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Extended Hartree–Fock–Bogoliubov theory for degenerate Bose systems

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Abstract

An extension of the Hartree–Fock–Bogoliubov (HFB) theory of degenerate Bose systems in which the coupling between one and two quasi-particles is taken into account is developed. The excitation operators are written as linear combinations of one and two HFB quasi-particles. Excitation energies and quasi-particle amplitudes are given by generalized Bogoliubov equations. The excitation spectrum has two branches. The first one is a discrete branch which is gapless and has a phonon character at large wavelength and, contrarily to HFB, is always stable. This branch is detached from a second, continuum branch whose threshold, at fixed total momentum, coincides with the two quasi-particle threshold of the HFB theory. The gap between the two branches at $P = 0$ is twice the HFB gap, which thus provides for the relevant energy scale. Numerical results for a specific case are given.

1. Introduction

The experimental realization of Bose–Einstein condensation in trapped neutral bosonic atoms has opened the opportunity for a comparison of microscopic theories of dilute systems with experimental data [1]. The standard approach is to solve the Gross–Pitaevskii (GP) equation for the condensate wavefunction and the linear Bogoliubov–de Gennes (BdG) equations for the collective excitations [2]. For $T = 0$ this theory has been successfully compared with the existing data [3–5]. Physically, the GP + BdG theory is a free quasi-particles theory. However it is not the 'best' such theory from a variational point of view, being superseded by the Hartree–Fock–Bogoliubov (HFB) theory [6], in which the nonlinear BdG equations are solved self-consistently and the GP and BdG equations are coupled. The two approaches agree when we neglect the depletion of the condensate in the self-consistent theory. This would suggest that HFB is the proper theory to use when the fluctuations become important, for example, in trapped gases through the mechanism of Feshbach resonance [7] or at finite temperature. It is however well known that the HFB theory has problems when applied to homogeneous systems [6]. Indeed, the excitation spectrum has a gap which violates the Hugenholtz–Pines theorem, which states that the excitation spectrum should be gapless [8]. The HFB theory is

also in contradiction with some thermodynamic data in ^{4}He (for example, the specific heat), which require that, in the large wavelength limit, the excitation spectrum should have a phonon behaviour [9].

In this paper we present an extension of the HFB theory leading to an excitation spectrum which, in particular, eliminates the gap problem. The key ingredient for this is the inclusion of two quasi-particle components together with their coupling to one quasi-particle components for the description of the excitation spectrum. Excitation energies and the structure of the corresponding modes are given by generalized Bogoliubov equations. The excitation spectrum includes a discrete stable phonon-like excitation branch. In addition to this discrete branch there is a continuum branch whose threshold is located at twice the HFB quasi-particle energy. This branch has, therefore, a gap at total momentum $\mathbf{P} = 0$ which is twice the HFB gap. Therefore, this gap sets an important energy scale for the excitation spectrum.

The use of this mechanism to solve the HFB gap problem has in fact being pioneered more than four decades ago by Takano [10]. A more recent work by Hutchinson *et al* [11] deals with the coupling between one and two quasi-particle components in a perturbative way, while the work of Kerman and Tommasini [12] deals with the same problem on the basis of the Gaussian functional approximation to a field theoretical variational procedure.

In this paper we use standard equations of motion techniques [13, 14], employed, for example, in [15] to study non-perturbatively the restoration of chiral symmetry in the linear σ model. This allows for a clear identification of the dynamical role played by various parts of the many-body Hamiltonian when expanded in terms of quasi-particles.

The paper is organized as follows. In section 2 we briefly discuss the basic properties of the HFB theory. In section 3 we derive the generalized Bogoliubov equations for the excitation energies and quasi-particle amplitudes. Our derivation allows for a clear identification of parts of the Hamiltonian responsible for the coupling between one and two quasi-particle components of the excitation operator. In section 4, we show that there exists a Goldstone mode at momentum equal to zero. Our proof of its existence is very simple and clearly related to the violation of number conservation. The results of a numerical application of the theory are discussed in section 5. Specifically we examine the properties of the excitation spectrum, its stability, and change in physical content as a function of the total momentum $\mathbf{P}$. We also make a comparison with the HFB and Bogoliubov approximations. Our conclusions are presented in section 6. All the expressions needed for numerical applications are given in appendices A and B.

2. HFB theory

The starting point is the Grand-Hamiltonian written in second quantization as

$$\hat{h} = \hat{H} - \mu\hat{N} = \sum_{\mathbf{k}} (e_k - \mu) a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \tfrac{1}{2} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} V(q) a^\dagger_{\mathbf{k}_1+\mathbf{q}} a^\dagger_{\mathbf{k}_2-\mathbf{q}} a_{\mathbf{k}_1} a_{\mathbf{k}_2}$$

where e_k is the free particle kinetic energy, $e_k = \hbar^2 k^2/2m$, $V(q)$ is the Fourier transform per unit volume of the atom–atom interaction potential

$$V(q) = \frac{1}{\Gamma} \int V(r)\, \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}} \mathrm{d}^3 r = \frac{\tilde{V}(q)}{\Gamma},$$

and the operators $a^\dagger_{\mathbf{k}}$ and $a_{\mathbf{k}}$ respectively create and annihilate atoms in a state with momentum $\hbar\mathbf{k}$, the corresponding wavefunction $\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{r})/\sqrt{\Gamma}$ satisfying periodic boundary conditions in volume Γ.

In a first step we perform a canonical transformation to quasi-particles by introducing a new set of creation and annihilation operators through the Bogoliubov rotation [16]

$$a_{\mathbf{k}} = c_{\mathbf{k}} + z_0\delta_{\mathbf{k},0} = u_{\mathbf{k}}\eta_{\mathbf{k}} - v_{\mathbf{k}}\eta^{\dagger}_{-\mathbf{k}} + z_0\delta_{\mathbf{k},0}, \tag{1}$$

where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are even functions of $\mathbf{k}$, $u_{\mathbf{k}} = u_{-\mathbf{k}}$, $v_{\mathbf{k}} = v_{-\mathbf{k}}$, and z_0 is a c-number. The constant z_0 appears as a shift in the equation for $\mathbf{k} = 0$ to account for the macroscopic condensate in the zero momentum state. In order to render the transformation canonical, the Bogoliubov factors have to obey the constraint

$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1.$$

It is straightforward to write the Grand-Hamiltonian $\hat{h}$ in the quasi-particle basis. After normal ordering, one obtains

$$\hat{h} = \hat{H} - \mu\hat{N} = h_0 + \hat{h}_1 + \hat{h}_2 + \hat{h}_3 + \hat{h}_4 \tag{2}$$

where the normal ordered operators $\hat{h_i}$ involve i quasi-particles. They are given explicitly in appendix A.

The amplitudes $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ and the shift z_0 are determined in HFB theory by minimizing the expectation value of $\hat{h}$, $\langle\Phi|\hat{h}|\Phi\rangle$ in the quasi-particle vacuum, that is, $\eta_{\mathbf{k}}|\Phi\rangle = 0$. Since the only term which contributes to the expectation value is the term h_0, the minimization is equivalent to the equations

$$\frac{\partial h_0}{\partial z_0} = 0, \qquad \frac{\partial h_0}{\partial v_{\mathbf{k}}} + \frac{\partial h_0}{\partial u_{\mathbf{k}}}\frac{\partial u_{\mathbf{k}}}{\partial v_{\mathbf{k}}} = 0 \tag{3}$$

with h_0 given by

$$\begin{aligned} h_0 = -z_0^2\mu + \frac{z_0^4}{2}V(0) + \sum_{\mathbf{k}}[e_k - \mu + (V(0) + V(k))z_0^2]v_{\mathbf{k}}^2 \\ - \sum_{\mathbf{k}} V(k)z_0^2 u_{\mathbf{k}}v_{\mathbf{k}} + \tfrac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2}(V(0) + V(|\mathbf{k}_1 - \mathbf{k}_2|))v_{\mathbf{k}_1}^2 v_{\mathbf{k}_2}^2 \\ + \tfrac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2} V(|\mathbf{k}_1 - \mathbf{k}_2|)u_{\mathbf{k}_1}v_{\mathbf{k}_1}u_{\mathbf{k}_2}v_{\mathbf{k}_2}. \end{aligned}$$

The two equations above can be written in a very compact way if we introduce the Hartree, exchange and pair potentials defined by the relations [17]

$$\begin{aligned} U_{\mathrm{h}} &= \sum_{\mathbf{k}_1} V(0)\langle\Phi|a^{\dagger}_{\mathbf{k}_1}a_{\mathbf{k}_1}|\Phi\rangle \\ U_{\mathrm{ex}}(\mathbf{k}) &= \sum_{\mathbf{k}_1} V(|\mathbf{k} - \mathbf{k}_1|)\langle\Phi|a^{\dagger}_{\mathbf{k}_1}a_{\mathbf{k}_1}|\Phi\rangle \\ U_{\mathrm{pair}}(\mathbf{k}) &= \sum_{\mathbf{k}_1} V(|\mathbf{k} - \mathbf{k}_1|)\langle\Phi|a_{\mathbf{k}_1}a_{-\mathbf{k}_1}|\Phi\rangle. \end{aligned}$$

