Derivation of the Gross-Pitaevskii Equation for Condensed Bosons from the Bogoliubov-de Gennes Equations for Superfluid Fermions

P. Pieri and G. C. Strinati

Dipartimento di Fisica, UdR INFM, Università di Camerino, I-62032 Camerino, Italy (Received 20 December 2002; published 15 July 2003)

We derive the time-independent Gross-Pitaevskii equation at zero temperature for condensed bosons, which form as bound-fermion pairs when the mutual fermionic attractive interaction is sufficiently strong, from the strong-coupling limit of the Bogoliubov–de Gennes equations that describe superfluid fermions in the presence of an external potential. Three-body corrections to the Gross-Pitaevskii equation are also obtained by our approach. Our results are relevant to the recent advances with ultracold fermionic atoms in a trap.

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Evolution from superfluid fermions to condensed composite bosons appears on the verge of being experimentally realized in terms of dilute ultracold fermionic atoms in a trap, although several experimental difficulties still remain to be overcome [1]. Dilute condensed bosons in harmonic traps, in particular, have already been studied extensively [2]. From a theoretical point of view, their macroscopic properties (such as the density profile) have been described by the time-independent Gross-Pitaevskii (GP) equation for the condensate wave function [3] (see also Refs. [4,5]). Superfluid fermions in the presence of a spatially varying external potential, on the other hand, are usually described in terms of the Bogoliubovde Gennes (BdG) equations [6], where a spatially varying gap function is obtained from a set of two-component fermion wave functions. Several problems (such as the calculation of the Josephson current [7]) have been approached in terms of the BdG equations for superfluid fermions.

Given the possible experimental connection between the properties of superfluid fermions with a strong mutual attraction and of condensed bosons, a corresponding theoretical connection between these two (GP and BdG) approaches seems appropriate at this time. In this way, one could even explore the interesting intermediatecoupling (crossover) region, where neither the fermionic nor the bosonic properties are fully realized [8].

In this Letter, we establish for the first time this connection by showing that the time-independent GP equation at zero temperature can be obtained as the strong-coupling limit (to be specified below) of the BdG equations. This result thus shows that the BdG equations, originally conceived for weak coupling, are also appropriate to describe the strong-coupling limit, whereby the fermionic gap function is suitably mapped onto the condensate wave function of the GP equation. Our derivation of the GP equation explains also the reason for the apparent similarity between the GP equation for condensed bosons and the Ginzburg-Landau equation for the superconducting order parameter near the critical temperature. Combining, in fact, the present derivation of the GP equation at low temperature in the strongcoupling limit with Gorkov's previous derivation [9] of the Ginzburg-Landau equation near the critical temperature in the weak-coupling limit, one realizes that these two different equations can be derived as two different limits of the same BdG equations. Our approach further enables us to obtain high-order corrections to the GP equation; in particular, the three-body correction is here explicitly derived.

We begin by considering the BdG equations for superfluid fermions in the presence of a spatially varying external potential $V(\mathbf{r})$:

$$\begin{bmatrix} \mathcal{H}(\mathbf{r}) & \Delta(\mathbf{r}) \\ \Delta(\mathbf{r})^* & -\mathcal{H}(\mathbf{r}) \end{bmatrix} \begin{bmatrix} u_n(\mathbf{r}) \\ v_n(\mathbf{r}) \end{bmatrix} = \epsilon_n \begin{bmatrix} u_n(\mathbf{r}) \\ v_n(\mathbf{r}) \end{bmatrix}.$$
 (1)

