-condensate states which are being progressively occupied as the temperature increases towards its critical value.

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Appendix A. Comparison with the Hartree-Fock-Bogolubov-Popov approximation

We show in this Appendix that the RPAE equation (24) for the normal modes of the condensate reduces to those obtained in the HFB-Popov approximation if we choose the excited states of the Gross-Pitaevskii operator for the reference gas of the condensate

and we neglect the coupling with the density fluctuations of the non-condensate.

The RPAE equation for the condensate can be put in a more explicit form by the use of equation (54) for the susceptibility into equation (24). This leads to an expansion of the condensate density change into normal modes:

$$\delta n_{e}(\mathbf{r},\omega) = \sum_{j\neq 0} \left[\Phi_{eq}^{*}(\mathbf{r})\phi_{j}(\mathbf{r})\Omega_{j}^{(-)}(\omega)f_{j}^{(-)}(\omega) - \Phi_{eq}(\mathbf{r})\phi_{j}^{*}(\mathbf{r})\Omega_{j}^{(+)}(\omega)f_{j}^{(+)}(\omega) \right]$$
(A1)

where

$$\Omega_j^{(\mp)}(\omega) = 1/(\omega \mp (e_j - \mu) + i\eta)$$
(A2)

with $\eta = 0^+$. The coefficients $f_j^{(-)}$ and $f_j^{(+)}$ in these equations give the selection rules for the excitations and are defined as follows:

$$f_j^{(-)}(\omega) \equiv \int d^3 r' \Phi_{eq}(\mathbf{r}') \phi_j^*(\mathbf{r}') \left(U_p^c(\mathbf{r}',\omega) + \alpha \delta n_c(\mathbf{r}',\omega) \right)$$
(A3)

and

$$f_j^{(+)}(\omega) \equiv \int d^3 r' \Phi_{eq}^*(\mathbf{r}') \phi_j(\mathbf{r}') \left(U_p^c(\mathbf{r}',\omega) + \alpha \delta n_c(\mathbf{r}',\omega) \right) . \tag{A4}$$

By substituting equation (A1) into equation (A3) we finally obtain a set of algebraic equations for the coefficients, which represent the RPAE equation expanded on a given basis:

$$f_j^{(-)} = B_j^{(-)} + \alpha \sum_{h \neq 0} \left(\Omega_h^{(-)} f_h^{(-)} R_{0j0h} - \Omega_h^{(+)} f_h^{(+)} R_{jh00} \right) \quad , \tag{A5}$$

and

$$f_j^{(+)} = B_j^{(+)} + \alpha \sum_{h \neq 0} \left(\Omega_h^{(-)} f_h^{(-)} R_{00jh} - \Omega_h^{(+)} f_h^{(+)} R_{0h0j} \right)$$
(A6)

These involve numerical coefficients defined by

$$B_j^{(-)} \equiv \int d^3 r' \ \phi_j^*(\mathbf{r}') U_p^c(\mathbf{r}',\omega) \Phi(\mathbf{r}') \quad , \tag{A7}$$

$$B_j^{(+)} \equiv \int d^3 r' \, \Phi^*(\mathbf{r}') U_p^c(\mathbf{r}',\omega) \phi_j(\mathbf{r}') \tag{A8}$$

and

$$R_{abcd} \equiv \int d^3 r' \ \phi_a^*(\mathbf{r}') \phi_b^*(\mathbf{r}') \phi_c(\mathbf{r}') \phi_d(\mathbf{r}') \quad . \tag{A9}$$

In equation (A9) we have used the notation $\Phi_{eq}(\mathbf{r}) = \phi_0(\mathbf{r})$. A similar treatment can be given in the general case when the non-condensate is also present.

In order to compare with equations (A5) and (A6), we start from the Bogolubov equations in the Popov approximation [18, 13]:

$$(\hat{L}^{GP} + \alpha n_c) u_{\lambda} - \alpha n_c v_{\lambda} = (\omega_{\lambda} + \mu) u_{\lambda} (\hat{L}^{GP} + \alpha n_c) v_{\lambda} - \alpha n_c u_{\lambda} = (-\omega_{\lambda} + \mu) v_{\lambda}$$
 (A10)

with \hat{L}^{GP} being the Gross-Pitaevskii operator defined in equation (32). Extending Esry's method at finite temperature [12], we expand the Bogolubov modes u_{λ} and v_{λ} on the reference gas basis ϕ_h :

$$u_{\lambda} = \sum_{h \neq 0} U_{h}^{(\lambda)} \phi_{h}$$
$$v_{\lambda} = \sum_{h \neq 0} V_{h}^{(\lambda)} \phi_{h}$$
(A11)

where ϕ_h are defined as the excited states of the Gross-Pitaevskii operator,

$$\hat{L}^{GP}\phi_h = e_h\phi_h . \tag{A12}$$

By substituting the expansion (A11) into the Bogolubov equations (A10) and using the orthogonality properties for ϕ_h $(h \neq 0)$, we find the equations for the coefficients $U_h^{(\lambda)}$ and $V_h^{(\lambda)}$:

$$\alpha \sum_{h \neq 0} R_{0j0h} U_h^{(\lambda)} - R_{jh00} V_h^{(\lambda)} = (\omega_\lambda - (e_j - \mu)) U_j^{(\lambda)}$$

$$\alpha \sum_{h \neq 0} R_{00jh} U_h^{(\lambda)} - R_{0h0j} V_h^{(\lambda)} = (\omega_\lambda + e_j - \mu) V_j^{(\lambda)}.$$
(A13)

For R_{ijkl} we have chosen the eigenfunctions to be real, consistently with the Popov approximation; moreover, $U_h^{(\lambda)}$ and $V_h^{(\lambda)}$ stand for $U_h(\omega = \omega_{\lambda})$ and $V_h(\omega = \omega_{\lambda})$. Equation (A13) agrees with the RPAE equations (A5) and (A6), when we set $U_j(\omega) = f_j^{(-)}(\omega) \Omega_j^{(-)}(\omega)$ and $V_j(\omega) = f_j^{(+)}(\omega) \Omega_j^{(+)}(\omega)$.

In this way we have also checked that in the limit of zero temperature our results are compatible with those of Esry [12], apart from terms of order 1/N where N is the total number of particles in the system.

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