

ASYMPTOTIC BEHAVIOUR OF CORRELATION FUNCTIONS IN THE TRAPPED BOSE GAS

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The functional integral method was applied for the calculation of the asymptotic behaviour of the correlation functions for the repulsive Bose gas in a paraboloidal trap. Results are reported here for the two-point correlation functions below the critical temperatures in $d = 3, 2$ and 1 dimensions. Only for $d = 3$ correlations are long range. The two-dimensional condensate is marginally stable in the sense that correlations decay by a power law.

The observation of Bose condensation in vapours of alkali atoms [1–3] held in magneto-optical traps, and recently [4] in atomic hydrogen, has stimulated enormous interest, both experimentally and theoretically, in this phenomenon. The natural starting point for studying the behaviour of such systems is the theory of the dilute weakly interacting Bose gas which was originated by Bogoliubov's 1947 paper [5]. Much of the theoretical work has been concerned with solutions of the Gross–Pitaevskii (GP) equation in the presence of the paraboloidal potential describing the trap [6–8]. Without the trap this equation is also called the Non-linear Schrödinger (NLS) equation [9] which, in one space dimension ($d = 1$), can be solved exactly at both classical and quantum level including [10, 11] calculation of the finite-temperature correlation functions for the repulsive case (coupling constant $g > 0$). For $d = 1$ as well as for the higher dimensions, the finite-temperature properties of the quantum NLS equation have otherwise been extensively analyzed [12] by functional integral methods. This way it is established, e.g., that without any trap no long-range correlations arise for $d < 3$.

Thus far it has remained an open question whether the presence of a trap potential will induce long-range order for $d < 3$. We'll establish here that, even in the presence of a paraboloidal trap, there is long-range order only for $d = 3$. To this end we have applied the previous [12, 13] functional integral methods to the case when a trap is included. An important new aspect is then that the trap breaks translational invariance; and this introduces wholly new many-body theoretical problems. Thus, rather than using periodic boundary conditions (b.c.s), we must expect to impose vanishing b.c.s at infinity, and so to work at «zero density» [14].

The functional integral method provides a framework within which, in principle, all thermodynamic properties of the trapped Bose gas can be determined. The main result reported here is the calculation of the asymptotic behaviour of the two-point correlation functions for trapped Bose gases at finite temperature for each of $d = 1, 2, 3$. Because there is no translational invariance these correlation functions no longer depend solely on the difference of two position vectors. It can still be concluded that long-range order arises, for $T < T_c$, in $d = 3$, and the first-order coherence function asymptotically approaches unity. In $d = 2$ and for $T < T_c$ the condensate is *marginally* stable for correlations decay algebraically, namely as a power law. In $d = 1$ correlations decay exponentially for $T < T_c$, and we have not yet analyzed any $T = 0$ limit. For $T > T_c$ there is a Gaussian decay in all dimensions.

One can write the finite-temperature correlation function $G(\mathbf{r}_1, \mathbf{r}_2) \equiv \langle \mathbf{T}_\tau \hat{\psi}(\mathbf{r}_1, \tau_1) \hat{\psi}^\dagger(\mathbf{r}_2, \tau_2) \rangle$ (where \mathbf{T}_τ means a thermal ordering in τ) as the ratio of two functional integrals,

$$G(\mathbf{r}_1, \mathbf{r}_2) = Z^{-1} \int e^S \psi(\mathbf{r}_1, \tau_1) \bar{\psi}(\mathbf{r}_2, \tau_2) D\psi D\bar{\psi}, \quad (1)$$

in which Z is a partition function $Z = \int e^S D\psi D\bar{\psi}$. The action S is

$$S = \int_0^\beta d\tau \int d^d r \left\{ \bar{\psi}(\mathbf{r}, \tau) K \psi(\mathbf{r}, \tau) - \frac{g}{2} \bar{\psi}(\mathbf{r}, \tau) \bar{\psi}(\mathbf{r}, \tau) \psi(\mathbf{r}, \tau) \psi(\mathbf{r}, \tau) \right\}. \quad (2)$$

The boundary conditions are vanishing at infinity for \mathbf{r} and periodic, period $\beta = (k_B T)^{-1}$, for τ . The action S yields the quantum many-body problem at $T > 0$ for a gas with repulsive pairwise δ -function interactions of strength g in \mathbf{R}^d . The differential operator $K = \partial_\tau - H$, and $H = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) - \mu$; μ is the chemical potential and $V(\mathbf{r}) = \frac{m}{2} \Omega^2 \mathbf{r}^2$ is the paraboloidal trap potential, taken with spherical symmetry for simplicity.