Each of these potentials can be written as the sum of two terms which can be interpreted as related respectively to the condensate and to the non-condensate:

$$\begin{aligned} U_{\mathrm{h}} &= U_{\mathrm{h}}^{\mathrm{c}} + U_{\mathrm{h}}^{\mathrm{nc}} = V(0)z_0^2 + \sum_{\mathbf{k}_1} V(0)\langle\Phi|c^{\dagger}_{\mathbf{k}_1}c_{\mathbf{k}_1}|\Phi\rangle \\ U_{\mathrm{ex}}(\mathbf{k}) &= U_{\mathrm{ex}}^{\mathrm{c}} + U_{\mathrm{ex}}^{\mathrm{nc}} = V(k)z_0^2 + \sum_{\mathbf{k}_1} V(|\mathbf{k} - \mathbf{k}_1|)\langle\Phi|c^{\dagger}_{\mathbf{k}_1}c_{\mathbf{k}_1}|\Phi\rangle \\ U_{\mathrm{pair}}(\mathbf{k}) &= U_{\mathrm{pair}}^{\mathrm{c}} + U_{\mathrm{pair}}^{\mathrm{nc}} = V(k)z_0^2 + \sum_{\mathbf{k}_1} V(|\mathbf{k} - \mathbf{k}_1|)\langle\Phi|c_{\mathbf{k}_1}c_{-\mathbf{k}_1}|\Phi\rangle. \end{aligned}$$

In terms of these potentials the equilibrium equations (3) can be written as

$$z_0[-\mu + U_{\rm h} + U^{\rm nc}_{\rm ex}(0) + U^{\rm nc}_{\rm pair}(0)] = 0, \tag{4}$$

$$\tanh 2\sigma_k = \frac{U_{\rm pair}(\mathbf{k})}{e_k + U_{\rm h} + U_{\rm ex}(\mathbf{k}) - \mu} \equiv \frac{U_{\rm pair}(\mathbf{k})}{\tilde{e}(\mathbf{k})} \tag{5}$$

with $u_{\mathbf{k}} = \cosh\sigma_{\mathbf{k}}$ and $v_{\mathbf{k}} = \sinh\sigma_{\mathbf{k}}$.

The quasi-particle vacuum $|\Phi\rangle$ does not have a definite number of particles. In order to control the number of particles we determine μ from the condition that the mean value of the number of particles in the state $|\Phi\rangle$ is N, $N = \langle\Phi|\hat{N}|\Phi\rangle$, which gives

$$N = z_0^2 + \sum_{\mathbf{k}} v_{\mathbf{k}}^2. \tag{6}$$

Thus, the set of equations (4)–(6) determines μ, z_0 and the Bogoliubov amplitudes $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$. Equations (4) and (5) can also be derived by demanding that $\hat{h}_1$ vanishes and that $\hat{h}_2$ is diagonal in the quasi-particle basis, $\hat{h}_2 = \sum_{\mathbf{k}} \omega(\mathbf{k})\eta^\dagger_{\mathbf{k}}\eta_{\mathbf{k}}$, with $\omega(\mathbf{k})$ the quasi-particle energies, $\omega(\mathbf{k})^2 = \tilde{e}(\mathbf{k})^2 - U_{\rm pair}(\mathbf{k})^2$.

One feature of the HFB theory is that the excitation energies show a gap in the limit $k \to 0$ [6],

$$\omega(0)^2 = -4\tilde{V}(0)n_0 U^{\rm nc}_{\rm pair}(0) \tag{7}$$

where $n_0 = z_0^2/\Gamma$ is the condensate density. The existence of an energy gap in the excitation spectrum does not conform with a phonon spectrum in superfluid systems and is also in contradiction with the Hugenholtz–Pines (HP) [8] theorem, which states that an excitation branch must exist such that the excitation energy vanishes when $k \to 0$.

An approximate way to satisfy the HP theorem is to neglect the so-called anomalous density $m_{\mathbf{k}} = \langle\Phi|c_{\mathbf{k}}c_{-\mathbf{k}}|\Phi\rangle$ in the HFB theory [6]. In this approximation $U^{\rm nc}_{\rm pair}(\mathbf{k})$ vanishes and the gap disappears. This approximation is known as the Popov approximation. In the next section we develop a theory which leads to a gapless dispersion equation while taking $m_{\mathbf{k}}$ fully into account. As it turns out, this theory also provides physical meaning for the quantity (7).

3. The quasi-particle RPA

As is well known in the physics of many-body systems, the random phase approximation (RPA) singles out as zero energy modes the generators of continuous symmetries which are broken in the underlying self-consistent mean-field approximation [13, 14], a feature akin to the appearance of Goldstone bosons in quantum field theories. One among the many ways of deriving the RPA equations is the linearization of the equations of motion [21]. In principle, if we can find operators satisfying the equations

$$[H, Q^\dagger_\alpha] = \Omega_\alpha Q^\dagger_\alpha, \tag{8}$$

$$Q_\alpha|\Psi_0\rangle = 0 \tag{9}$$

with the normalization condition

$$\langle\Psi_0|[Q_\beta, Q^\dagger_\alpha]|\Psi_0\rangle = \delta_{\beta,\alpha},$$

the state $|\Psi_0\rangle$ being the exact ground state of H, we have an exact excited state of the many-body system since, from the above equations, it follows that $|\Psi_\alpha\rangle = Q^\dagger_\alpha|\Psi_0\rangle$ is an eigenstate of H with excitation energy Ω_α. This cannot be carried out in general, however, and we are bound to use approximations regarding both Q_α and $|\Psi_0\rangle$ in solving equations (8) and (9). In the method of linearization of the equations of motion we make an ansatz for the excitation

operators, writing it as a linear combination of basic excitations, and we linearize the left-hand side of equation (8) with respect to these operators.

We look for excitation operators which are a combination of one and two HFB quasi-particles,

$$Q^\dagger_{\mathbf{P}} = x_{\mathbf{P}}\eta^\dagger_{\mathbf{P}} + y_{\mathbf{P}}\eta_{-\mathbf{P}} + \sum_{\mathbf{q}\geqslant 0} X_{\mathbf{q},\mathbf{P}}\frac{\eta^\dagger_{\mathbf{q}+\mathbf{P}/2}\eta^\dagger_{-\mathbf{q}+\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q},0}}} + Y_{\mathbf{q},\mathbf{P}}\frac{\eta_{-\mathbf{q}-\mathbf{P}/2}\eta_{\mathbf{q}-\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q},0}}}. \tag{10}$$

In this expression $Q^\dagger_{\mathbf{P}}$ creates an excitation with momentum $\mathbf{P}$ which is a linear combination of one and two HFB quasi-particles, $\eta^\dagger_{\mathbf{P}}$, $\eta_{-\mathbf{P}}$, and $\eta^\dagger_{\mathbf{q}+\mathbf{P}/2}\eta^\dagger_{-\mathbf{q}+\mathbf{P}/2}$, $\eta_{-\mathbf{q}-\mathbf{P}/2}\eta_{\mathbf{q}-\mathbf{P}/2}$ respectively. The two quasi-particle terms carry moreover the relative momentum $\mathbf{q}$. The coefficients $x_{\mathbf{P}}$, $y_{\mathbf{P}}$, $X_{\mathbf{q},\mathbf{P}}$ and $Y_{\mathbf{q},\mathbf{P}}$ are even functions of $\mathbf{P}$. As the pair creation and annihilation are invariant by the replacement $\mathbf{q}\to-\mathbf{q}$, $X_{\mathbf{q},\mathbf{P}}$ and $Y_{\mathbf{q},\mathbf{P}}$ are even functions of $\mathbf{q}$ and we restrict the sum in order that each pair appears only once. Note that this ansatz does not include terms of the type $\eta^\dagger_{\mathbf{k}}\eta_{\mathbf{k}'}$, $\mathbf{k}\neq\mathbf{k}'$. Although from a technical point of view their inclusion presents no problem, it may be expected on physical grounds that the most important correlation processes involve creation and annihilation of quasi-particle pairs on the HFB vacuum. The excitations corresponding to the omitted terms cannot be created on this vacuum, so they will be able to play any role in higher order correlation processes only.

