A Variational derivation of the time-dependent Hartree-Fock Bogoliubov-De Gennes equations for ultracold trapped Bose gases

Benarous Mohamed†, Boudjemaa Abd-El-Aali‡, Chachou-Sameut Houria

1- Laboratory of Theoretical Physics and Material Physics, Faculty of Science, Hassiba Benbouali University of Chlef, B.P 151, Route de Sendjas, Chlef, Algeria.

*Corresponding author. GSM: 213559907262; Tel./Fax: 21327773260; E-mail: benarous_med@yahoo.fr, m.benarous@univ-chlef.dz

Abstract

We use the time dependent variational principle of Balian and Vénérioni to derive the dynamics of an ultracold trapped boson gas. The Hartree-Fock-Bogoliubov-De Gennes equations appear as a special case of our formalism. The latter is not only free of known inconsistencies of the previous approach but allows also for a consistent determination of various correlation functions.

Keywords: Ultracold trapped gases, Bose-Einstein condensation, variational formalism, HFB-. BdG equations

1. Introduction

A long standing problem in ultra-cold boson gases and in general in many body problems, is that while the Gross-Pitaevskii equation can be derived from variational principles, its finite temperature extensions, which take into account the dynamics of the thermal cloud and that of the anomalous average, seem to resist such a formulation. In particular, up to now, one does not know how to derive variationally and in a consistent way, the non local version of the ”Hartree-Fock-Bogoliubov-De Gennes equations”.

In a recent paper[1], we have derived variationally a set of dynamical coupled equations (which we called TDHFB for Time-Dependent Hartree-Fock-Bogoliubov) for dilute trapped boson gases below the transition. These equations were shown to generalize in a consistent way the Gross-Pitaevskii equations[2] in that they introduce a non trivial coupling between the order parameter, the thermal cloud and the anomalous density. Furthermore, they exhibit an intrinsic dynamics of these last two quantities which has never been written down before (an exception is perhaps the paper of Chernyak et al[3] which discusses a somewhat similar set of equations but uses a notation different from ours). This dynamics induces an effect on the condensate density which is highly needed in order to go beyond the HFB-Popov approximations. Indeed, the discrepancies between the HFB-Popov computed properties and the experimental results that show up at temperatures as high as 60% of the transition temperature seem to be related to the absence of a feedback effect of the dynamics of both the thermal cloud and the anomalous density on the condensate density.

The paper is organized as follows. In section 2, we present our main tool which is the time-dependent variational principle of R. Balian and M. Vénéroni (BV) proposed earlier in the context of the nuclear many-body problem[4]. Then, we derive the nonlocal TDHFB equations and show how they can be related to the HFB-BdG equations. In section 3, we discuss some of their formal properties and show how the inconsistencies of the naïve approach nicely disappear.
2. The BV variational principle and the TDHFB equations

The BV variational principle requires the choice of a trial space for the density operator. We choose to consider a gaussian time-dependent density-like operator. This Ansatz which belongs to the class of the generalized coherent states allows us to perform the calculation (since there exists a Wick’s theorem) while retaining some fundamental aspects such as the pairing between atoms.

The derivation of the Time-Dependent Hartree-Fock Bogoliubov (TDHFB) equations is performed along the following steps. First we define $\Psi^+$ and $\Psi$ as the boson creation and destruction operator fields, satisfying the usual canonical commutation relations. Then we consider a two-body grand canonical Hamiltonian of trapped bosons with mass $M$:

$$
H = \int \frac{\hbar^2}{2M} \Delta + V_{\text{ext}}(\vec{r}) - \mu \right] \Psi(\vec{r}) \\
+ \frac{1}{2} \int_{\vec{r},\vec{r}'} \Psi^+(\vec{r})\Psi^+(\vec{r}')V(\vec{r},\vec{r}')\Psi(\vec{r})\Psi(\vec{r}').
$$

(2.1)

$V_{\text{ext}}(\vec{r})$ is the trapping potential and $\mu$ is the chemical potential. With the Gaussian Ansatz, we define the boson field expectation value (or order parameter), the non-condensate density and the anomalous density as:

$$
\Phi(\vec{r}) = \langle \Psi(\vec{r}) > \\
\tilde{n}(\vec{r},\vec{r}') = \langle \Psi^+(\vec{r})\Psi(\vec{r}') > - \langle \Psi^+(\vec{r}) \rangle \langle \Psi(\vec{r}') > \\
\tilde{m}(\vec{r},\vec{r}') = \langle \Psi(\vec{r})\Psi(\vec{r}') > - \langle \Psi(\vec{r}) > \langle \Psi(\vec{r}') >
$$

(2.2)

