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Off-diagonal long-range behavior of interacting Bose systems

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The off-diagonal long-range behavior of interacting Bose systems is studied in one, two, and three dimensions and also for the interdimensional case. The one-dimensional result is new while the two- and three-dimensional results present a rederivation of known results. A qualitative analysis of the interdimensional case is presented showing the way by which the behavior of the single-particle reduced density matrix is changed when going from $\nu-1$ dimensions to ν dimensions.

I. INTRODUCTION

In a recent paper by the author,[1] an approximate expression for the single-particle reduced density matrix was obtained in terms of the measurable structure factor and excitation spectrum. The aim of this paper is to use that expression and the known behavior of the structure factor and excitation spectrum at large wavelengths to derive the behavior of the single-particles reduced density matrix at large distances and to compare the results with previous derivations.

In Sec. II the behavior of the one-dimensional system is discussed. The $T=0$ result shows that at large distances the single-particle reduced density matrix behaves like an inverse power law of the distance where the power is determined by the density and the velocity of sound. Considering the partly soluble model of impenetrable bosons[2-5] it is found that the obtained behavior obeys an inequality derived by Lenard[3] and in fact agrees with his conjecture about the actual behavior. At finite temperature the result of this section disagrees with the approximate result of Kane and Kadanoff,[6] who assumed the existence of Bose-Einstein condensation at $T=0$.

The problem of a phase transition in a two-dimensional system possessing a continuous symmetry has been the subject of many experimental and theoretical papers.[7-13] Proofs were given that no ordering can occur in such a system.[7-9] On the other hand some evidence appeared that although the order parameter remains zero, these systems undergo a phase transition at some finite temperature.[10-13]

The arguments given by Berezinsky[11] and Lasher[12] for the existence of a phase transition in a two-dimensional interacting Bose system were based on the behavior of the single-particle reduced density matrix at low temperatures and large distances. In Sec. III their result is obtained by a different method and this supports the idea that a phase transition does occur at a finite temperature.

In Sec. IV the three-dimensional system is discussed and the obtained behavior of the single-particle reduced density matrix agrees with previous results of Chester and Reatto.[14] It is argued that this result should serve as a consistency condition to be obeyed by numerical calculations in which the condensed fraction is obtained by estimating the asymptotic behavior of the single-particle reduced density matrix, and where uncertainty in the results is mainly due to using a finite system for the calculations.[15-17]

In Sec. V the interdimensional behavior is obtained. It is qualitatively shown that for a ν-dimensional system that is infinite in $\nu-1$ dimensions and finite in one, the single-particle reduced density matrix shows $(\nu-1)$-dimensional behavior at very large distances, while ν-dimensional behavior is encountered at distances very large compared to the characteristic microscopic distance and very small compared to the extent of the finite dimension.

II. ONE-DIMENSIONAL SYSTEM

The approximate expression for the single-particle reduced density matrix obtained in Ref. 1 is given for low temperatures by[18]

$$\langle \psi^\dagger(0)\psi(\vec{r})\rangle = \bar{\rho}\left\{\exp\left[\frac{1}{N}\sum_{\vec{q}\neq 0}\frac{S_q^2-1}{4S_q}\,(1-\cos\vec{q}\cdot\vec{r})\left(1+\frac{2}{e^{\beta\omega_q}-1}\right)\right]\right.$$
$$\left.\times\left(1-\frac{1}{N}\sum_{\vec{p}\neq 0}\frac{(S_p-1)(1-e^{-i\vec{p}\cdot\vec{r}})}{2(1-e^{-\beta\omega_p})}+\frac{(S_p+1)(1-e^{-i\vec{p}\cdot\vec{r}})}{2(e^{\beta\omega_p}-1)}\right)\right\}, \qquad (1)$$

where $\bar{\rho}$ is the density of particles, N is the number of particles, S_q is the structure factor, and ω_q is the excitation energy. In the volume limit this function is given by