The coefficients in (10) are determined by the method of the equations of motion in the version of [13] and [14], which provides for a systematic way of achieving the linearization referred to above. In this way equations (8) and (9) lead to

$$\langle\Psi_0|[Q_{\mathbf{P}}, H, Q^\dagger_{\mathbf{P}}]|\Psi_0\rangle = \Omega_P\langle\Psi_0|[Q_{\mathbf{p}}, Q^\dagger_{\mathbf{P}}]|\Psi_0\rangle$$

where $[A, B, C]$ is the symmetrized double commutator $\frac{1}{2}([A,[B,C]] + [[A,B],C])$. Requiring that $\Omega_{\mathbf{P}}$ be stationary under variation of the excitation operators one obtains

$$\langle\Phi|[\delta Q_{\mathbf{P}}, H, Q^\dagger_{\mathbf{P}}]|\Phi\rangle = \Omega_P\langle\Phi|[\delta Q_{\mathbf{P}}, Q^\dagger_{\mathbf{P}}]|\Phi\rangle \tag{11}$$

where $\delta Q_{\mathbf{P}}$ is the hermitian conjugate of the operator given by the variation of the coefficients in (10) and, as usual, we replaced the ground state $|\Psi_0\rangle$ by the HFB vacuum $|\Phi\rangle$.

Performing the variation indicated in equation (11), we get for the excitation energies Ω_P and for the coefficients in equation (10), collected in matrix form as

$$\mathcal{X} = \begin{pmatrix} x_{\mathbf{P}} \\ X_{\mathbf{P}} \end{pmatrix} \qquad \text{and} \qquad \mathcal{Y} = \begin{pmatrix} y_{\mathbf{P}} \\ Y_{\mathbf{P}} \end{pmatrix}, \tag{12}$$

the equation

$$\begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^* & \mathcal{A}^* \end{pmatrix}\begin{pmatrix} \mathcal{X} \\ \mathcal{Y} \end{pmatrix} = \Omega_P\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \mathcal{X} \\ \mathcal{Y} \end{pmatrix}. \tag{13}$$

For each $\mathbf{P}$ the number of modes equals the number of operator pairs plus one, $n_{\text{pairs}} + 1$. Actually this number is denumerably infinite, the modes being labelled by a quantum number λ. In equation (12), $X_{\mathbf{P}}(Y_{\mathbf{P}})$ stands for the set of n_{pairs} coefficients $X_{\mathbf{q},\mathbf{P}}(Y_{\mathbf{q},\mathbf{P}})$ and $\mathcal{A}$ and $\mathcal{B}$ are respectively Hermitian and symmetric matrices of dimension $n_{\text{pairs}} + 1$. The coefficients are subject to the normalization condition

$$\langle\Phi|[Q^\lambda_{\mathbf{P}}, Q^{\dagger\tau}_{\mathbf{P}}]\Phi\rangle = x^{\lambda^*}_{\mathbf{P}}x^\tau_{\mathbf{P}} - y^{\lambda^*}_{\mathbf{P}}y^\tau_{\mathbf{P}} + \sum_{\mathbf{q}\geqslant 0}\left(X^{\lambda^*}_{\mathbf{q},\mathbf{P}}X^\tau_{\mathbf{q},\mathbf{P}} - Y^{\lambda^*}_{\mathbf{q},\mathbf{P}}Y^\tau_{\mathbf{q},\mathbf{P}}\right) = \delta_{\lambda,\tau}. \tag{14}$$

The hermitian matrix $\mathcal{A}$ is conveniently written as

$$\mathcal{A} = \begin{pmatrix} \mathcal{A}^{11} & \mathcal{A}^{12} \\ \mathcal{A}^{21} & \mathcal{A}^{22} \end{pmatrix},$$

the diagonal blocks $\mathcal{A}^{11}$ and $\mathcal{A}^{22}$ being hermitian matrices with dimensionality 1 and n_{pairs} respectively. They are given by

$$\mathcal{A}^{11}(\mathbf{P}) = \langle\Phi|[\eta_{\mathbf{P}}, H, \eta^{\dagger}_{\mathbf{P}}]|\Phi\rangle,$$

and

$$\mathcal{A}^{22}(\mathbf{q}', \mathbf{q}; \mathbf{P}) = \langle\Phi|\left[\frac{\eta_{\mathbf{q}'+\mathbf{P}/2}\eta_{-\mathbf{q}'+\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q}',0}}}, H, \frac{\eta^{\dagger}_{\mathbf{q}+\mathbf{P}/2}\eta^{\dagger}_{-\mathbf{q}+\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q},0}}}\right]|\Phi\rangle.$$

The coupling matrices $\mathcal{A}^{12}$ and $\mathcal{A}^{21}$ are hermitian conjugates with dimensions $1 \times n_{\text{pairs}}$ and $n_{\text{pairs}} \times 1$ respectively, their elements being given by

$$\mathcal{A}^{12}(\mathbf{q}; \mathbf{P}) = \langle\Phi|\left[\eta_{\mathbf{P}}, H, \frac{\eta^{\dagger}_{\mathbf{q}+\mathbf{P}/2}\eta^{\dagger}_{-\mathbf{q}+\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q},0}}}\right]|\Phi\rangle.$$

The symmetric matrix $\mathcal{B}$ can be split in a similar way as

$$\mathcal{B} = \begin{pmatrix} \mathcal{B}^{11} & \mathcal{B}^{12} \\ \mathcal{B}^{21} & \mathcal{B}^{22} \end{pmatrix}.$$

The diagonal blocks $\mathcal{B}^{11}$ and $\mathcal{B}^{22}$ are symmetric matrices whose elements are given by

$$\mathcal{B}^{11}(\mathbf{P}) = \langle\Phi|[\eta_{\mathbf{P}}, H, \eta_{-\mathbf{P}}]|\Phi\rangle,$$

and

$$\mathcal{B}^{22}(\mathbf{q}', \mathbf{q}; \mathbf{P}) = \langle\Phi|\left[\frac{\eta_{\mathbf{q}'+\mathbf{P}/2}\eta_{-\mathbf{q}'+\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q}',0}}}, H, \frac{\eta_{-\mathbf{q}-\mathbf{P}/2}\eta_{\mathbf{q}-\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q},0}}}\right]|\Phi\rangle.$$

The coupling matrices $\mathcal{B}^{12}$ and $\mathcal{B}^{21}$ are transposes of each other and have elements

$$\mathcal{B}^{12}(\mathbf{q}; \mathbf{P}) = \langle\Phi|\left[\eta_{\mathbf{P}}, H, \frac{\eta_{-\mathbf{q}-\mathbf{P}/2}\eta_{\mathbf{q}-\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q},0}}}\right]|\Phi\rangle.$$

Note that the matrices labelled 12 and 21 couple one and two quasi-particle excitations whereas the matrices labelled 11 and 22 act only inside the one and two quasi-particle subspaces, respectively. As shown in appendix B, the coupling matrices depend only on $\hat{h}_3$ (see equation (2)), which is therefore responsible for the coupling between the one and two quasi-particle components. On the other hand the one and two quasi-particle diagonal blocks depend only on $\hat{h}_2$ and $\hat{h}_4$. All the matrix elements are given in detail in appendix B. If the coupling terms $\hat{h}_3$ and $\hat{h}_4$ are set to zero we have that $\mathcal{B} = 0$ and $\mathcal{A}$ is diagonal with eigenvalues $\omega(\mathbf{P})$ and $\omega_2(\mathbf{q}, \mathbf{P}) = \omega(\mathbf{q} + \mathbf{P}/2) + \omega(-\mathbf{q} + \mathbf{P}/2)$ which correspond to one and two free quasi-particle energies.

Since the static quantities are real, the matrix elements of $\mathcal{A}$ and $\mathcal{B}$ are real and the RPA equations can be written in a more compact and symmetrical form by introducing the new variables

$$\begin{aligned} &\phi_1(\mathbf{P}) = x_{\mathbf{P}} + y_{\mathbf{P}}, \\ &\phi_2(\mathbf{q}; \mathbf{P}) = X_{\mathbf{q},\mathbf{P}} + Y_{\mathbf{q},\mathbf{P}}, \\ &\pi_1(\mathbf{P}) = (x_{\mathbf{P}} - y_{\mathbf{P}}) \qquad \text{and} \\ &\pi_2(\mathbf{q}; \mathbf{P}) = (X_{\mathbf{q},\mathbf{P}} - Y_{\mathbf{q},\mathbf{P}}). \end{aligned}$$

Collecting ϕ_1, ϕ_2 and π_1, π_2 in the $n_{\text{pairs}} + 1$ component vectors

$$\mathcal{Q} = \begin{pmatrix} \phi_1(\mathbf{P}) \\ \phi_2(\mathbf{q}; \mathbf{P}) \end{pmatrix} \qquad \mathcal{P} = \begin{pmatrix} \pi_1(\mathbf{P}) \\ \pi_2(\mathbf{q}; \mathbf{P}) \end{pmatrix}$$

we can rewrite the equations (13) in the compact form [11, 12]

$$\begin{aligned}\Omega\mathcal{Q} &= \mathcal{A}_-\mathcal{P}\\ \Omega\mathcal{P} &= \mathcal{A}_+\mathcal{Q}\end{aligned} \tag{15}$$

where $\mathcal{A}_+$ and $\mathcal{A}_-$ are symmetric matrices given in terms of $\mathcal{A}$ and $\mathcal{B}$ as

$$\begin{aligned}\mathcal{A}_+ &= \mathcal{A}+\mathcal{B}\\ \mathcal{A}_- &= \mathcal{A}-\mathcal{B}.\end{aligned} \tag{16}$$