For $T < T_c$ we shall put $\psi(\mathbf{r}, \tau) = \psi_0(\mathbf{r}) + \psi_1(\mathbf{r}, \tau)$ [7, 12, 15] and likewise for $\bar{\psi}$: where the condensate variable $\psi_0(\mathbf{r})$ will not depend on τ , and ψ_1 is

that due to thermal fluctuations. In this Letter we shall only consider terms in S up to quadratic (bilinear) in $\psi_1, \bar{\psi}_1$ and can therefore explicitly integrate out the thermal fluctuations. This way we arrive at $S_{\text{eff}}[\psi_o, \bar{\psi}_o] = \ln \int e^S D\psi_1 D\bar{\psi}_1$, and

$$\begin{aligned} & S_{\text{eff}}[\psi_o, \bar{\psi}_o] + \beta F_{nc}(\mu) \\ &= \beta \int d^d r \{ \bar{\psi}_o(\mathbf{r}) [\frac{\hbar^2}{2m} \nabla^2 + \mu - \tilde{V}(\mathbf{r})] \psi_o(\mathbf{r}) - \frac{g}{2} \bar{\psi}_o(\mathbf{r}) \bar{\psi}_o(\mathbf{r}) \psi_o(\mathbf{r}) \psi_o(\mathbf{r}) \}. \end{aligned} \quad (3)$$

In S_{eff} , $\tilde{V}(\mathbf{r}) = V(\mathbf{r}) + 2g\rho_{nc}(\mathbf{r})$ is a renormalized trap potential, while $\rho_{nc}(\mathbf{r})$ is the density profile of the thermal particles in the ideal gas approximation — as is consistent with terms only quadratic in $\psi_1, \bar{\psi}_1$ retained. More precisely, at this level of approximation (Hartree–Fock–Bogoliubov) this density profile derives from the fundamental solution of the $d + 1$ -dimensional operator K : $K\mathcal{G}(\mathbf{r}, \tau; \mathbf{r}', \tau') = -\delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau')$, and Green's function \mathcal{G} can be expressed in the form

$$\mathcal{G}(\mathbf{r}, \tau; \mathbf{r}', \tau') = \sum_{\mathbf{n}} \frac{u_{\mathbf{n}}(\mathbf{r})u_{\mathbf{n}}(\mathbf{r}')}{e^{\beta E_{\mathbf{n}}} - 1} e^{E_{\mathbf{n}}(\tau - \tau')}, \tau > \tau'. \quad (4)$$

For $d = 3$ the vectors $\mathbf{n} = (n_1, n_2, n_3)$, and the $u_{\mathbf{n}}(\mathbf{r})$ and $E_{\mathbf{n}}$ are the eigenfunctions and eigenenergies, respectively, of the $d = 3$ harmonic oscillator Hamiltonian H ; and similarly for $d = 1, 2$. Then $\rho_{nc}(\mathbf{r}) = \mathcal{G}'(\mathbf{r}, \tau; \mathbf{r}, \tau)$, where prime means $\mathbf{n} = (0, 0, 0)$ is omitted. The free energy of the thermal particles $F_{nc}(\mu)$ is simply $F_{nc}(\mu) = \beta^{-1} \sum_{\mathbf{n}}' \ln(1 - e^{-\beta E_{\mathbf{n}}})$.

At this point it is possible to calculate the actual temperatures T_c . The leading, i.e., zeroth order term is found by replacing $\rho_{nc}(\mathbf{r})$ by a constant $\rho_{nc}(0)$: this defines the renormalized chemical potential $\Lambda = \mu - 2g\rho_{nc}(0)$, and $\Lambda = 0$ determines T_c [6]. At first order in g we can add the appropriate terms arising in S_{eff} . Beyond this we also need to include fluctuations ψ_1 to an order higher than quadratic.