$$\langle \psi^\dagger(0)\psi(\vec{r})\rangle = \rho e^{f_1(\vec{r})+f_2(\vec{r})} f_3(\vec{r}) , \tag{2}$$

where

$$f_1(\vec{r}) = \frac{1}{(2\pi)^\nu \bar{\rho}} \int d^\nu q \, \frac{S_q^2 - 1}{4S_q} \, (1 - \cos \vec{q}\cdot\vec{r}) , \tag{3}$$

$$f_2(\vec{r}) = \frac{2}{(2\pi)^\nu \bar{\rho}} \int d^\nu q \, \frac{S_q^2 - 1}{4S_q(e^{\beta\omega_q} - 1)} \, (1 - \cos \vec{q}\cdot\vec{r}) , \tag{4}$$

$$f_3(\vec{r}) = 1 - \frac{1}{(2\pi)^\nu \bar{\rho}} \int d^\nu q \left(\frac{(S_q - 1)(1 - \cos \vec{q}\cdot\vec{r})}{2(1 - e^{-\beta\omega_q})} + \frac{(S_q + 1)(1 - \cos \vec{q}\cdot\vec{r})}{2(e^{\beta\omega_q} - 1)} \right) , \tag{5}$$

and ν denotes the dimension of the system.

Assuming that for small $|q|$, S_q is linear in $|q|$, and ω_q is given by the Feynman relation

$$\omega_q = \hbar^2 q^2 / 2mS_q , \tag{6}$$

one can easily verify the following equations for the one-dimensional system:

$$\lim_{|\vec{r}| \to \infty} f_1(\vec{r}) = -\infty , \tag{7}$$

$$\lim_{|\vec{r}| \to \infty} f_3(\vec{r}) = C_1 \quad (C_1 \neq \pm\infty, \; C_1 \neq 0) , \tag{8}$$

$$f_2(\vec{r})_{T=0} = 0 , \tag{9}$$

$$\lim_{|\vec{r}| \to \infty} f_2(\vec{r})_{T>0} = -\infty . \tag{10}$$

Equations (7)–(10) imply that Bose-Einstein condensation exists neither at finite temperature nor in the ground state.

Let us see how $f_1(\vec{r})$ behaves for large but finite $|\vec{r}|$. To estimate this behavior one may cut off the integral of the oscillating part at some small $q = \alpha/r$, where α is independent of r (see Ref. 19)

$$f_1(\vec{r}) \simeq \frac{1}{\pi\bar{\rho}} \int_0^{\alpha/r} dq \, \frac{S_q^2 - 1}{4S_q} \, (1 - \cos qr) + \frac{1}{\pi\bar{\rho}} \int_{\alpha/r} dq \, \frac{S_q^2 - 1}{4S_q} , \tag{11}$$

$$\frac{1}{\pi\bar{\rho}} \int_0^{\alpha/r} dq \, \frac{S_q^2 - 1}{4S_q} \, (1 - \cos qr) \simeq -\frac{mc}{2\pi\rho\hbar} \int_0^{\alpha} \frac{dt}{t} \, (1 - \cos t) \quad \text{for large } r , \tag{12}$$

where c is the sound velocity at $T = 0$.

Using the same considerations

$$\frac{1}{\pi\bar{\rho}} \int_{\alpha/r} dq \, \frac{S_q^2 - 1}{4S_q} = -\frac{mc}{2\pi\bar{\rho}\hbar} \ln \frac{\alpha}{r} + R_1 , \tag{13}$$

where R_1 contains the r-independent contribution from the upper limit of the integral as well as lower r-dependent contributions. Consequently,

$$\langle \psi^\dagger(0)\psi(r)\rangle = \bar{\rho} C_{1,\,T=0} \, e^R \, (\alpha/r)^{mc/2\pi\bar{\rho}\hbar} , \tag{14}$$

where R is given by

$$R = f_1(r) - (mc/2\pi\bar{\rho}\hbar) \ln \alpha/r \tag{15}$$

and, according to the previous arguments, approaches a finite constant when r becomes very large.

