Fully quantum mechanical moment of inertia of a mesoscopic ideal Bose gas

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(preprint, March 21, 2022)

I. INTRODUCTION

Despite recent achievements in preparing Bose condensed atomic gases [1,2] the question of superfluidity still escapes direct experimental observation. This is partly due to the difficulty to define and/or access the appropriate experimental observables.

Our understanding of superfluidity is formed by the physics of macroscopic systems such as liquid helium. In those systems standard theoretical methods could be applied that required a thermodynamic limit procedure.

However, for the finite size systems prepared with trapped atomic Bose gases the standard answers had to be made more precise. E.g., one can speak of a phase transition, but a discontinuous change of system observables does not occur in mesoscopic systems. The phase transition was linked to the ground state population, but the most striking effect of superfluidity cannot be observed in a direct way.

In a spatially homogeneous situation the phenomenon of superfluidity is defined as the suppression of friction for a linear motion slower than the velocity of sound [3]. This phenomenon is constrained to a fraction of the fluid only, the so-called superfluid fraction. In linear response theory the latter is calculated via the quantum mechanical dispersion of the momentum distribution.

The suppression of friction itself can be traced back to the appearance of excitations with a linear dispersion relation for an interacting Bose gas in the presence of a condensate. It is thus inseparably connected with inter-particle interactions. Nevertheless the superfluid fraction mentioned above does not vanish for an ideal Bose gas due to Bose-Einstein statistics at least for mesoscopic samples.

In the case of a atomic cloud trapped e.g. in a harmonic potential a similar qualitative change of the spectrum of low lying excitations can not be observed, and the understanding of superfluidity in rotational motion of trapped atoms is more subtle. Instead of regarding the response to a Galilei shift one has to consider the response of the gas to rotations. The response coefficient then is the moment of inertia of the trapped gas.

The approach of Brosens et. al. to the moment of inertia is based on the classical expectation value \( \langle x^2 + y^2 \rangle \). Their analysis focuses on the difference in the moment of inertia of a totally classical Boltzmann gas in a trap and the expectation value of \( (x^2 + y^2) \) for a Bose gas (cf. Eq. (4)). Therefore they miss the true superfluid effects that may only be analyzed by calculating the moment of inertia from quantum mechanical response to rotations.

By contrast, Stringari’s work [3] is based on linear response theory. He obtained the different contributions from the condensate and the thermal cloud to the response coefficient both for an ideal and an interacting Bose gas. His use of the grand canonical ensemble is certainly justified for the study of 10^6 particles, a characteristic number for present BEC experiments.

Instead of considering the relation between rotations and superfluidity one might investigate the relation between dissipation and superfluidity like in [4] where the onset of dissipation is analyzed depending on the velocity of an external perturbation. The numerical work in [4] favors vortex creation as the main dissipation mechanism but it is still under debate at which critical velocity dissipation sets in.

The rotational properties have recently been analyzed in various works either focusing on vortices [5,6] or on the so-called scissors mode [7,8]. The analysis of this mode led to a connection between the quadrupole excitations and the moment of inertia of the normal fluid fraction [9] which might open a way to measure the moment of inertia.

In this paper we present a calculation of the fully quantum mechanical moment of inertia for a mesoscopic cloud.
of non-interacting atoms in a cylindrically symmetrical trap. Finite size effects are allowed for by calculating the canonical ensemble averages appropriate for this regime. In this respect, our calculations are complementary to [8] and show markedly different results for the superfluid fraction. It is of particular interest that all relevant averages are expressed using permutation cycles which have already played a crucial role in previous Path-Integral-Monte-Carlo (PIMC) studies [16,17]. Our analytical results are compared to and corroborated by numerically exact results computed by the PIMC method.

In Section II we first present the method of permutation cycles and apply it to the evaluation of the moment of inertia in Section III. In Sec. IV, we finally compare the results obtained by the different methods.

II. CANONICAL AVERAGES

We want to perform our calculations using the permutation cycle analysis introduced by Feynman [18] and the canonical ensemble. Let us consider $N$ particles living in an exterior potential $V(r)$ ($r \in R^R$), so the single particle Hamiltonian is given as usual by

$$H = \frac{p^2}{2m} + V(r). \quad (1)$$

With the help of the eigenvalues $E_i$ and eigenfunctions $|\phi_i\rangle$ $H$ can also be written as

$$H = \sum_i E_i |\phi_i\rangle \langle \phi_i| . \quad (2)$$

The total Hamiltonian for $N$ particles is then given by the sum $H_N = \sum_{j=1}^N H^{(j)}$ over all the particles.