The free energy F of the trapped Bose gas is calculated from $-\beta F(\mu) = \ln \int e^{S_{\text{eff}}} D\psi_0 D\bar{\psi}_0$. By the steepest descents for large β (low T) we find that

$$F(\mu) = F_{nc}(\mu) - \frac{g}{2} \int d^d r |\Phi(\mathbf{r})|^4. \quad (5)$$

In Eq.(5) the fields $\Phi, \bar{\Phi}$ are the quasi-classical fields satisfying the extremum condition $\delta(S_{\text{eff}}[\Phi, \bar{\Phi}]) = 0$. This condition is equivalent to the stationary Gross–Pitaevskii equations

$$\frac{\hbar^2}{2m} \nabla^2 \Phi(\mathbf{r}) + (\mu - \tilde{V}(\mathbf{r}))\Phi(\mathbf{r}) - g |\Phi(\mathbf{r})|^2 \Phi(\mathbf{r}) = 0, \quad (6)$$

and the similar equation for $\bar{\Phi}$. At this quasi-classical approximation we already find through the presence of $\tilde{V}(\mathbf{r})$ the Hartree–Fock–Bogoliubov (HFB) corrections to the Gross–Pitaevskii equation introduced earlier [6].

We turn next to the calculation of the finite-temperature correlation function, Eq. (1). By integrating out the thermal fluctuations included up to terms quadratic in $\psi_1, \bar{\psi}_1$ we find that

$$G(\mathbf{r}_1, \mathbf{r}_2) \simeq \frac{\int e^{S_{\text{eff}}[\psi_o(\mathbf{r}_1), \bar{\psi}_o(\mathbf{r}_2)]} D\psi_o D\bar{\psi}_o}{\int e^{S_{\text{eff}}} D\psi_o D\bar{\psi}_o} \equiv C(\mathbf{r}_1, \mathbf{r}_2). \quad (7)$$

At low enough temperatures these remaining functional integrals can be evaluated by the steepest descents where again we work consistently at the HFB level. At this level the correlation functions can be expressed in the form

$$C(\mathbf{r}_1, \mathbf{r}_2) \simeq e^{-S_{\text{eff}}[\Phi_0, \bar{\Phi}_0] + S_{\text{eff}}[\Phi_1, \bar{\Phi}_1] + \ln \Phi_1(\mathbf{r}_1) \bar{\Phi}_1(\mathbf{r}_2)}, \quad (8)$$

and the fields $\Phi_0, \bar{\Phi}_0$ satisfy Eq. (6). Evidently the fields $\Phi_1, \bar{\Phi}_1$ are determined by $\delta(S_{\text{eff}}[\Phi_1, \bar{\Phi}_1] + \ln \Phi_1(\mathbf{r}_1) \bar{\Phi}_1(\mathbf{r}_2)) = 0$, and this variational equation also leads to a pair of equations with additional sources from the $\ln(\Phi_1 \bar{\Phi}_1)$. This pair of equations is

$$\begin{aligned} -\frac{\hbar^2}{2m} \nabla^2 \Phi_1(\mathbf{r}) - (\mu - \tilde{V}(\mathbf{r})) \Phi_1(\mathbf{r}) + g \Phi_1^2(\mathbf{r}) \bar{\Phi}_1(\mathbf{r}) &= \frac{\delta(\mathbf{r} - \mathbf{r}_2)}{\beta \bar{\Phi}_1(\mathbf{r}_2)}, \\ -\frac{\hbar^2}{2m} \nabla^2 \bar{\Phi}_1(\mathbf{r}) - (\mu - \tilde{V}(\mathbf{r})) \bar{\Phi}_1(\mathbf{r}) + g \bar{\Phi}_1^2(\mathbf{r}) \Phi_1(\mathbf{r}) &= \frac{\delta(\mathbf{r} - \mathbf{r}_1)}{\beta \Phi_1(\mathbf{r}_1)}. \end{aligned} \quad (9)$$

For simplicity, we shall solve them only at the Thomas–Fermi approximation: this is expected to be valid at low enough temperatures [6–8]. The stationary Gross–Pitaevskii equation Eq. (6) is now reduced to a simple algebraic equation and we then easily find the expected inverted paraboloidal density profile which is

$$\rho_0(\mathbf{r}) \equiv \Phi_0(\mathbf{r}) \bar{\Phi}_0(\mathbf{r}) = \frac{1}{g} (\mu - \tilde{V}(\mathbf{r})) \Theta(\mu - \tilde{V}(\mathbf{r})), \quad (10)$$

in which Θ is the Heaviside step function. Evidently $\rho_0(\mathbf{r})$ can be interpreted as the condensate density expressed in terms of order parameters $\Phi_0, \bar{\Phi}_0$. The radius of the condensate R_c can now be determined from the condition $\mu - \tilde{V}(R_c) = 0$.