It is interesting to compare this result with the results obtained by Lenard[3] for the momentum distribution for the model of impenetrable bosons. Lenard was able to show that for all r

$$\langle \psi^\dagger(0)\psi(r)\rangle \leq (e/\pi\bar{\rho}r)^{1/2} , \tag{16}$$

and conjectured that at large r,

$$\langle \psi^\dagger(0)\psi(r)\rangle \propto (1/r)^{1/2} . \tag{17}$$

The sound velocity in that model is given by

$$c = \pi\bar{\rho}\hbar/m . \tag{18}$$

Hence the power law predicted by Eq. (14) agrees with Lenard's conjecture. For $T > 0$ one has to look at the behavior of $f_2(r)$ at large r. The Feynman relation may be used, and the exponentials may be expanded (for small q) to obtain

$$f_2(r) \simeq -\frac{2}{\pi\bar{\rho}} \int_0^{\alpha/r} \frac{dq}{4S_q(e^{\beta\omega_q} - 1)} \, (1 - \cos qr) - \frac{2}{\pi\bar{\rho}} \int_{\alpha'/r} dq \, \frac{S_q^2 - 1}{4S_q(e^{\beta\omega_q} - 1)}$$
$$= -\frac{m}{\pi\hbar^2\beta\bar{\rho}} \, r \int_0^{\alpha'} \frac{dt}{t^2} (1 - \cos t) - \frac{m}{\pi\hbar^2\beta\bar{\rho}} \, r \int_{\alpha'} \frac{dt}{t^2} = -\frac{m}{\pi\bar{\rho}\hbar^2\beta} \, Cr , \tag{19}$$

where C is a constant to leading order in r.

For large r,

$$\langle \psi^\dagger(0)\psi(r)\rangle_{T>0} = \bar{\rho} C_{1,\,T>0} \, e^R (\alpha/r)^{mc/2\pi\bar{\rho}\hbar} \times \exp[-(m/\pi\hbar^2\beta\bar{\rho})Cr] . \tag{20}$$

This result differs from the result of Kane and Kadanoff which may be written

$$\langle \psi^\dagger(0)\psi(r)\rangle_{T>0} = n_0 e^{-r/r_0} , \tag{21}$$

where r_0 is a decreasing function of temperature that tends to infinity at zero temperature. In their derivation as well as in the final result it is assumed that n_0, the condensed density at $T=0$, is finite. This assumption contradicts some approximate results and some rigorous model calculations that show that the one dimensional interacting Bose system is not Bose condensed even in the ground state.[1,3,4]

III. TWO-DIMENSIONAL SYSTEM

In two dimensions the following equations hold:

$$\lim_{|\vec{r}|\to\infty} f_1(\vec{r}) = A_2 \quad (A_2 \neq \pm\infty,\ A_2 \neq 0)\ , \tag{22}$$

$$\lim_{|r|\to\infty} f_3(\vec{r}) = C_2 \quad (C_2 \neq \pm\infty,\ C_2 \neq 0)\ , \tag{23}$$

$$f_2(\vec{r})_{T=0} = 0\ , \tag{24}$$

$$\lim_{|\vec{r}|\to\infty} f_2(\vec{r})_{T>0} = -\infty\ . \tag{25}$$

Equations (21)–(23) imply that at $T=0$ Bose-Einstein condensation does exist, while Eqs. (21), (23), and (24) imply that at any finite temperature Bose-Einstein condensation does not exist. For $T=0$ one may write

$$\begin{aligned}\langle\psi^\dagger(0)\psi(r)\rangle_{T=0} &= e^{f_1(\vec{r})} f_3(\vec{r}) \\ &= e^{f_1(\infty)} f_3(\infty) e^{f_1(\vec{r})-f_1(\infty)} \\ &\quad\times \{1+[f_3(\vec{r})-f_3(\infty)]/f_3(\infty)\}\ .\end{aligned} \tag{26}$$