The central physical quantity in statistical mechanics is the partition function $Z_N(\beta)$ at inverse temperature $\beta = 1/(kT)$. For a gas of $N$ bosons $Z_N(\beta)$ is given by

$$Z_N(\beta) = \frac{1}{N!} \int dR \rho(R,PR), \quad R = (r_1, \ldots, r_N) \quad (3)$$

where $\rho(R, PR) = \langle R | e^{-\beta H_N} | PR \rangle$ is the density matrix between the point $R$ and the permuted point $PR = (r_{P1}, \ldots, r_{PN})$ and $P$ is a permutation of the first $N$ integer numbers. As the total Hamiltonian $H_N$ is a sum of independent single-particle Hamiltonians the integral factorizes

$$Z_N(\beta) = \frac{1}{N!} \sum_{P \in S_N} \prod_{j=1}^N \int dP r_j \rho_1(r_j, r_{Pj}). \quad (4)$$

Here, $\rho_1(r, r_{P}) = \langle r_j | e^{-\beta H} | r_{Pj} \rangle$ is the single-particle density matrix. Now, we break up the permutations into so-called "cycles", that is subsets of the number from $1$ to $N$ that are invariant under the action of a permutation $P$. If we break up $P$ in this way, we may get $C_q$ cycles of length $q$; as we are working in the canonical ensemble these numbers are restricted by $\sum_{q=1}^N qC_q = N$. Rearranging the integrand of (4) one arrives at

$$Z_N(\beta) = \sum_{C_1, \ldots, C_N} \prod_{q=1}^N \frac{Z_1(q\beta)^{C_q}}{C_q q^{qC_q}} \quad (5)$$

for the partition function (see [19]). Here, the sum over all combinations of "cycle populations" $C_1, \ldots, C_N$ is restricted by $\sum_{q=1}^N qC_q = N$.

By calculating the derivative with respect to $\beta E_i$ one gets the formula for $\langle N_i \rangle$ for later evaluations (see also [19])

$$\langle N_i \rangle = -\frac{1}{Z_N(\beta)} \frac{\partial Z_N(\beta)}{\partial \beta E_i} . \quad (6)$$

We now apply this expression to (3) and use the fact that $Z_1(q\beta) = \sum_i e^{-q\beta E_i}$ to finally obtain

$$\langle N_i \rangle = \sum_{q=1}^N \frac{e^{-q\beta E_i}}{Z_1(q\beta)} \langle qC_q \rangle . \quad (7)$$

So we need to know the mean number of $q$-cycles $\langle C_q \rangle$ to compute $\langle N_i \rangle$.

Evidently, $\langle C_q \rangle$ is defined by

$$\langle C_q \rangle = \frac{1}{Z_N(\beta)} \sum_{C_1, \ldots, C_N} \prod_{r=1}^N \frac{Z_1(r\beta)^{C_r}}{C_r r^{C_r}} \cdot \langle qC_q \rangle . \quad (8)$$

To calculate this expression, we split the product into the factors with $r \neq q$ and the factor with $r = q$. Note also that terms with $C_q = 0$ do not contribute. So one gets

$$\langle C_q \rangle = \frac{1}{Z_N(\beta)} \sum_{C_1, \ldots, C_N} \prod_{r=1}^N \frac{Z_1(r\beta)^{C_r}}{C_r r^{C_r}} \cdot \frac{Z_1(q\beta)^{C_q-1}}{(C_q - 1) q^{C_q-1}} \cdot \frac{Z_1(q\beta)}{q} . \quad (9)$$

As $C_q > 0$, we can substitute $C_q - 1$ by $C_q$ and do the sum again from $C_q = 0 \to \infty$. But this means that we consider one $q$-cycle less, so $\sum_{r} rC_r = N - q$. We end up with the final formula for the cycle occupation number

$$\langle C_q \rangle = \frac{Z_{N-q}(\beta)}{Z_N(\beta)} \frac{Z_1(q\beta)}{q} . \quad (10)$$

where $Z_{N-q}(\beta)$ originates from the sum over the products in (3). This equation together with the constraint on the $C_q$'s constitute the well-known recursion relations for $Z_N(\beta)$ [19].

2
III. SUPERFLUIDITY IN A HARMONIC TRAP

In this section we want to compute the superfluid fraction $\rho_s/\rho$ of a gas of noninteracting bosons in a harmonic trap. This will be done by using the permutation cycles introduced in the last section.

The superfluid fraction can be defined via the response of the system to infinitesimal rotations just like in the usual case for translations [10]. The superfluid part shows no response to rotations at all while its density distribution contributes to the classical moment of inertia. Therefore, one has

$$\frac{\rho_s}{\rho} = 1 - \frac{\rho_n}{\rho}, \quad (11)$$

with the normal fluid fraction defined by the quotient of the quantum mechanical and the classical moment of inertia for rotations around the symmetry axis (z-axis)

$$\frac{\rho_n}{\rho} = \frac{I_{qm}}{I_{class}}. \quad (12)$$

One can calculate $I_{qm}$ via the response to rotations [10], this yields

$$I_{qm} = \beta (\langle L_z^2 \rangle - \langle L_z \rangle^2) \quad (13)$$

or

$$I_{qm} = \beta (L_z^2), \quad (14)$$

because we only consider non-rotating situations with $\langle L_z \rangle = 0$. The classical moment of inertia is defined as usual by

$$I_{class} = m \sum_{j=1}^{N} \left( x_j^2 + y_j^2 \right). \quad (15)$$

We now want to compute both [14] and [15] by using the permutation cycles of section [11].