Here

$$\mathcal{H}(\mathbf{r}) = -\frac{\nabla^2}{2m} + V(\mathbf{r}) - \mu \qquad (2)$$

is the single-particle Hamiltonian reckoned on the (fermionic) chemical potential μ (*m* being the fermionic mass and $\hbar = 1$ throughout), while

$$\Delta(\mathbf{r}) = - \upsilon_0 \sum_n u_n(\mathbf{r}) \upsilon_n(\mathbf{r})^* [1 - 2f(\boldsymbol{\epsilon}_n)] \quad (3)$$

is the gap function that has to be self-consistently determined [6], where $f(\epsilon_n) = [\exp(\beta \epsilon_n) + 1]^{-1}$ is the Fermi function with inverse temperature β [the sum in Eq. (3) being limited to positive eigenvalues ϵ_n only]. The negative constant v_0 in Eq. (3) originates from the attractive interaction acting between fermions with opposite spins (or fermionic atoms with two different internal states) and taken of the contact-potential form $v_0 \,\delta(\mathbf{r} - \mathbf{r}')$, which can be conveniently regularized in terms of the scattering length a_F of the associated two-body problem [10,11]. Correspondingly, the gap function has *s*-wave component only with spinless structure. Solution of the BdG equations (1) is equivalent to considering the associated Green's function equation (in matrix form):

$$\begin{bmatrix} i\omega_s - \mathcal{H}(\mathbf{r}) & -\Delta(\mathbf{r}) \\ -\Delta(\mathbf{r})^* & i\omega_s + \mathcal{H}(\mathbf{r}) \end{bmatrix} \hat{\mathcal{G}}(\mathbf{r}, \mathbf{r}'; \omega_s) = \hat{\mathbf{1}}\delta(\mathbf{r} - \mathbf{r}'),$$
(4)

where $\omega_s = (2s + 1)\pi/\beta$ (s integer) is a fermionic Matsubara frequency, $\hat{\mathbf{1}}$ is the unit dyadic, and $\hat{\mathbf{G}}$ is the single-particle Green's function in Nambu's notation [12]. Solutions of Eqs. (1) and (4) are, in fact, related by the expression

$$\hat{\boldsymbol{\mathcal{G}}}(\mathbf{r},\mathbf{r}';\boldsymbol{\omega}_{s}) = \sum_{n} \begin{bmatrix} u_{n}(\mathbf{r}) \\ \boldsymbol{\upsilon}_{n}(\mathbf{r}) \end{bmatrix} \frac{1}{i\boldsymbol{\omega}_{s} - \boldsymbol{\epsilon}_{n}} \begin{bmatrix} u_{n}(\mathbf{r}')^{*}, \boldsymbol{\upsilon}_{n}(\mathbf{r}')^{*} \end{bmatrix} \\ + \sum_{n} \begin{bmatrix} -\boldsymbol{\upsilon}_{n}(\mathbf{r})^{*} \\ u_{n}(\mathbf{r})^{*} \end{bmatrix} \frac{1}{i\boldsymbol{\omega}_{s} + \boldsymbol{\epsilon}_{n}} \begin{bmatrix} -\boldsymbol{\upsilon}_{n}(\mathbf{r}'), u_{n}(\mathbf{r}') \end{bmatrix}.$$
(5)

We adopt at this point Gorkov's procedure [9] for expressing the solution of Eq. (4) in terms of the noninteracting Green's function \tilde{G}_0 that satisfies the equation

$$[i\omega_s - \mathcal{H}(\mathbf{r})]\tilde{\mathcal{G}}_0(\mathbf{r},\mathbf{r}';\omega_s) = \delta(\mathbf{r}-\mathbf{r}') \qquad (6)$$

and subject to the *same* external potential $V(\mathbf{r})$. We are thus led to consider the two coupled integral equations:

$$\mathcal{G}_{11}(\mathbf{r},\mathbf{r}';\boldsymbol{\omega}_s) = \tilde{\mathcal{G}}_0(\mathbf{r},\mathbf{r}';\boldsymbol{\omega}_s) + \int d\mathbf{r}'' \tilde{\mathcal{G}}_0(\mathbf{r},\mathbf{r}'';\boldsymbol{\omega}_s) \Delta(\mathbf{r}'')$$
$$\times \mathcal{G}_{21}(\mathbf{r}'',\mathbf{r}';\boldsymbol{\omega}_s), \tag{7}$$

$$\mathcal{G}_0(\mathbf{r}-\mathbf{r}';\omega_s|\mu) = \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{i\omega_s-\mathbf{k}^2/(2m)+\mu} =$$

