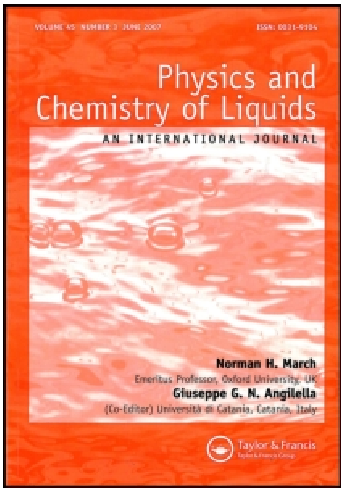

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Momentum Distribution for an Inhomogeneous Bose Fluid at $T = 0$ with Both Confinement and Particle Interactions Modelled as Harmonic

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MOMENTUM DISTRIBUTION FOR AN INHOMOGENEOUS BOSE FLUID AT $T = 0$ WITH BOTH CONFINEMENT AND PARTICLE INTERACTIONS MODELLED AS HARMONIC

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Because of experimental interest in the effects of particle interactions in Bose condensates, such as a dilute atomic vapour of ^{87}Rb, we have worked out the momentum distribution in an N-Boson many-body assembly at $T = 0$, for which both confinement and interbosonic interactions are modelled as purely harmonic. The half-width of the Gaussian momentum distribution is displayed as a function of N and of the strength and sign of the harmonic interactions. The bosonic kinetic energy is finally treated.

Keywords: N-Boson fluid; Momentum density

Condensation in confined bosonic vapours consisting of alkali atoms [1–4] is the motivation for renewed theoretical studies of many-body effects in interacting assemblies of confined Bosons. Thus, the recent investigation of Amoruso *et al.* [5] has resulted in a comparison between collective excitations of a Fermion vapour and those in a dilute Bose-condensed cloud at zero temperature, in the latter case assuming contact interactions.

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Our interest in the present Letter is related, but different, in that we focus on the momentum distribution for another interacting N-Boson model in its ground state. The model considered below has been studied earlier in a different context by various authors [6–8]. What is important for present purposes is that the reduced density matrices can be established analytically for this model of N Bosons with harmonic confinement, along with Boson–Boson interactions which are also harmonic. Specifically then, the model Hamiltonian H is given by

$$H = \frac{1}{2}\sum_{i=1}^{N}(-\nabla_i^2 + \omega^2 r_i^2) \pm \frac{1}{2}\gamma^2 \sum_{i<j}^{N} r_{ij}^2, \tag{1}$$

the choice of sign allowing either attractive or repulsive interactions between the Bosons.

We shall, because of the studies in Refs. [6–8], merely quote the result for the first-order density matrix ρ_1 (see, for example, Eq. (2.34) of Ref. [8]) as

$$\rho_1(\mathbf{r},\mathbf{r}') = N\left[\frac{\omega_N N\omega/\pi}{(N-1)\omega + \omega_N}\right]^{3/2} \exp[-a_1(\mathbf{r}^2 + \mathbf{r}'^2) + a_2\mathbf{r}\cdot\mathbf{r}'] \tag{2}$$

where ω_N^2 is defined by

$$\omega_N^2 = \omega^2 \pm N\gamma^2. \tag{3}$$

In Eq. (2), a_1 and a_2 have the explicit forms

$$a_1 = \frac{1}{4N}\frac{(N-1)(\omega^2 + \omega_N^2) + 2(N^2 - N + 1)\omega\omega_N}{(N-1)\omega + \omega_N} \tag{4}$$

and

$$a_2 = \frac{1}{2N}\frac{(N-1)(\omega - \omega_N)^2}{(N-1)\omega + \omega_N}. \tag{5}$$

We assume that for repulsive interactions the coupling is not so strong as to break confinement.

We next note that the ground-state density profile $n(\mathbf{r}) \equiv \rho_1(\mathbf{r}, \mathbf{r})$ enters the first-order density matrix ρ_1 in Eq. (2) through

$$\rho_1(\mathbf{r}, \mathbf{r}') = \exp\left\{ -\frac{1}{N}[\omega + (N-1)\omega_N]\left(\frac{\mathbf{r}-\mathbf{r}'}{2}\right)^2 \right\} n\left(\frac{\mathbf{r}+\mathbf{r}'}{2}\right). \quad (6)$$

To see how Eq. (6) arises from Eq. (2), we note first, as is readily verified from Eqs. (4) and (5), that

$$a_1 - \frac{1}{2}a_2 = \frac{1}{2}\frac{N\omega\omega_N}{(N-1)\omega + \omega_N}. \quad (7)$$

Using sum and difference coordinates $\mathbf{R} = (\mathbf{r}+\mathbf{r}')/2$ and $(\mathbf{r}-\mathbf{r}')/2$ respectively in Eq. (2), it follows after some manipulation in which the identity (7) is utilized that ρ_1 in Eq. (2) has the equivalent form (6).