The elements of these matrices can be written explicitly as

$$\mathcal{A}_-^{11} = \mathcal{A}_+^{11} = \omega(\mathbf{P}) \tag{17}$$

$$\begin{aligned}\mathcal{A}_-^{12}(\mathbf{q},\mathbf{P}) = {}& \frac{z_0}{\sqrt{1+\delta_{\mathbf{q},0}}}C_0(\mathbf{P})\{C_0(-)C_0(+)[V(+)+V(-)]+[C_0(+)C_0(-)\\ & - C_0^{-1}(+)C_0^{-1}(-)]V(\mathbf{P})\}\end{aligned} \tag{18}$$

$$\mathcal{A}_+^{12}(\mathbf{q},\mathbf{P}) = \frac{z_0}{2\sqrt{1+\delta_{\mathbf{q},0}}}C_0^{-1}(\mathbf{P})\{[C_0^{-1}(+)C_0(-)+C_0(+)C_0^{-1}(-)][V(+)+V(-)]\} \tag{19}$$

$$\begin{aligned}\mathcal{A}_-^{22}(\mathbf{q},\mathbf{q}',\mathbf{P}) = {}& [\omega(+)+\omega(-)]\delta_{\mathbf{q},\mathbf{q}'}\\ & + \frac{1}{2\sqrt{(1+\delta_{\mathbf{q},0})(1+\delta_{\mathbf{q}',0})}}\{[C_0^{-1}(+')C_0^{-1}(-')C_0^{-1}(+)C_0^{-1}(-)\\ & + C_0(+')C_0(-')C_0(+)C_0(-)][V(|\mathbf{q}-\mathbf{q}'|)+V(|\mathbf{q}+\mathbf{q}'|)]+[C_0^{-1}(+')C_0^{-1}(-')\\ & - C_0(+')C_0(-')][C_0^{-1}(+)C_0^{-1}(-)-C_0(+)C_0(-)]V(\mathbf{P})\}\end{aligned} \tag{20}$$

$$\begin{aligned}\mathcal{A}_+^{22}(\mathbf{q},\mathbf{q}',\mathbf{P}) = {}& [\omega(+)+\omega(-)]\delta_{\mathbf{q},\mathbf{q}'}\\ & + \frac{1}{2\sqrt{(1+\delta_{\mathbf{q},0})(1+\delta_{\mathbf{q}',0})}}[C_0^{-1}(+')C_0(-')C_0^{-1}(+)C_0(-)\\ & + C_0(+')C_0^{-1}(-')C_0(+)C_0^{-1}(-)]V(|\mathbf{q}-\mathbf{q}'|)+[C_0^{-1}(+')C_0(-')C_0^{-1}(-)C_0(+)\\ & + C_0(+')C_0^{-1}(-')C_0(-)C_0^{-1}(+)]V(|\mathbf{q}+\mathbf{q}'|),\end{aligned} \tag{21}$$

where we used the notation $\pm = \pm\mathbf{q}+\mathbf{P}/2$ and $\pm' = \pm\mathbf{q}'+\mathbf{P}/2$. These expressions show the remarkable result that all the matrix elements depend on just a single function of the static quantities, namely

$$C_0(\mathbf{q}) = u_{\mathbf{q}} - v_{\mathbf{q}}.$$

The solutions to the coupled equations (15) give the 'dressed' excitation modes which will now have one and two quasi-particle contributions. The results for the excitation energies will lead to a discrete branch and a continuum whose threshold coincides with the two quasi-particle threshold of the HFB theory. The discrete branch is detached from the continuum and due to the coupling between the one and two quasi-particles will be pushed down and become gapless. This fact can be proved for any pseudo-potential, as will be shown in the next section.

4. The Goldstone mode

Equations (13) have a zero energy solution $\Omega_0 = 0$ with zero-norm when $\mathbf{P} = 0$, which will be referred to as the Goldstone mode [18]. To identify this solution one considers the generator of the symmetry violated by the theory which, in our case, is the $U(1)$ symmetry generated by the number operator. This operator, when written in the HFB basis, has components that are present in the general ansatz for the excitation operators, equation (10). These components will be identified with the excitation operator of the Goldstone mode $\hat{Q}_{\mathrm{G}}$.

In order to find $\hat{Q}_{\rm G}$ we thus start by writing the number operator

$$\hat{N} = \sum_{\mathbf{k}} a^{\dagger}_{\mathbf{k}} a_{\mathbf{k}}$$

in terms of the HFB quasi-particles $\eta^{\dagger}_{\mathbf{k}}$, $\eta_{\mathbf{k}}$, which gives

$$\hat{N} = N + z_0(u_0 - v_0)(\eta_0 + \eta^{\dagger}_0) - \sum_{\mathbf{k}\geqslant 0} \frac{2u_{\mathbf{k}}v_{\mathbf{k}}}{1+\delta_{\mathbf{k},0}}(\eta^{\dagger}_{\mathbf{k}}\eta^{\dagger}_{-\mathbf{k}} + \eta_{\mathbf{k}}\eta_{-\mathbf{k}}) + \sum_{\mathbf{k}}(u^2_{\mathbf{k}} + v^2_{\mathbf{k}})\eta^{\dagger}_{\mathbf{k}}\eta_{\mathbf{k}}. \tag{22}$$

Comparing with the general ansatz equation (10) we identify the excitation operator of the Goldstone mode as

$$\hat{Q}_{\rm G} = z_0(u_0 - v_0)(\eta_0 + \eta^{\dagger}_0) - \sum_{\mathbf{k}\geqslant 0} \frac{2u_{\mathbf{k}}v_{\mathbf{k}}}{1+\delta_{\mathbf{k},0}}(\eta^{\dagger}_{\mathbf{k}}\eta^{\dagger}_{-\mathbf{k}} + \eta_{\mathbf{k}}\eta_{-\mathbf{k}}). \tag{23}$$

Our task is then to prove that, when $\mathbf{P} = 0$, there is a zero-energy solution of (13) with norm zero for which

$$x_0 = y_0 = z_0(u_0 - v_0) \qquad \text{and} \qquad X_{\mathbf{q},0} = Y_{\mathbf{q},0} = -\frac{2u_{\mathbf{q}}v_{\mathbf{q}}}{\sqrt{1+\delta_{\mathbf{q},0}}}.$$

To this effect, we use the fact that equation (13) is equivalent to the coupled equations (15). For $\Omega_0 = 0$ and $\mathcal{P} = 0$ these coupled equations reduce to

$$\mathcal{A}_+ \mathcal{Q}_{\rm G} = 0$$

with

$$\mathcal{Q}_{\rm G} = \begin{pmatrix} \phi_1(0) \\ \phi_2(\mathbf{q};0) \end{pmatrix} = \begin{pmatrix} 2x_0 \\ 2X_{\mathbf{q},0} \end{pmatrix}.$$

From the expression of the matrix elements of $\mathcal{A}_+$, equations (19) and (21) (at $\mathbf{P} = 0$), it follows that $\mathcal{Q}_{\rm G}$ given as in equation (23) is a zero-energy solution of equations (15) provided one has

$$\tfrac{1}{2}\omega_0(u_0 - v_0)^2 + U^{\rm nc}_{\rm pair}(0) = 0$$
$$U_{\rm pair}(\mathbf{q}) - 2\omega_{\mathbf{q}}u_{\mathbf{q}}v_{\mathbf{q}} = 0.$$

These identities are in fact easily seen to hold when use is made of the relations, satisfied by the static quantities,

$$u^2_{\mathbf{q}} = \frac{1}{2}\left(\frac{\tilde{e}_{\mathbf{q}}}{\omega_q} + 1\right), \qquad v^2_{\mathbf{q}} = \frac{1}{2}\left(\frac{\tilde{e}_{\mathbf{q}}}{\omega_{\mathbf{q}}} - 1\right) \qquad \text{and} \qquad 2u_{\mathbf{q}}v_{\mathbf{q}} = \frac{U_{\rm pair}(\mathbf{q})}{\omega_{\mathbf{q}}}.$$

In the equations of motion method the connection between the Goldstone mode excitation operator $\hat{Q}_{\rm G}$ and the number operator $\hat{N}$ goes as follows. Since $[\hat{h}, \hat{N}] = 0$ one has

$$\langle\Phi|[\delta\hat{Q}, [\hat{h}, \hat{N}]]|\Phi\rangle = 0. \tag{24}$$

At first glance there is a difficulty to conclude from the above equation that $\hat{Q}_{\rm G}$ is a zero-energy solution of equation (11), caused by the presence of the term $\sum_{\mathbf{k}}(u^2_{\mathbf{k}} + v^2_{\mathbf{k}})\eta^{\dagger}_{\mathbf{k}}\eta_{\mathbf{k}}$ in equation (22) which does not belong to the general RPA ansatz, equation (10). However, this term does not give any contribution to (24) and since in our case the double-commutator is identical to the symmetrized double-commutator one has

$$\langle\Phi|[\delta\hat{Q}, \hat{h}, \hat{Q}_{\rm G}]|\Phi\rangle = 0$$

showing that the last term in equation (22) does not play any role and indeed $\hat{Q}_{\rm G}$ is a zero-energy solution of equation (9).