that holds for any coupling. With the above conditions, it can be verified that the expression

$$\tilde{\mathcal{G}}_0(\mathbf{r}, \mathbf{r}'; \boldsymbol{\omega}_s) \simeq \mathcal{G}_0(\mathbf{r} - \mathbf{r}'; \boldsymbol{\omega}_s | \boldsymbol{\mu} - [V(\mathbf{r}) + V(\mathbf{r}')]/2),$$
(11)

whereby the chemical potential μ in expression (10) is replaced by the local form $\mu - [V(\mathbf{r}) + V(\mathbf{r}')]/2$, satisfies Eq. (6) in the presence of the external potential. (The midpoint rule, albeit superfluous for most of the following arguments owing to the slowness of the potential over the distance a_F , has been adopted for later convenience in the derivation of the current density.) The novel approximate expression (11) allows one to deal readily with the external scalar potential, and plays in the present context an analogous role to the eikonal approximation for Gorkov's problem in the presence of an external magnetic field [9].

In particular, for the corresponding one-dimensional problem with a generic (albeit nonpathological) potential V(x) that satisfies the first two above conditions $[a_F]$

$$\mathcal{G}_{21}(\mathbf{r}, \mathbf{r}'; \boldsymbol{\omega}_s) = -\int d\mathbf{r}'' \, \tilde{\mathcal{G}}_0(\mathbf{r}'', \mathbf{r}; -\boldsymbol{\omega}_s) \Delta(\mathbf{r}'')^* \\ \times \, \mathcal{G}_{11}(\mathbf{r}'', \mathbf{r}'; \boldsymbol{\omega}_s) \tag{8}$$

for the normal (G_{11}) and anomalous (G_{21}) single-particle Green's functions. Equations (7) and (8), together with the self-consistency equation

$$\Delta^*(\mathbf{r}) = v_0 \frac{1}{\beta} \sum_{s} \mathcal{G}_{21}(\mathbf{r}, \mathbf{r}; \omega_s)$$
(9)

are fully equivalent to the original BdG equations (1) and (3), and hold for any coupling.

We pass now to specifically consider the *strong*coupling limit of Eqs. (7)–(9), and show under what circumstances they reduce to the GP equation for spinless composite bosons with mass 2m and subject to the potential $2V(\mathbf{r})$. In this limit, the fermionic chemical potential approaches $-\varepsilon_0/2$, where $\varepsilon_0 = (ma_F^2)^{-1}$ is the binding energy of the composite boson which represents the largest energy scale of the problem.

In the present context, achieving the strong-coupling limit implies that the conditions $|V(\mathbf{r})| \ll |\mu|$, $a_F |\nabla V(\mathbf{r})| \ll |V(\mathbf{r})|$, and $a_F^2 |\nabla^2 V(\mathbf{r})| \ll |V(\mathbf{r})|$ hold for all relevant values of \mathbf{r} . In the strong-coupling limit, $a_F \sim (2m|\mu|)^{-1/2}$ represents the characteristic length scale for the noninteracting Green's function of the associated homogeneous problem [with $V(\mathbf{r}) = 0$], as it can be seen from the expression

$$\frac{m}{2\pi |\mathbf{r} - \mathbf{r}'|} \exp\{i \operatorname{sgn}(\omega_s) \sqrt{2m(\mu + i\omega_s)} |\mathbf{r} - \mathbf{r}'|\}$$
(10)

therein being replaced by $a = (2m|\mu|)^{-1/2}$, one can readily verify that our expression (11), namely,

$$\tilde{\mathcal{G}}_{0}(x, x'; \omega_{s}) = -\frac{me^{-\sqrt{2m(|\mu| + [V(x) + V(x')]/2 - i\omega_{s})}|x - x'|}}{\sqrt{2m(|\mu| + [V(x) + V(x')]/2 - i\omega_{s})}},$$
(12)

is fully equivalent to the solution of the (one-dimensional version of the) Green's function Eq. (6) as obtained in terms of the asymptotic $(a \rightarrow 0^+)$ WKB approximation [13]. This identification holds in the relevant range $|x - x'| \leq a$ and provided $|\omega_s| \ll |\mu|$ (that can be always satisfied for sufficiently large $|\mu|$).