One can now obtain the zero-temperature Wigner distribution function, $f_W(\mathbf{R}, \mathbf{p})$, by taking the Fourier transform with respect to $(\mathbf{r}-\mathbf{r}')/2$ in Eq. (6). Then the 'mixed' density matrix f_W is found to take the form

$$f_W(\mathbf{R}, \mathbf{p}) = A^2 \exp(-\alpha_N p^2) n(\mathbf{R}) \quad (8)$$

where α_N is essentially the inverse of the constant multiplying $(\mathbf{r}-\mathbf{r}')^2$ in Eq. (6). The momentum distribution, $P(\mathbf{p})$ say, is readily obtained by integration over $\mathbf{R}$ as

$$P(\mathbf{p}) = \int f_W(\mathbf{R}, \mathbf{p}) d\mathbf{R} = NA^2 \exp(-\alpha_N p^2) \quad (9)$$

where $\int n(\mathbf{R}) d\mathbf{R} = N$ has been used, while A^2 in Eqs. (8) and (9) is a remaining normalization factor. The result for $P(\mathbf{p})$ is thus proved to be of Gaussian shape, as for the non-interacting, harmonically confined Bosons, but with a half-width that depends not only on N and the force constant of confinement (proportional to ω^2) but also on the strength (and of course the sign) of the Boson–Boson interactions through ω_N^2 defined in Eq. (3).

In summary, in the N-Boson model already studied in $\mathbf{r}$ space in Refs. [6–8], the Wigner function factorizes into the form (8) and since the $\mathbf{R}$ dependence enters only through the density profile $n(\mathbf{R})$, the momentum distribution follows using only the normalization of the density profile $n(\mathbf{R})$ to the number of Bosons N. The momentum distribution remains Gaussian, as for harmonic confinement with $\gamma^2=0$: but the half width is altered by the sign and strength of the harmonic interbosonic interactions characterizing the model.

The final point we wish to stress concerns the quantum-mechanical average of the kinetic energy operator in Eq. (1). Clearly this can be immediately related to $\langle p^2P(\mathbf{p})/2\rangle$, the kinetic energy per Boson, T_γ/N say, to yield

$$\frac{T_\gamma}{N}=\frac{3}{4}\left[\left(1-\frac{1}{N}\right)\omega_N+\frac{\omega}{N}\right]. \tag{10}$$

Switching off the interactions by letting $\gamma^2\to 0$, one finds the expected 'confinement' result $T_0/N=3\omega/4$ as follows from the virial theorem with total energy per particle as the zero-point value $3\omega/2$. Evidently, the kinetic energy change per Boson due to the interactions is given by

$$\frac{T_\gamma-T_0}{N}=\frac{3}{4}\left(1-\frac{1}{N}\right)(\omega_N-\omega). \tag{11}$$

In addition to these results following readily from the momentum density formulation, it is of interest to note an alternative route to the kinetic energy. This $\mathbf{r}$ space treatment is now in terms of the particle density $n(\mathbf{r})$, the expectation value of the total kinetic energy operator in Eq. (1) being

$$\left\langle -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2\right\rangle=\int n(\mathbf{r})\left\{C+\frac{1}{2}\frac{N\omega\omega_N}{(N-1)\omega+\omega_N}\ln n(\mathbf{r})\right\}d\mathbf{r} \tag{12}$$

where C is the known constant:

$$C=\frac{3}{4N}\frac{(N-1)(\omega^2+\omega_N^2)+2(N^2-N+1)\omega\omega_N}{(N-1)\omega+\omega_N}-\frac{1}{2}\frac{N\omega\omega_N}{(N-1)\omega+\omega_N}\ln\left\{N\left[\frac{N\omega\omega_N/\pi}{(N-1)\omega+\omega_N}\right]^{3/2}\right\}. \tag{13}$$

While Eqs. (12) and (13) must obviously be equivalent to $\langle p^2P(\mathbf{p})/2\rangle$ evaluated from the Gaussian momentum density (9) when the explicit form of $n(\mathbf{r})$ is inserted into Eq. (12) from Eq. (2), the result (12), going back at least as far as Cohen and Lee [8], is of basic interest for the density functional theory (DFT) of interacting Bosons in the ground state. While the constant C in Eq. (12) involves again simply the normalization integral for the density profile $n(\mathbf{r})$, we wish finally to emphasize, as a possible future direction for research in this currently important area of interacting Bosons, that the contribution involving $\int n(\mathbf{r}) \ln n(\mathbf{r}) d\mathbf{r}$ is of the form of the so-called Shannon information entropy, which has been discussed elsewhere in relation to DFT [9].

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