The function $f_1(\vec{r})-f_1(\infty)$ is given for large r by[19]

$$\begin{aligned} f_1(r)-f_1(\infty) &= -\frac{1}{(2\pi)^2\bar{\rho}} \int d^2q\, \frac{S_q^2-1}{4S_q} \cos\vec{q}\cdot\vec{r} \\ &= \frac{mc}{4\pi\bar{\rho}\hbar}\frac{1}{r}\ .\end{aligned} \tag{27}$$

It is also easy to check that for large r

$$f_3(r)-f_3(\infty) \propto 1/r^3\ , \tag{28}$$

so that one can write for large r

$$\langle\psi^\dagger(0)\psi(r)\rangle = n_0[1+(mc/4\pi\bar{\rho}\hbar)(1/r)]\ , \tag{29}$$

where n_0 is the density of the condensate at $T=0$.

At $T>0$ one has to study the behavior of $f_2(r)$. Using the Feynman relation and expanding the exponentials for small $|q|$ and also using the same arguments as for computing $f_1(r)$ for the one dimensional case, it is easily seen that

$$f_2(r) = -(m/2\pi\bar{\rho}\hbar^2\beta)\ln\alpha''/r + R'\ , \tag{30}$$

where R' is a constant to leading order in r. As a result

$$\langle\psi^\dagger(0)\psi(r)\rangle = \bar{\rho}e^{f_1(\infty)+R'} f_3(\infty)\,(\alpha''/r)^{m/2\pi\bar{\rho}\beta\hbar^2}\ . \tag{31}$$

It is easily seen that

$$\lim_{\beta\to\infty} \bar{\rho}e^{f_1(\infty)+R'} f_3(\infty) = n_0\ , \tag{32}$$

so that at very low temperatures Eq. (30) is identical with the results of Berezinsky and Lasher who used this kind of behavior in their arguments for the existence of a phase transition in the above system. The alternative derivation presented above supports the belief that the approximate results of Berezinsky and Lasher are correct and thus supports the idea that the system undergoes a phase transition at some finite temperature. The author hopes to come back to discuss superfluidity at low temperatures in future work.

IV. THREE-DIMENSIONAL SYSTEM

For $T=0$ the single-particle reduced density matrix can be written again as

$$\begin{aligned}\langle\psi^\dagger(0)\psi(r)\rangle &= e^{f_1(\infty)} f_3(\infty) e^{f_1(r)-f_1(\infty)} \\ &\quad\times\{1+[f_3(r)-f_3(\infty)]/f_3(\infty)\}\end{aligned} \tag{33}$$

for large r (Ref. 19):

$$\begin{aligned} f_1(r)-f_1(\infty) &= -\frac{1}{(2\pi)^3\bar{\rho}} \int d^3q\, \frac{S_q^2-1}{4S_q} \cos\vec{q}\cdot\vec{r} \\ &= \frac{2mc}{\bar{\rho}\hbar}\,\pi\,\frac{1}{r^2}\ .\end{aligned} \tag{34}$$

The other function needed is

$$f_3(r)-f_3(\infty) \propto 1/r^4 \quad \text{for large } r\ , \tag{35}$$

so that

$$\langle\psi^\dagger(0)\psi(r)\rangle = n_0[1+(mc/4\pi^2\rho\hbar)(1/r^2)]\ . \tag{36}$$

Numerical calculations of n_0 are really calculations of the single-particle reduced density matrix that are done for a finite system for large r that must be small compared to the size of the system. This procedure is a source of uncertainty in the results. Equation (36) suggests a consistency criterion that should be obeyed by the numerical results:

$$\lim_{r\to\infty} r^2\,\frac{\langle\psi^\dagger(0)\psi(r)\rangle - n_0}{n_0} = \frac{mc}{4\pi^2\bar{\rho}\hbar}\ , \tag{37}$$

so that in a numerical calculation, the size of the system must be large, compared to a region of large enough r where Eq. (36) should be obeyed.