In the HFB case we could proceed in the same fashion. However, in this case the terms which do not belong to the HFB ansatz, equation (1), do contribute to the matrix element (11) and, as a consequence, the HFB equations do not have a zero-energy mode and the excitation spectrum always has a gap.

5. Numerical results

In this section we present and discuss the results obtained by solving equations (15) numerically in a specific case. This will illustrate quantitatively the predictions of the theory outlined above and allow for comparison with results of the HFB and Bogoliubov approximations. To this effect, we simply adopt the purely repulsive Gaussian pseudo-potential written in momentum space and used for similar purposes in [19, 20]. This pseudo-potential is parameterized as

$$\tilde{V}(k) = \frac{4\pi\hbar^2 a}{m} \exp\left(-\frac{\sigma^2 k^2}{2}\right)$$

where, as usual, the pseudo-potential at zero relative momentum $\tilde{V}(0)$ and the scattering length a are related by $a = m\tilde{V}(0)/4\pi\hbar^2$. Unlike in the case of the usual contact pseudo-potential, this choice allows for a straightforward solution of the self-consistent static equations (4)–(6). The use of the same pseudo-potential in equations (15) will then highlight the new features brought about by the inclusion of two quasi-particle terms.

We measure lengths in units of a and energies in units of $\hbar^2/(2ma^2)$. The width of the pseudo-potential is chosen to be of the order of the scattering length $\sigma = 2.8a$ as in [20]. The only parameter left is the total density ρ. We report on calculations done with two different values chosen to be such that $a^3\rho = 10^{-2}$ and 10^{-3}. These choices of the 'dilution parameter' fall between the values corresponding to the dilute gas experiments and to liquid helium. These values of $a^3\rho$ can be achieved with trapped gaseous condensates in experiments conducted close to a Feshbach resonance [7].

The parameter values having been specified, we calculate the energy of the discrete branch, the continuum threshold and the structure of the excitation operators of the discrete branch. The first step in these calculations is to self-consistently solve the static equations (4)–(6) in order to construct the matrices $\mathcal{A}_+$ and $\mathcal{A}_-$ defined in equation (16). The next step is to solve the coupled equations (15). A standard way to proceed would be taking the thermodynamic limit in both cases and solving the resulting coupled integral equations. In this paper, we took a different route: we solved iteratively the discrete self-consistent static equations (4)–(6) and the matrix eigenvalue equations (15) in a box with volume Γ. The value of the volume Γ is increased (with constant density) and the whole calculation is repeated until volume independence is observed, indicating that the thermodynamic limit has been sufficiently reached for the required quantities.

We begin discussing in detail the results for $a^3\rho = 10^{-2}$, since the qualitative behaviour of the calculated quantities does not depend on the value of the density. They are summarized in figure 1. We start by looking at the discrete branch in figure 1 (top). In the long-wavelength limit this branch is gapless, as shown in section 4, has a phonon-like dispersion relation, i.e. $\Omega_P = cP$, and is always stable. We have also verified numerically that the continuum threshold starts at the minimum value for the two quasi-particles HFB energies, $\omega_2(\mathbf{q}, \mathbf{P}) = \omega(\mathbf{q} + \mathbf{P}/2) + \omega(-\mathbf{q} + \mathbf{P}/2)$ at a fixed value of $\mathbf{P}$, which in our case always occurs at $\mathbf{q} = 0$.

These results may be compared with those of the HFB and Bogoliubov approximations. In the HFB approximation we have free quasi-particles, and the one and two quasi-particle branches are decoupled. As shown in figure 1 (middle), both branches have a gap and the lowest is not linear in $\mathbf{P}$ in the limit of long wavelengths. It is possible to show that the one quasi-particle branch always crosses the lower limit of the two quasi-particle continuum at some value of $\mathbf{P}$. In fact, at small P the energy of the one quasi-particle branch is always below the two quasi-particle threshold due to the existence of the gap, $\omega_2(0, 0) = 2\omega(0)$, whereas for large P just the opposite happens, $\omega_2(0, \mathbf{P}) \approx P^2/2 < \omega(\mathbf{P}) \approx P^2$. The one quasi-particle

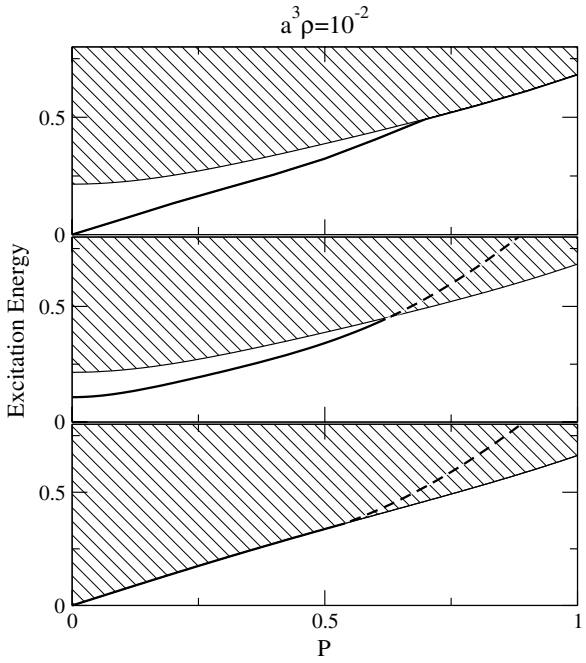

Figure 1. The excitation spectrum according to the RPA (top), to the HFB theory (middle), and in the Bogoliubov approximation (bottom) for $a^3\rho = 10^{-2}$. In the top part the solid lines show the dispersion of the discrete branch and the continuum threshold, whereas in the middle and bottom parts the lower solid/dashed line is the dispersion of the decoupled one quasi-particle branch. The dashed part corresponds to the region where the energy of the one quasi-particle branch is greater than the threshold of the two quasi-particle continuum. The excitation energy is measured in units of $\hbar^2/(2ma^2)$ and the momenta in units of $\hbar/a$. See the text for details.

branch always becomes eventually unstable as a consequence of the crossing. In the case $a^3\rho = 10^{-2}$, the crossing point happens at $P = 0.63a^{-1}$. The one quasi-particle branch is therefore stable for $P < 0.63a^{-1}$, becoming unstable above this value of P. Comparison with figure 1 (top) shows that the discrete branch 'avoids' the crossing moving away from that point and rapidly approaching the two quasi-particle threshold above the HFB crossing point. This effect is displayed in grater detail in figure 2(c).

In the Bogoliubov approximation, shown in figure 1 (bottom), the two branches are gapless and phonon-like in the long-wavelength limit. In this approximation the one quasi-particle branch is always unstable [21]. For $a^3\rho = 10^{-2}$ and momenta $P < 0.54a^{-1}$ the one quasi-particle branch and the two quasi-particle threshold are degenerate. In this case the one quasi-particle decays into two quasi-particles, one of which carries all the momentum and energy. This is possible because the one quasi-particle branch is gapless. For $P > 0.54a^{-1}$ the one quasi-particle branch lies above the continuum threshold that occurs for zero relative momentum $\mathbf{q} = 0$.

In conclusion, we found that the energy of the discrete branch of the present theory interpolates between the Bogoliubov one quasi-particle spectrum and the HFB two quasi-particle threshold, with a relatively sharp transition region near the onset of instability of the HFB one quasi-particle spectrum, as illustrated in figures 2(a), (c) for $a^3\rho = 10^{-2}$ and in figures 3(a), (c) for $a^3\rho = 10^{-3}$. From these graphs we also see that the sound velocities are practically equal to the sound velocities of the Bogoliubov approximation.

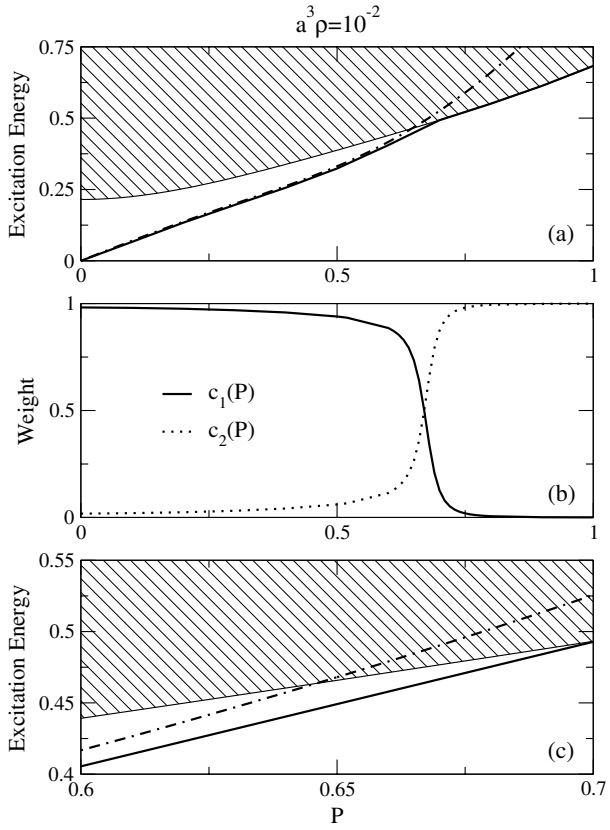

Figure 2. Part (a) shows the dispersion of the RPA discrete excitation mode, the continuum threshold (solid lines) and the dispersion of the Bogoliubov one quasi-particle excitations (dot–dashed line). In (b) $c_1(\mathbf{P})$ (solid line) and $c_2(\mathbf{P})$ (dashed line) measure respectively the one and two quasi-particles content of the discrete branch as a function of P, for $a^3\rho = 10^{-2}$. Part (c) is a zoom of (a) near the transition region. Units are as in figure 1.