Derivation of the GP equation from the BdG equations in the strong-coupling limit exploits the expression (11) and proceeds by using Eq. (7) to expand perturbatively Eq. (8) up to third order in $\Delta(\mathbf{r})$ [the ratio $\Delta(\mathbf{r})/|\mu|$ providing the small parameter for this expansion]. Equation (9) yields eventually the following integral equation for the gap function:

$$-\frac{1}{\nu_0}\Delta(\mathbf{r})^* = \int d\mathbf{r}_1 Q(\mathbf{r}, \mathbf{r}_1)\Delta(\mathbf{r}_1)^* + \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \ R(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2.\mathbf{r}_3) \times \Delta(\mathbf{r}_1)^* \Delta(\mathbf{r}_2)\Delta(\mathbf{r}_3)^*$$
(13)

with the notation

$$Q(\mathbf{r},\mathbf{r}_1) = \frac{1}{\beta} \sum_{s} \tilde{\mathcal{G}}_0(\mathbf{r}_1,\mathbf{r};-\omega_s) \,\tilde{\mathcal{G}}_0(\mathbf{r}_1,\mathbf{r};\omega_s) \qquad (14)$$

and

$$R(\mathbf{r}, \mathbf{r}_{1}, \mathbf{r}_{2}, \mathbf{r}_{3}) = -\frac{1}{\beta} \sum_{s} \tilde{\mathcal{G}}_{0}(\mathbf{r}_{1}, \mathbf{r}; -\omega_{s}) \tilde{\mathcal{G}}_{0}(\mathbf{r}_{1}, \mathbf{r}_{2}; \omega_{s})$$
$$\times \tilde{\mathcal{G}}_{0}(\mathbf{r}_{3}, \mathbf{r}_{2}; -\omega_{s}) \tilde{\mathcal{G}}_{0}(\mathbf{r}_{3}, \mathbf{r}; \omega_{s}).$$
(15)

The expression (11) implies that, in strong coupling, $Q(\mathbf{r}, \mathbf{r}_1)$ vanishes for $|\mathbf{r} - \mathbf{r}_1| \ge a_F$. Since [as a consequence of the above conditions on the external potential] $\Delta(\mathbf{r})$ is slowly varying over the length scale a_F , we can set $\Delta(\mathbf{r}_1)^* \simeq \Delta(\mathbf{r})^*$ on the right-hand side of Eq. (13) and write

$$\int d\mathbf{r}_1 Q(\mathbf{r}, \mathbf{r}_1) \Delta(\mathbf{r}_1)^* \simeq \left[a_0(\mathbf{r}) + \frac{1}{2} b_0(\mathbf{r}) \nabla^2 \right] \Delta(\mathbf{r})^*, \quad (16)$$

$$a_0(\mathbf{r}) = \int d\mathbf{r}_1 Q(\mathbf{r}, \mathbf{r}_1) = \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{\frac{k^2}{m} + 2|\boldsymbol{\mu}(\mathbf{r})|}$$
$$\simeq -\frac{1}{\nu_0} + \frac{m^2 a_F}{8\pi} [\boldsymbol{\mu}_B - 2V(\mathbf{r})]$$
(17)

and

$$b_0(\mathbf{r}) = \frac{1}{3} \int d\mathbf{r}_1 \ Q(\mathbf{r}, \mathbf{r}_1) |\mathbf{r}_1 - \mathbf{r}|^2 \simeq \frac{m a_F}{16 \pi}.$$
 (18)