The estimation of the long-range behavior at $T>0$ is entirely equivalent to this estimation at $T=0$ in two dimensions, since one may expand the exponentials and use the Feynman relation at small $|q|$. The expression for large and finite r is[20]

$$\langle\psi^\dagger(0)\psi(r)\rangle = n_{0,\,T>0}[1+(m/4\pi\hbar^2\bar{\rho}\beta)(1/r)]\ , \tag{38}$$

where $n_{0,\,T>0}$ is the density of the condensate at the given temperature. In obtaining Eq. (38) one uses again the fact that $f_3(r)-f_3(\infty)$ is very short ranged.

V. INTERDIMENSIONAL BEHAVIOR

It is interesting to understand how the behavior of the single-particle reduced density matrix depends continuously on the dimensionality of the system, namely, how does it change when one increases the thickness of a ν-dimensional box that is small compared to its other dimensions. Let us consider a specific example.

Let a system of N bosons enclosed in a box of sides $L \times L \times D$, parallel, respectively, to the xy and z axes, with periodic boundary conditions, be described by the Hamiltonian[21]

$$H = \sum_{\vec{k}} \tfrac{1}{2} k^2 a_k^\dagger a_k + \frac{1}{2L^2 D} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \nu(\vec{q}) a_{k_1+q}^\dagger a_{k_1-q}^\dagger a_{k_2-q} a_{k_1} a_{k_2} , \quad (39)$$

where the allowed $\vec{k}$'s are

$$\vec{k} = [(2\pi/L) n_1, (2\pi/L) n_1, (2\pi/D) n_3] . \quad (40)$$

n_1, n_2, n_3, are integers and a and $a^\dagger$ are boson creation and destruction operators, respectively.

It is easily verified using the procedures described in Ref. 1 that the single-particle reduced density matrix is given by Eq. (1), where the summation is restricted to the allowed vectors of Eq. (39). Since it is obvious that now the single-particle reduced density matrix will depend on the direction of $\vec{r}$ as well as on its magnitude, let us take $\vec{r}$ perpendicular to the z axis.

At $T=0$ and $L \to \infty$

$$f_1(\vec{r}) = B - \frac{1}{\bar{\rho} D (2\pi)^2} \int d^2 q \, \frac{S_q^2 - 1}{4 S_q} \cos \vec{q} \cdot \vec{r} - \frac{2}{\bar{\rho} D (2\pi)^2} \sum_{n=1}^{\infty} g_n(\vec{r}) , \quad (41)$$

where

$$g_n(\vec{r}) = \int d^2 q \, \frac{S^2[\vec{q} + (2\pi n/D)\hat{k}] - 1}{4 S[\vec{q} + (2\pi n/D)\hat{k}]} \cos \vec{q} \cdot \vec{r} , \quad (42)$$

$$B = \frac{1}{\bar{\rho} D (2\pi)^2} \sum_{n=-\infty}^{\infty} \int d^2 q \, \frac{S^2[\vec{q} + (2\pi n/D)\hat{k}] - 1}{4 S[\vec{q} + (2\pi n/D)\hat{k}]} . \quad (43)$$

q is perpendicular to the z axis and $\hat{k}$ is a unit vector in the z direction. Assuming that the structure factor depends linearly on the absolute value of the wave vector, one obtains that at very large distances the behavior of $f_1(\vec{r})$ is two dimensional because the functions $g_n(r)$ approach zero faster than any decreasing power of r when r tends to infinity. On the other hand one expects that for small D the behavior will be two dimensional going over to three-dimensional behavior when D is increased. In order to clarify what happens, let us employ a qualitative, crude, picture.