The solution of Eqs. (9) is more complicated. Notice first that the fields $\Phi_1, \bar{\Phi}_1$, appearing in these equations will be complex valued fields in general. But they are two independent fields with independent variations. We can therefore seek first of all solutions in the form

$$\Phi_1(\mathbf{r}) = \sqrt{\rho(\mathbf{r})} e^{\phi(\mathbf{r})}, \quad \bar{\Phi}_1(\mathbf{r}) = \sqrt{\rho(\mathbf{r})} e^{-\phi(\mathbf{r})},$$

where $\phi(\mathbf{r})$ can be complex valued, but will be found below to describe the real contribution to the correlation functions of the complex phases of the wave functions. We can furthermore assume that, away from the boundaries, $\rho(\mathbf{r})$ is a slowly varying function of position \mathbf{r} so that $\nabla^2\sqrt{\rho}$ and $\nabla\sqrt{\rho}$ are both small and can be neglected. This will not be true of $(\nabla\phi)^2$ or $\rho\nabla^2\phi$, so that Eqs. (9) become

$$g\rho(\mathbf{r}) - (\mu - \tilde{V}(\mathbf{r})) - \frac{\hbar^2}{2m}(\nabla\phi(\mathbf{r}))^2 = 0, \quad (11)$$

$$\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r}) = \frac{1}{2\beta\rho(\mathbf{r}_1)}\delta(\mathbf{r} - \mathbf{r}_1) - \frac{1}{2\beta\rho(\mathbf{r}_2)}\delta(\mathbf{r} - \mathbf{r}_2). \quad (12)$$

The first of these equations Eq. (11) has the solution $\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \frac{\hbar^2}{2mg}(\nabla\phi)^2$. Within the Thomas–Fermi approximation, $\rho(\mathbf{r})$ in Eq. (12) is then $\rho_0(\mathbf{r})$. We then express the solution of this equation in terms of a function $f(\mathbf{r}, \mathbf{r}')$:

$$\phi(\mathbf{r}; \mathbf{r}_1, \mathbf{r}_2) = f(\mathbf{r}, \mathbf{r}_1) - f(\mathbf{r}, \mathbf{r}_2).$$

The functional form of $f(\mathbf{r}, \mathbf{r}')$ depends on the dimensionality of the system. We find that

$$f(\mathbf{r}, \mathbf{r}') = -\frac{a}{2\pi\beta\rho_0(\mathbf{r}')} \frac{1}{R} \quad (d = 3), \quad (13)$$

$$f(\mathbf{r}, \mathbf{r}') = \frac{a}{\pi\beta\rho_0(\mathbf{r}')} \ln R \quad (d = 2), \quad (14)$$

$$f(\mathbf{r}, \mathbf{r}') = \frac{a}{\beta\rho_0(\mathbf{r}')} R \quad (d = 1) \quad (15)$$

with $a \equiv \frac{m}{2\hbar^2}$ and $R \equiv |\mathbf{r} - \mathbf{r}'|$. It is already clear that the correlation functions can no longer depend on $R = |\mathbf{r} - \mathbf{r}'|$ alone: they depend also on both \mathbf{r}_1 and \mathbf{r}_2 separately, consistent with the breakdown of translational invariance induced by the trap.

We consider first the correlation function in $d = 3$. In this case the points $\mathbf{r} = \mathbf{r}_1$ and $\mathbf{r} = \mathbf{r}_2$ in $\phi(\mathbf{r}; \mathbf{r}_1, \mathbf{r}_2)$ are singular and introduce a divergence problem. This difficulty can be avoided first of all by considering a first-order «coherence function» $G^{(1)}(\mathbf{r}_1, \mathbf{r}_2)$ (compare, e.g., [16, 17]) which we define here as

$$G^{(1)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{G(\mathbf{r}_1, \mathbf{r}_2)}{\langle\psi(\mathbf{r}_1, \tau_1)\rangle\langle\psi^\dagger(\mathbf{r}_2, \tau_2)\rangle} \simeq \frac{C(\mathbf{r}_1, \mathbf{r}_2)}{\langle\psi_o(\mathbf{r}_1)\rangle\langle\bar{\psi}_o(\mathbf{r}_2)\rangle}, \quad (16)$$

for identically the same singularities appear [12] in the direct calculation of the order parameters $\langle \psi(\mathbf{r}, \tau) \rangle, \langle \psi^\dagger(\mathbf{r}, \tau) \rangle$. Notice that in Eq. (16) we have already replaced $\langle \psi \rangle$, the order parameter of the trapped Bose gas, by $\langle \psi_o \rangle$ since average over thermal fluctuations vanishes: $\langle \psi_1 \rangle = 0$. For $T < T_c$, when the order parameter is nonzero, we find that