Here, $\mu(\mathbf{r}) = \mu - V(\mathbf{r})$ and we have introduced the bosonic chemical potential $\mu_B = 2\mu + \varepsilon_0$ such that $\mu_B \ll \varepsilon_0$. Note that $[V(\mathbf{r}) + V(\mathbf{r}_1)]/2$ in the local chemical potential has been replaced by $V(\mathbf{r})$ at the relevant order, since the external potential is slowly varying over the distance a_F . Disposal of the ultraviolet divergence in Eq. (17) via the regularization of the contact potential [10,11] in terms of a_F and use of the strong-coupling assumption $\beta\mu \rightarrow -\infty$ have led to the approximate expressions (17) and (18). By a similar token, we obtain

$$d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \ R(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \ \Delta(\mathbf{r}_1)^* \ \Delta(\mathbf{r}_2) \ \Delta(\mathbf{r}_3)^* \simeq c_0 |\Delta(\mathbf{r})|^2 \Delta(\mathbf{r})^*$$
(19)

with $c_0 \simeq -(m^2 a_F/8\pi)^2 8\pi a_F/(2m)$. Entering the approximate expressions (16)–(19) into the integral Eq. (13) for the gap function and introducing the *condensate wave function* $\Phi(\mathbf{r}) = \sqrt{(m^2 a_F)/8\pi} \Delta(\mathbf{r})$, we obtain eventually

$$-\frac{1}{4m}\nabla^2\Phi(\mathbf{r}) + 2V(\mathbf{r})\Phi(\mathbf{r}) + \frac{8\pi a_F}{2m}|\Phi(\mathbf{r})|^2\Phi(\mathbf{r}) = \mu_B\Phi(\mathbf{r}).$$
(20)

This is just the *time-independent Gross-Pitaevskii equation* for composite bosons of mass $m_B = 2m$, chemical potential μ_B , subject to the external potential $2 V(\mathbf{r})$, and mutually interacting via the short-range repulsive potential $4\pi a_B/m_B$ where $a_B = 2a_F$. It was pointed out in Ref. [11] that this value of a_B corresponds to treating the scattering of composite bosons within the Born approximation, while improvement of this approximation to include the *t*-matrix scattering results in a mere reduction of the bosonic scattering length by a factor of order unity. Note that the two-body binding energy ε_0 has been eliminated from explicit consideration via the bound-state equation. Note also that the nontrivial rescaling between the gap function and the condensate wave function has been fixed by the nonlinear term in Eq. (20).

Equation (20) has been formally obtained from the original BdG equations in the limit $\beta \mu \rightarrow -\infty$. In this respect, it would seem that this equation holds even near the condensation temperature T_c , where the GP equation is instead known not to be valid. On physical grounds, however, at finite temperature excitations of bosons out of the condensate (that are not included in the present treat-

ment) are expected to be important especially in the strong-coupling regime of the BdG equations, thus restricting the range of validity of Eq. (20) near zero temperature.

The physical interpretation of the condensate wave function can be obtained from the general expression for the density $n(\mathbf{r}) = (2/\beta)\sum_s \exp(i\omega_s \eta)G_{11}(\mathbf{r}, \mathbf{r}; \omega_s)$, where G_{11} is obtained by combining Eqs. (7) and (8) and expanding perturbatively up to second order in $\Delta(\mathbf{r})$. Recalling that the fermionic contribution $(2/\beta)\sum_s \exp(i\omega_s \eta)G_0(\mathbf{r}, \mathbf{r}; \omega_s)$ vanishes in the strongcoupling limit, one is left with the expression

$$n(\mathbf{r}) \simeq -2|\Delta(\mathbf{r})|^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{\beta} \sum_s \mathcal{G}_0(\mathbf{k}, \omega_s)^2 \mathcal{G}_0(\mathbf{k}, -\omega_s)$$
$$\simeq -2|\Delta(\mathbf{r})|^2 \left(-\frac{m^2 a_F}{8 \pi}\right) = 2|\Phi(\mathbf{r})|^2$$
(21)

evaluated in terms of the wave-vector representation of G_0 . Since the bosonic density $n_B(\mathbf{r})$ is just half the fermionic density $n(\mathbf{r})$, from Eq. (21) we obtain that

 $n_B(\mathbf{r}) = |\Phi(\mathbf{r})|^2$, as usual with the GP equation. The normalization condition $N = \int d\mathbf{r} n(\mathbf{r})$ (or, equivalently, its bosonic counterpart) fixes, in turn, the overall chemical potential μ (or directly μ_B in the strong-coupling limit).