We extracted information on the composition of the excitation operator as a function of the total momentum $\mathbf{P}$ by calculating the quantity

$$c_1(\mathbf{P}) = x_{\mathbf{P}}^2 - y_{\mathbf{P}}^2$$

which corresponds to the relative weight of the one quasi-particle component. Analogously for the two quasi-particle component we can define

$$c_2(\mathbf{P}) = \sum_{\mathbf{q}\geqslant 0}(X_{\mathbf{q},\mathbf{P}}^2 - Y_{\mathbf{q},\mathbf{P}}^2).$$

These two relative weights are related through the normalization condition (14) which requires $c_1(\mathbf{P}) + c_2(\mathbf{P}) = 1$.

Figures 2(b) and 3(b) show the values of $c_1(P)$ and $c_2(P)$ as a function of the total momentum P for $a^3\rho = 10^{-2}$ and 10^{-3} respectively. In the long-wavelength regime the excitation operator is predominantly a one quasi-particle operator. In the short-wavelength regime, on the other hand, it becomes predominantly a two quasi-particle operator as it approaches the continuum threshold asymptotically. Note that there is a sharp transition between these two regimes, the effect being more pronounced at higher densities. Comparing

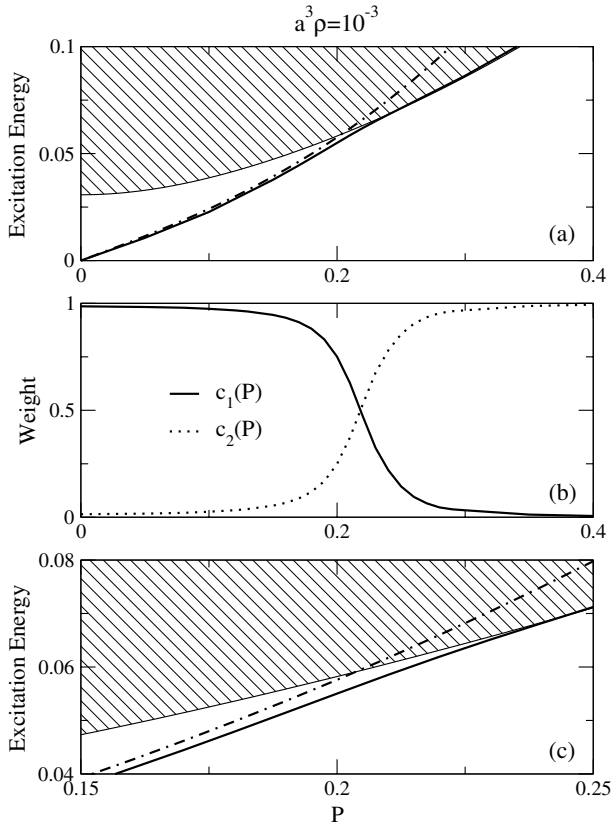

Figure 3. The same as figure 2, but for $a^3\rho = 10^{-3}$.

figures 2(a), (b) and 3(a), (b), we see that the change from a predominantly one quasi-particle to a predominantly two quasi-particle physical content of the discrete branch of the excitation spectrum and of its corresponding excitation operator occurs in the same momentum range. At least in the cases shown in figures 2 and 3 this range corresponds in order of magnitude to the inverse 'healing length' $\hbar/\xi$, with $\xi = (8\pi a\rho)^{-1/2}$.

6. Conclusion

In this paper we presented an extension of the HFB theory, cast in terms of well known method of equations of motion in order to access the excitation spectrum of a condensed many-boson system. The key ingredient for the extension is the coupling of the one and two HFB quasi-particle components to form the excitation modes. These are determined by solving the appropriate generalized Bogoliubov equations for the relevant amplitudes and excitation energies.

The generalized Bogoliubov equations are shown to have a Goldstone mode at zero transferred momentum, whose structure is related to that generated by the particle number operator. Correspondingly, an examination of the properties of the excitation spectrum reveals a detached gapless excitation branch with phonon-like dispersion at small momenta and a continuum branch starting at the two quasi-particle threshold of the HFB theory. The detached

branch has a predominantly one quasi-particle character at small momenta, where it closely approximates the Bogoliubov one quasi-particle spectrum. At high momenta it approaches the continuum threshold and eventually acquires a predominantly two quasi-particle character in what can be seen as an avoided crossing situation, due to the coupling between one and two quasi-particle components included in the calculation. The transition from one to two quasi-particle character is relatively sharp and occurs near the onset of instability of the HFB one quasi-particle spectrum. Differently from the Bogoliubov and HFB approximations the detached phonon-like branch is always stable.

The presence of the continuum branch serves, in particular, to give physical significance to the HFB one quasi-particle energy gap, this being the quantity which sets the appropriate energy scale for the continuum threshold.

The features revealed in this theory are closely linked to the depletion of the condensate caused by the two body interaction effects. They should be particularly relevant, therefore, in cases where such depletion effect become important. This happens for larger condensate densities and/or larger values of the relevant scattering length (implying stronger effective interaction) a situation that may be realized experimentally, for example, by taking advantages of Feshbach resonances.

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Appendix A. Grand-Hamiltonian in normal order

The Grand-Hamiltonian can be split as

$$\hat{h} = \hat{h}_0 + \hat{h}_1 + \hat{h}_2 + \hat{h}_3 + \hat{h}_4 \tag{A.1}$$

where $\hat{h}_i$ corresponds to the normal ordered component with i quasi-particle operators. We will split further each one of the terms $\hat{h}_i$ as

$$\hat{h}_i = \sum_{j=0}^{i} \hat{h}_{i-j,j}$$

where $i - j$ stands for the number of quasi-particle creation operators and j for the number of annihilation operators. In what follows we give explicit expressions of this form for each of the terms in (A.1).

A.1. $\hat{h}_0$

$$\begin{aligned}\hat{h}_0 = -z_0^2\mu + \frac{z_0^4}{2}V(0) + \sum_{\mathbf{k}}[e_k - \mu + (V(0) + V(k))z_0^2]v_{\mathbf{k}}^2 \\ - \sum_{\mathbf{k}} V(k)z_0^2 u_{\mathbf{k}} v_{\mathbf{k}} + \tfrac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2}(V(0) \\ + V(|\mathbf{k}_1 - \mathbf{k}_2|))v_{\mathbf{k}_1}^2 v_{\mathbf{k}_2}^2 + \tfrac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2} V(|\mathbf{k}_1 - \mathbf{k}_2|)u_{\mathbf{k}_1} v_{\mathbf{k}_1} u_{\mathbf{k}_2} v_{\mathbf{k}_2}.\end{aligned}$$

A.2. $\hat{h}_1$

$$\hat{h}_1 = h_{10}\eta_0^\dagger + h_{01}\eta_0$$

with

$$h_{10} = h_{01} = (-\mu + U_{\rm h} + U_{\rm ex}^{\rm nc}(0) + U_{\rm pair}^{\rm nc}(0))z_0(x_0 - y_0).$$

It follows from this expression that $\hat{h}_1 = 0$ as a consequence of the equilibrium equation (4).