The TDHFB equations are a direct consequence of the BV variational principle. They were first written in a local form in [2] then in a non-local form in [5]. They read:

$$
i\hbar \tilde{\Phi}(\vec{r}) = H^{\text{op}}(\vec{r})\Phi(\vec{r}) \\
i\hbar \tilde{n}(\vec{r},\vec{r}') = [H^{\text{op}}(\vec{r}) - H^{\text{op}}(\vec{r}')] \tilde{n}(\vec{r},\vec{r}') \\
i\hbar \tilde{m}(\vec{r},\vec{r}') = [H^{\text{op}}(\vec{r}) + H^{\text{op}}(\vec{r}')] \tilde{m}(\vec{r},\vec{r}')
$$

(2.3)

where

$$
a(\vec{r},\vec{r}') = \langle \psi^+(\vec{r})\psi(\vec{r}') \rangle = \tilde{n}(\vec{r},\vec{r}') + \Phi^*(\vec{r})\Phi(\vec{r}')
$$

and

$$
b(\vec{r},\vec{r}') = \langle \psi(\vec{r})\psi(\vec{r}') \rangle = \tilde{m}(\vec{r},\vec{r}') + \Phi(\vec{r})\Phi(\vec{r}').
$$

In the case of a contact potential $V(\vec{r},\vec{r}') = \delta(\vec{r} - \vec{r}')$, they simplify to yield:

2*Corresponding Author: Pr. Mohamed Benarous, Laboratory for Theoretical Physics and Material Physics, Faculty of Science, Hassiba Benbouali University of Chlef, Algeria. (m.benarous@univ-chlef.dz, benarous_med@yahoo.fr)
\[ i\hbar \hat{\Phi}(r) = [H^{sp}(r) + g(n_c(r) + 2\tilde{n}(r))] \Phi(r) + g\tilde{m}(r)\Phi^*(r), \]
\[ i\hbar \hat{\tilde{n}}(r, r') = \left[ (H^{sp}(r) + 2gn(r)) - (H^{sp}(r') + 2gn(r')) \right] \tilde{n}(r, r') + g \left[ b(r', r')\tilde{m}^*(r, r') - b^*(r, r)\tilde{m}(r, r') \right], \]
\[ i\hbar \hat{m}(r, r') = \left[ (H^{sp}(r) + 2gn(r)) + (H^{sp}(r') + 2gn(r')) \right] m(r, r') + g \left[ b(r', r')\tilde{m}^*(r, r') + b^*(r, r)\tilde{m}(r, r') \right], \]
where \( n_c(r) = |\Phi(r)|^2, \tilde{n}(r, r) = \tilde{n}(r, r) \) and \( \tilde{m}(r) = \tilde{m}(r, r) \) are respectively the condensate density, the non-condensate density and the anomalous density.

Obviously, there is a diverging term in the third equation of (2.4) which does not allow for a direct computation of the local limit. However, in the quasi-homogeneous limit, we may set
\[ \tilde{n}(r, r') = -\frac{1}{2} \sum_k (1 + 2n_k) \left( U_k(r)V_k(r') + U_k^*(r)V_k^*(r') \right), \]
\[ \tilde{m}(r, r') = \sum_k \left( n_k U_k^*(r)U_k(r') + (1 + n_k)V_k^*(r)V_k(r') \right), \]
where \( U_k \) and \( V_k \) are linearly independent space functions and \( n_k \) is the occupation probability given at equilibrium by the Bose-Einstein distribution. Upon inserting (2.5) into (2.4), we readily get
\[ i\hbar \hat{U}_k(r) = \left[ H^{sp}(r) + 2gn(r) \right] U_k(r) - gb(r, r)V_k^*(r), \]
\[ i\hbar \hat{V}_k(r) = \left[ H^{sp}(r) + 2gn(r) \right] V_k(r) - gb(r, r)U_k^*(r), \]
which are clearly the Bogoliubov–De Gennes equations [6,7]. Our equations (2.4) are clearly still valid even in the non-homogeneous case.

3. Results and discussion

There are a number of important implications of these equations. First of all, for a general Hamiltonian (without specifying the two-body interactions), the equations are energy and number conserving. This is to be contrasted to the literature where the conservation of the total number of atoms is not guaranteed a priori and one has to introduce heuristically a symmetry-breaking operator[6]. On the other hand, when considering a contact potential (hard sphere model) and taking correctly the local limit, one recovers the HFB-BdG equations but only in the quasi-homogeneous case. This means in particular that the G(eneralized)HFB equations [5] are only valid in the quasi-homogeneous case. On the contrary, our equations do not require quasi-homogeneity. Moreover, the UV divergences that appear in the anomalous density are more simply handled.

*Corresponding Author:* Pr. Mohamed Benarous, Laboratory for Theoretical Physics and Material Physics, Faculty of Science, Hassiba Benbouali University of Chlef, Algeria. (m.benarous@univ-chlef.dz, benarous_med@yahoo.fr)
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