$$\begin{aligned} G^{(1)}(\mathbf{r}_1, \mathbf{r}_2) &\simeq e^{-\frac{1}{2}(f(\mathbf{r}_1, \mathbf{r}_2) + f(\mathbf{r}_2, \mathbf{r}_1))} \\ &= \exp\left\{\frac{a}{4\pi\beta\rho_0(\mathbf{r}_1, \mathbf{r}_2)} \frac{1}{R}\right\}, \end{aligned} \quad (17)$$

where $\rho_0^{-1}(\mathbf{r}_1, \mathbf{r}_2) \equiv \rho_0^{-1}(\mathbf{r}_1) + \rho_0^{-1}(\mathbf{r}_2)$. Evidently that $G^{(1)}(\mathbf{r}_1, \mathbf{r}_2) \rightarrow 1$ for large R , thus indicating long-range order and long-range coherence, and there are thus features of a coherent state in this sense. The coherence length is given by $\frac{a}{4\pi\beta\rho_0(\mathbf{r}_1, \mathbf{r}_2)}$ and depends on both \mathbf{r}_1 and \mathbf{r}_2 separately. Notice that we have assumed \mathbf{r}_1 and \mathbf{r}_2 are not close to the boundaries of the condensate so that always $\rho_0(\mathbf{r}) > 0$ in the above expression.

Let us consider the *uniform* Bose gas ($V(\mathbf{r}) = 0$) and study the long distance ($R \rightarrow \infty$) behaviour of the correlation function:

$$G^{(1)}(\mathbf{r}_1, \mathbf{r}_2) - 1 \simeq \frac{m}{4\pi\hbar^2\beta} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$

Going over to the momentum representation one can see that for the small temperatures the Fourier transform of this function is divergent at small momenta as $|\mathbf{k}|^{-2}$ thus forbidding transitions for a lower symmetry phase at $d = 1, 2$ which is the famous Bogoliubov's result [18].

For $d = 2$ the singularity in $f(\mathbf{r}, \mathbf{r}')$ is logarithmic and the divergence is renormalizable. For $d = 1$ the function f is nonsingular. Thus we can directly evaluate the correlation functions, and find that

$$G(\mathbf{r}_1, \mathbf{r}_2) \simeq \sqrt{\rho_0(\mathbf{r}_1)\rho_0(\mathbf{r}_2)} \exp\left\{-\frac{a}{2\pi\beta\rho_0(\mathbf{r}_1, \mathbf{r}_2)} \ln R\right\}, \quad (d = 2); \quad (18)$$

$$G(\mathbf{r}_1, \mathbf{r}_2) \simeq \sqrt{\rho_0(\mathbf{r}_1)\rho_0(\mathbf{r}_2)} \exp\left\{-\frac{a}{2\beta\rho_0(\mathbf{r}_1, \mathbf{r}_2)} R\right\}, \quad (d = 1). \quad (19)$$

It is obvious that these correlation functions both vanish for large R and that there is no long-range order in $d = 1$ or in $d = 2$. In the case $d = 2$ the condensate is marginally stable in that correlations decay algebraically, namely by a power law. The exponent of this power-law is proportional to T so that at very low temperatures, correlations may thus prevail over almost macroscopic distances. In real magneto-optical traps for $d = 3$ we still expect the condensate to be stable

even for extremely anisotropic trap potentials, as in, e.g., the experiments [4] on atomic hydrogen. The three correlation functions (Eqs.(17–19)) coincide with those obtained under translational invariance without the trap to the extent that for $\Omega \rightarrow 0, V(\mathbf{r}) \rightarrow 0$, and we can expect $2g\rho_{nc}(\mathbf{r}) \rightarrow \text{Const} = 2g\rho_{nc}$.

Thus in summary we have demonstrated that the functional integration techniques can be extended to Bose gases in a confining trap potential, and form a convenient framework in which to consider the thermal properties of the condensate. We have shown in particular that true long-range order only arises in $d = 3$. In $d = 2$ the condensate is only marginally stable, but the related power-law decay of correlations becomes increasingly weak as temperature decreases. We expect to define multipoint correlation functions similarly to Eq.(16) and find these ~ 1 for large separations of points.

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