A.3. $\hat{h}_2$

$$\hat{h}_2 = \sum_k h_{11}(\mathbf{k})\eta_{\mathbf{k}}^\dagger\eta_{\mathbf{k}} + h_{20}(\mathbf{k})\eta_{\mathbf{k}}^\dagger\eta_{-\mathbf{k}}^\dagger + h_{02}(\mathbf{k})\eta_{\mathbf{k}}\eta_{-\mathbf{k}}$$

with

$$h_{11}(\mathbf{k}) = \tilde{e}(\mathbf{k})\cosh 2\sigma_{\mathbf{k}} - U_{\rm pair}(\mathbf{k})\sinh 2\sigma_{\mathbf{k}},$$
$$h_{20}(\mathbf{k}) = h_{02}(\mathbf{k}) = -\tilde{e}(\mathbf{k})\sinh 2\sigma_{\mathbf{k}} + U_{\rm pair}(\mathbf{k})\cosh 2\sigma_{\mathbf{k}}.$$

From the equilibrium equation (5) it follows that the non-diagonal components $h_{20}(\mathbf{k})$ and $h_{02}(\mathbf{k})$ vanish, and also that the coefficient of the diagonal component $h_{11}(\mathbf{k})$ is equal to $\omega(\mathbf{k})$, leading to

$$\hat{h}_2 = \sum_k \omega(\mathbf{k})\eta_{\mathbf{k}}^\dagger\eta_{\mathbf{k}}$$

A.4. $\hat{h}_3$

$$\hat{h}_3 = \sum_{\mathbf{k},\mathbf{k}'}\{h_{1,2}(\mathbf{k},\mathbf{k}')\eta_{\mathbf{k}+\mathbf{k}}^\dagger\eta_{\mathbf{k}}\eta_{\mathbf{k}'} + h_{2,1}(\mathbf{k},\mathbf{k}')\eta_{\mathbf{k}'}^\dagger\eta_{\mathbf{k}}^\dagger\eta_{\mathbf{k}+\mathbf{k}'}$$
$$+ h_{3,0}(\mathbf{k},\mathbf{k}')\eta_{\mathbf{k}+\mathbf{k}'}^\dagger\eta_{-\mathbf{k}}^\dagger\eta_{-\mathbf{k}'}^\dagger + h_{0,3}(\mathbf{k},\mathbf{k}')\eta_{\mathbf{k}+\mathbf{k}'}\eta_{-\mathbf{k}}\eta_{-\mathbf{k}'}\}$$

with

$$h_{1,2}(\mathbf{k},\mathbf{k}') = h_{2,1}(\mathbf{k},\mathbf{k}') = \frac{z_0}{2}\{[u_{\mathbf{k}+\mathbf{k}'}u_{\mathbf{k}'} + v_{\mathbf{k}+\mathbf{k}'}v_{\mathbf{k}'}][u_{\mathbf{k}} - v_{\mathbf{k}}]V(k)$$
$$+ [u_{\mathbf{k}+\mathbf{k}'}u_{\mathbf{k}} + v_{\mathbf{k}+\mathbf{k}'}v_{\mathbf{k}}][u_{\mathbf{k}'} - v_{\mathbf{k}'}]V(k')$$
$$- [u_{\mathbf{k}+\mathbf{k}'} - v_{\mathbf{k}+\mathbf{k}'}][u_{\mathbf{k}}v_{\mathbf{k}'} + v_{\mathbf{k}}u_{\mathbf{k}'}]V(|\mathbf{k}+\mathbf{k}'|)\} \qquad \text{(A.2)}$$
$$h_{3,0}(\mathbf{k},\mathbf{k}') = h_{0,3}(\mathbf{k},\mathbf{k}') = \frac{z_0}{2}\left\{[u_{\mathbf{k}+\mathbf{k}'}v_{\mathbf{k}}v_{\mathbf{k}'} - v_{\mathbf{k}+\mathbf{k}'}u_{\mathbf{k}}u_{\mathbf{k}'}][V(k) + V(k')]\right\}.$$

Note that all the coefficients obey the symmetry property $h_{i,j}(\mathbf{k},\mathbf{k}') = h_{i,j}(-\mathbf{k},-\mathbf{k}') = h_{i,j}(\mathbf{k}',\mathbf{k})$.

A.5. $\hat{h}_4$

$$\hat{h}_4 = \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} h_{1,3}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\eta_{\mathbf{k}_2-\mathbf{q}}^\dagger\eta_{-\mathbf{k}_1-\mathbf{q}}\eta_{\mathbf{k}_1}\eta_{\mathbf{k}_2} + h_{3,1}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\eta_{\mathbf{k}_1}^\dagger\eta_{\mathbf{k}_2}^\dagger\eta_{-\mathbf{k}_1-\mathbf{q}}^\dagger\eta_{\mathbf{k}_2-\mathbf{q}}$$
$$+ h_{4,0}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\eta_{\mathbf{k}_1+\mathbf{q}}^\dagger\eta_{\mathbf{k}_2-\mathbf{q}}^\dagger\eta_{-\mathbf{k}_1}^\dagger\eta_{-\mathbf{k}_2}^\dagger + h_{0,4}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\eta_{\mathbf{k}_1+\mathbf{q}}\eta_{\mathbf{k}_2-\mathbf{q}}\eta_{-\mathbf{k}_1}\eta_{-\mathbf{k}_2}$$
$$+ h_{2,2}(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\eta_{\mathbf{k}_1+\mathbf{q}}^\dagger\eta_{\mathbf{k}_2-\mathbf{q}}^\dagger\eta_{\mathbf{k}_1}\eta_{\mathbf{k}_2}$$

with

$$h_{3,1}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}) = h_{1,3}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{q})$$
$$= -[u_{\mathbf{k}_2-\mathbf{q}} v_{\mathbf{k}_1+\mathbf{q}} u_{\mathbf{k}_1} u_{\mathbf{k}_2} + v_{\mathbf{k}_2-\mathbf{q}} u_{\mathbf{k}_1+\mathbf{q}} v_{\mathbf{k}_1} v_{\mathbf{k}_2}] V(q)$$
$$\hat{h}_{4,0}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}) = \hat{h}_{0,4}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}) = \tfrac{1}{2} u_{\mathbf{k}_1+\mathbf{q}} u_{\mathbf{k}_2-\mathbf{q}} v_{\mathbf{k}_1} v_{\mathbf{k}_2} V(q)$$
$$\hat{h}_{2,2}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}) = \tfrac{1}{2}\{[u_{\mathbf{k}_1+\mathbf{q}} u_{\mathbf{k}_1} + v_{\mathbf{k}_1+\mathbf{q}} v_{\mathbf{k}_1}][u_{\mathbf{k}_2-\mathbf{q}} u_{\mathbf{k}_2} + v_{\mathbf{k}_2-\mathbf{q}} v_{\mathbf{k}_2}] V(q)$$
$$+ [u_{\mathbf{k}_2-\mathbf{q}} u_{\mathbf{k}_1} v_{\mathbf{k}_1+\mathbf{q}} v_{\mathbf{k}_2} + u_{\mathbf{k}_1+\mathbf{q}} u_{\mathbf{k}_2} v_{\mathbf{k}_2-\mathbf{q}} v_{\mathbf{k}_1}] V(|\mathbf{k}_1 + \mathbf{k}_2|)\}.$$

The coefficients $h_{i,j}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{q})$ for $\{i, j\} = \{4, 0\}, \{0, 4\}$ and $\{2, 2\}$ obey the symmetry property

$$h_{i,j}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}) = h_{i,j}(\mathbf{k}_2, \mathbf{k}_1, -\mathbf{q}) = h_{i,j}(-\mathbf{k}_1, -\mathbf{k}_2, -\mathbf{q}).$$

Appendix B. RPA matrices

In this appendix we evaluate the matrix elements of $\mathcal{A}$ and $\mathcal{B}$. The key property to be used in order to calculate the involved average value of symmetrized double commutators is that $|\Phi\rangle$ is the quasi-particle vacuum. In order to work with more compact expressions we introduce the quantities

$$C_0(\mathbf{k}) = u_{\mathbf{k}} - v_{\mathbf{k}}$$
$$C_1(\mathbf{k}, \mathbf{k}') = C_1(\mathbf{k}', \mathbf{k}) = C_1(-\mathbf{k}, -\mathbf{k}') = u_{\mathbf{k}} u_{\mathbf{k}'} + v_{\mathbf{k}} v_{\mathbf{k}'}$$
$$C_2(\mathbf{k}, \mathbf{k}') = C_2(\mathbf{k}', \mathbf{k}) = C_2(-\mathbf{k}, -\mathbf{k}') = u_{\mathbf{k}} v_{\mathbf{k}'} + v_{\mathbf{k}} u_{\mathbf{k}'}.$$

C_1 and C_2 are usually called coherence factors and are well known in the study of Bose systems [9].

B.1. Sub-matrices of $\mathcal{A}$

(i) $\mathcal{A}^{11}$

$$\mathcal{A}^{11}(\mathbf{P}) = \langle\Phi|[\eta_{\mathbf{P}}, H, \eta^{\dagger}_{\mathbf{P}}]|\Phi\rangle.$$

From the property that $|\Phi\rangle$ is the quasi-particle vacuum it follows immediately that only $\hat{h}_2$ contributes to this matrix element, with the result $\mathcal{A}^{11}(\mathbf{P}) = \omega(\mathbf{P})$.