Let $S(Q)$ be linear in Q for $Q < Q_1$ and let n be a fixed integer. If D is large enough, there is a range of $|q|$ obeying

$$(2\pi n'/D)^2 \ll q^2 \ll Q_1^2 - (2\pi n'/D)^2 \quad \text{for all } n' \leq n , \quad (44)$$

where $|q|$ is the absolute value of the two-dimensional vector $\vec{q}$. In this range $S(\vec{q} + (2\pi n'/D)\hat{k})$ is proportional to $|Q|$. For small $|q|$ it approaches a constant. This means that there is a range of r's

$$2\pi/[Q_1^2 - (2\pi n/D)^2]^{1/2} \ll r \ll D/n , \quad (45)$$

for which $g_{n'}(r)$ is proportional to r^{-1} with a proportionality constant that does not depend on n'. Also $g_{n'}(r)$ is effectively cut off at $r \sim D/n'$. In order to estimate the long-range behavior of $f_1(r)$, let us assume a sharp cut off at $r = D/n'$, then

$$f_1(r) \simeq B - \frac{c'}{r} \left[1 + 2 \sum_{n'=1}^{\infty} \theta\left(\frac{D}{n'} - r\right) \right] . \quad (46)$$

Let $R_m = D/M$ be in the range defined by Eq. (45):

$$f_1(R_m) = B - (c'/R_m)(1 + 2m) = B - c'D(1/DR_m + 1/R_m^2) . \quad (47)$$

By Eq. (44), $R_m \ll D$, so that Eq. (47) implies a r^{-2} correction to the constant term that is characteristic of the three-dimensional system. Equation (45) implies also $R_m \gg 1/Q_1$, that is of the order of the microscopic length parameters of the potential and the density which are more or less of the same order of magnitude in a realistic situation. For all other cases of interdimensional behavior one arrives at the same conclusions. The very-long-range behavior is $\nu-1$- and ν-dimensional behavior starts to be built up at distances large compared with microscopic distances and small compared with the thickness of the system.

VI. CONCLUSIONS

The long-range behavior of the single-particle reduced density matrix was obtained in one, two and three dimensions for the interacting Bose system. The basic assumption was that for small $|q|$ the structure factor is linear in $|q|$ and that the structure factor and excitation spectrum are connected by the Feynman relation. This assumption is very plausible since it is based on general arguments that are dimension independent and it was also verified by model calculations.

The one dimensional results are new. The one dimensional result at $T=0$ was found to agree with a model calculation. At finite temperature the result of this paper differs from a previous result that assumed the existence of Bose-Einstein condensation in the ground state in contradiction with approximate and exact model calculations. The results obtained for two and three dimensions are not new and their importance lies in increasing the credibility of the results as well as of the employed approximation schemes. The interdimensional behavior was also studied and it was qualitatively shown that for a system of finite thickness in one dimension and infinite in all the others the ν-dimensional behavior is encountered at distances that are small compared with the thickness and large compared with the characteristic microscopic distances.

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[18]Equation (1) is expected to hold for r's large compared to $1/|Q_c|$, where Q_c is the wave vector of largest norm for which the Feynman relation $\omega_q = \hbar^2 q^2/2mS_q$ is obeyed to a good approximation. This implies r's large compared to the microscopic distances appearing in the description of the system, i.e., the range of the potential and the interparticle distance.

[19]The distance r may always be taken large enough so that the dominant contribution to the q integration comes from the region of very small $|q|$ for which $S_q = \hbar|q|/2mc$.

[20]As stated in Sec. II. this expression should be valid at low temperatures. Comparing it to the hydrodynamic result

$$\langle\Psi^\dagger(r)\Psi(0)\rangle = n_0[1+(m/4\pi\hbar^2\rho_S\beta)(1/r)],$$

where ρ_S is the superfluid particle density, we see that the reduction of the superfluid density, important at higher temperature, is not taken into account.

[21]The particles may be said to interact via a two-body potential $v(r)$ defined by

$$v(q) = \int v(r) e^{i\vec{q}\cdot\vec{r}}\, d^3r$$

only when D is large compared to the range of $v(r)$.