By a similar token, the current density can be obtained from the general expression $\mathbf{j}(\mathbf{r}) = \frac{1}{im} (\nabla - \nabla') \frac{1}{\beta} \times \sum_{s} e^{i\omega_{s}\eta} \mathcal{G}_{11}(\mathbf{r}, \mathbf{r}'; \omega_{s})|_{\mathbf{r}=\mathbf{r}'}$ by combining Eqs. (7) and (8) as before. The independent-particle contribution to the current now vanishes exactly with the midpoint rule (11). After long but straightforward manipulations one obtains for the remaining contributions in the limit $\beta \mu \rightarrow -\infty$:

$$\mathbf{j}(\mathbf{r}) \simeq \frac{1}{2im} \left[\Phi(\mathbf{r})^* \nabla \Phi(\mathbf{r}) - \Phi(\mathbf{r}) \nabla \Phi(\mathbf{r})^* \right], \quad (22)$$

which is, as expected, twice the value of the quantummechanical expression of the current for a composite boson with mass $m_B = 2m$ and wave function $\Phi(\mathbf{r})$.

It is clear from the above derivation that higher-order corrections to the GP Eq. (20) can also be obtained by expanding Eqs. (7) and (8) to higher than the third order in $\Delta(\mathbf{r})$. In particular, to fifth order in $\Delta(\mathbf{r})$ the following term adds to the right-hand side of Eq. (8) (with $\mathbf{r} = \mathbf{r}'$) once summed over ω_s :

$$-|\Delta(\mathbf{r})|^{4}\Delta(\mathbf{r})^{*}\int \frac{d\mathbf{k}}{(2\pi)^{3}}\frac{1}{\beta}\sum_{s}\mathcal{G}_{0}(\mathbf{k},\,\omega_{s})^{3}\mathcal{G}_{0}(\mathbf{k},\,-\omega_{s})^{3}.$$
(23)

Evaluating the integral in Eq. (23) in the strong-coupling limit and recalling the above rescaling between the gap function and the condensate wave function, one finds that the term $g_3 |\Phi(\mathbf{r})|^4 \Phi(\mathbf{r})$ adds to the left-hand side of the GP Eq. (20), where the *three-body interaction* $g_3 =$ $-30\pi^2 a_F^4/m$ is attractive. As an example, taking for m_B the mass of ⁸⁵Rb and the typical value $a_B \sim 250$ a.u., one gets $|g_3|/\hbar \sim 10^{-27}$ cm⁶ s⁻¹ with the correct order of magnitude [14]. A single calculation with a fermionic point-contact potential has thus provided both a repulsive bosonic two-body term and a *real* three-body term, which has been shown to be of importance to give quantitative agreement with experiments with ultracold bosons in a trap [14]. Even further higher-order corrections can be evaluated in this way with not much additional burden.

The results of the present Letter could be applied to determine the evolution of the density profile for a system of superfluid fermionic atoms in a trap when the effective fermionic attraction is increased. It has recently been shown [15] that, as far as the gross features of the density profile are concerned, this problem can be dealt with by solving the coupled mean-field BCS equations for the gap and the density within a local-density approximation. Such an approach reduces to the (bosonic) Thomas-Fermi approximation in the strong-coupling limit, thus missing the contribution of the kinetic energy. The present derivation of the GP equation from the BdG equations shows, in this respect, that solution of the BdG equations for fermionic atoms in a trap represents a refined approach that correctly treats the kinetic energy for all couplings.

In conclusion, the time-independent GP equation at zero temperature for composite bosons (formed as bound-fermion pairs) has been obtained from the BdG equations for superfluid fermions subject to an external potential, in the strong-coupling limit of the mutual fermionic attraction.

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