(ii) $\mathcal{A}^{12} = (\mathcal{A}^{21})^{\dagger}$

$$\mathcal{A}^{12}(\mathbf{q}; \mathbf{P}) = \langle\Phi|\left[\eta_{\mathbf{P}}, H, \frac{\eta^{\dagger}_{\mathbf{q}+\mathbf{P}/2}\eta^{\dagger}_{-\mathbf{q}+\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q},0}}}\right]|\Phi\rangle.$$

The only contribution to this matrix element comes from $\hat{h}_3$ through the term $\hat{h}_{1,2}$, giving

$$\mathcal{A}^{12}(\mathbf{q}; \mathbf{P}) = -2\frac{h_{1,2}(\mathbf{q}+\mathbf{P}/2, -\mathbf{q}+\mathbf{P}/2)}{\sqrt{1+\delta_{\mathbf{q},0}}}.$$

Using the expression for $h_{1,2}$ given in equation (A.2) this can be rewritten in terms of the coherence factors C_1, C_2 as

$$\mathcal{A}^{12}(\mathbf{q}; \mathbf{P}) = \frac{1}{\sqrt{1+\delta_{\mathbf{q},0}}}\{C_0(+)C_1(\mathbf{P}, -)V(+) + C_0(-)C_1(\mathbf{P}, +)V(-)$$
$$- C_0(P)C_2(+, -)V(P)\}$$

where we used the notation $\pm \equiv \pm\mathbf{q} + \mathbf{P}/2$.

(iii) $\mathcal{A}^{22}$

$$\mathcal{A}^{22}(\mathbf{q}', \mathbf{q}; \mathbf{P}) = \langle\Phi| \left[\frac{\eta_{\mathbf{q}'+\mathbf{P}/2}\eta_{-\mathbf{q}'+\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q}',0}}}, H, \frac{\eta^{\dagger}_{\mathbf{q}+\mathbf{P}/2}\eta^{\dagger}_{-\mathbf{q}+\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q},0}}} \right] |\Phi\rangle.$$

The terms involving $\hat{h}_{1,1}$ and $\hat{h}_{2,2}$ of $\hat{h}_2$ and $\hat{h}_4$ respectively contribute to this matrix element, leading to

$$\begin{aligned}\mathcal{A}^{22}(\mathbf{q}', \mathbf{q}; \mathbf{P}) &= [\omega(-\mathbf{q}+\mathbf{P}/2) + \omega(\mathbf{q}+\mathbf{P}/2)]\delta_{\mathbf{q},\mathbf{q}'} \\ &\quad + \frac{1}{\sqrt{(1+\delta_{\mathbf{q},0})(1+\delta_{\mathbf{q}',0})}} \\ &\quad \times \{h_{2,2}(\mathbf{q}+\mathbf{P}/2, -\mathbf{q}+\mathbf{P}/2, \mathbf{q}'-\mathbf{q}) + h_{2,2}(\mathbf{q}'+\mathbf{P}/2, -\mathbf{q}'+\mathbf{P}/2, \mathbf{q}-\mathbf{q}') \\ &\quad + h_{2,2}(-\mathbf{q}+\mathbf{P}/2, \mathbf{q}+\mathbf{P}/2, \mathbf{q}'+\mathbf{q}) + h_{2,2}(-\mathbf{q}'+\mathbf{P}/2, \mathbf{q}'+\mathbf{P}/2, \mathbf{q}+\mathbf{q}')\}.\end{aligned}$$

Using the expression for $h_{2,2}$ calculated in appendix A we get

$$\begin{aligned}\mathcal{A}^{22}(\mathbf{q}', \mathbf{q}; \mathbf{P}) &= [\omega(-) + \omega(+)]\delta_{\mathbf{q},\mathbf{q}'} + \frac{1}{\sqrt{(1+\delta_{\mathbf{q},0})(1+\delta_{\mathbf{q}',0})}} \\ &\quad \times \{C_2(+', -')C_2(+, -)V(P) + C_1(+, +')C_1(-, -')V(|\mathbf{q}-\mathbf{q}'|) \\ &\quad + C_1(+', -)C_1(+, -')V(|\mathbf{q}+\mathbf{q}'|)\}.\end{aligned}$$

B.2. Sub-matrices of $\mathcal{B}$

(i) B^{11}

$$\mathcal{B}^{11}(\mathbf{P}) = \langle\Phi|[\eta_{\mathbf{P}}, H, \eta_{-\mathbf{P}}]|\Phi\rangle = 0.$$

since, by inspection, we see that there are no terms in the Hamiltonian that contribute to this matrix element.

(ii) $\mathcal{B}^{12} = (\mathcal{B}^{21})^{\mathrm{T}}$

$$\mathcal{B}^{12}(\mathbf{q}; \mathbf{P}) = \langle\Phi| \left[\eta_{\mathbf{P}}, H, \frac{\eta_{-\mathbf{q}-\mathbf{P}/2}\eta_{\mathbf{q}-\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q},0}}} \right] |\Phi\rangle.$$

In this case the only contribution comes from $\hat{h}_3$ through the term $\hat{h}_{3,0}$, so

$$\begin{aligned}\mathcal{B}^{12}(\mathbf{q}; \mathbf{P}) &= -\frac{2}{\sqrt{1+\delta_{\mathbf{q},0}}}[h_{3,0}(\mathbf{q}+\mathbf{P}/2, -\mathbf{q}+\mathbf{P}/2) \\ &\quad + h_{3,0}(-\mathbf{q}+\mathbf{P}/2, -\mathbf{P}) + h_{3,0}(\mathbf{q}+\mathbf{P}/2, -\mathbf{P})]\end{aligned}$$

which can be written in terms of the coherence factors as

$$\begin{aligned}\mathcal{B}^{12}(\mathbf{q}; \mathbf{P}) &= -\frac{1}{\sqrt{1+\delta_{\mathbf{q},0}}}[C_0(+)C_2(\mathbf{P}, -)V(+) \\ &\quad + C_0(-)C_2(\mathbf{P}, +)V(-) + C_0(P)C_2(+, -)V(P)].\end{aligned}$$

(iii) B^{22}

$$B^{22}(\mathbf{q}', \mathbf{q}; \mathbf{P}) = \langle\Phi| \left[\frac{\eta_{\mathbf{q}'+\mathbf{P}/2}\eta_{-\mathbf{q}'+\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q}',0}}}, H, \frac{\eta_{\mathbf{q}-\mathbf{P}/2}\eta_{-\mathbf{q}-\mathbf{P}/2}}{\sqrt{1+\delta_{\mathbf{q},0}}} \right] |\Phi\rangle.$$

The only non-vanishing contribution to this matrix element comes from $\hat{h}_4$ through the term $\hat{h}_{4,0}$, giving

$$\begin{aligned}B^{22}(\mathbf{q}', \mathbf{q}; \mathbf{P}) = &-h_{0,4}(-\mathbf{q} + \mathbf{P}/2, -\mathbf{q}' - \mathbf{P}/2, \mathbf{q} - \mathbf{q}') \\ &- h_{0,4}(\mathbf{q} + \mathbf{P}/2, -\mathbf{q}' - \mathbf{P}/2, -\mathbf{q}' - \mathbf{q}) \\ &- h_{0,4}(-\mathbf{q} + \mathbf{P}/2, \mathbf{q} + \mathbf{P}/2, -\mathbf{q}' + \mathbf{q}) - h_{0,4}(\mathbf{q} + \mathbf{P}/2, -\mathbf{q} + \mathbf{P}/2, -\mathbf{q} - \mathbf{q}') \\ &- h_{0,4}(-\mathbf{q} + \mathbf{P}/2, \mathbf{q}' - \mathbf{P}/2, \mathbf{q}' + \mathbf{q}) - h_{0,4}(\mathbf{q} + \mathbf{P}/2, \mathbf{q}' - \mathbf{P}/2, \mathbf{q}' - \mathbf{q}) \\ &- h_{0,4}(-\mathbf{q} + \mathbf{P}/2, \mathbf{q} + \mathbf{P}/2, \mathbf{q} + \mathbf{q}') - h_{0,4}(\mathbf{q} + \mathbf{P}/2, -\mathbf{q} + \mathbf{P}/2, \mathbf{q}' - \mathbf{q}) \\ &- h_{0,4}(\mathbf{q}' - \mathbf{P}/2, -\mathbf{q} + \mathbf{P}/2, \mathbf{P}) - h_{0,4}(\mathbf{q}' - \mathbf{P}/2, \mathbf{q} + \mathbf{P}/2, \mathbf{P}) \\ &- h_{0,4}(-\mathbf{q}' - \mathbf{P}/2, -\mathbf{q} + \mathbf{P}/2, \mathbf{P}) - h_{0,4}(-\mathbf{q}' - \mathbf{P}/2, \mathbf{q} + \mathbf{P}/2, \mathbf{P}) \\ &+ \{q \rightleftharpoons q'\}, \{P \to -P\}\end{aligned}$$

which can be written in terms of the coherence factors as

$$\begin{aligned}B^{22}(\mathbf{q}', \mathbf{q}; \mathbf{P}) = &-\frac{1}{\sqrt{(1 + \delta_{\mathbf{q},0})(1 + \delta_{\mathbf{q}',0})}}\{C_2[+, +']C_2[-, -'][V(|\mathbf{q} + \mathbf{q}'|) \\ &+ V(|\mathbf{q} - \mathbf{q}'|)] + C_2[+, -]C_2[+', -']V(P)\}.\end{aligned}$$

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