We consider the single-particle Hamiltonian for a deformed, harmonic potential in three dimensions

$$H = \frac{p^2}{2m} + \frac{1}{2} m \left( \omega_x^2 (x^2 + y^2) + \omega_z^2 z^2 \right). \quad (16)$$

Its eigenfunctions can be classified by three quantum numbers $n_r = 0, 1, 2, \ldots$, $m = 0, \pm 1, \ldots$, $n_z = 0, 1, \ldots$ with

$$H|n_r, m, n_z\rangle = \{ h \omega_x (2n_r + |m| + 1) + h \omega_z (n_z + 1/2) \}|n_r, m, n_z\rangle; \quad (17)$$

they are also eigenfunctions of the angular momentum operator around the z-direction

$$l_z|n_r, m, n_z\rangle = m h|n_r, m, n_z\rangle. \quad (18)$$

The total angular momentum is given by the sum over the angular momentum operators for the $N$ particles in the trap

$$L_z = \sum_{j=1}^{N} l_z^{(j)}. \quad (19)$$

We first turn to $\langle L_z^2 \rangle$. Instead of expressing the sum over all states in the thermodynamic averaging as integrals over the particle positions like in [19] we here use the basis of the single-particle states in [17] to calculate the expectation value of $L_z^2$ (we use $i_j = (n_{r,j}, m_j, n_{z,j})$ to denote the states of particle $j$)

$$\langle L_z^2 \rangle = \frac{1}{Z_N N!} \sum_{p \in S_N} \sum_{i_1, \ldots, i_N} \langle i_1, \ldots, i_N | l_z^{(j)} l_z^{(k)} e^{-\beta H_N} | i_{P1}, \ldots, i_{PN} \rangle. \quad (20)$$

Again, one can factorize the matrix element to a product of matrix elements for only one particle. The factors are either of the form $\langle i_j | e^{-\beta H^{(q)}} | i_{Pj} \rangle = e^{-\beta E_{ij} \delta_{ij,ip_j}}$ or $\langle i_j | l_z^{(q)} e^{-\beta H^{(j)}} | i_{Pj} \rangle = h m_j e^{-\beta E_{ij} \delta_{ij,ip_j}}$ or

$$\langle i_j | l_z^{(q)} e^{-\beta H^{(j)}} | i_{Pj} \rangle = (h m_j)^2 e^{-\beta E_{ij} \delta_{ij,ip_j}}. \quad (21)$$

If now the sum of the permutations is expressed as a sum over all cycle occupations one can see, that due to the Kronecker-δs in the factors, all particles on the same $q$-cycle have the same state. For one $q$-cycle, there are again three different possibilities: if there is no $i_j$ associated to one of the particles on the cycle, then [20] gets the contribution

$$\sum_{i_j} e^{-\beta E_{ij}} = Z_1(q\beta). \quad (21)$$

Or there may be only one such $l_z^{(j)}$. Then the contribution is

$$\sum_{i_j} h m_j e^{-\beta E_{ij}} = 0, \quad (22)$$

which vanishes due to the symmetry $E_{n_r, m, n_z} = E_{-n_r, -m, n_z}$. The third possibility is to have two angular momentum operators acting on two particles on the same $q$-cycle. This contributes a factor

$$\sum_{i_j} (h m_j)^2 e^{-\beta E_{ij}} = \frac{2h^2 e^{-\beta h_\perp \omega_{||}}}{(1 - e^{-\beta h_\perp \omega_{||}})^2} Z_1(q\beta). \quad (23)$$

So all $q$-cycles contribute a factor of $Z_1(q\beta)$, those involving two angular momentum operators additionally contribute a factor of $\frac{2h^2 e^{-\beta h_\perp \omega_{||}}}{(1 - e^{-\beta h_\perp \omega_{||}})^2}$. Before we can write down the formula for $\langle L_z^2 \rangle$ we must count the number of ways how the two $l_z$-operators may
be distributed among the cycles: for a given number \( C_q \) of \( q \)-cycles there are \( qC_q \) particles sitting on these cycles. They can be paired with \( q \) other particles on their own cycle (including themselves), so there are \( q^2C_q \) ways to pair the two angular momentum operators to get (23). This leads to

\[
\langle L_z^2 \rangle = \frac{1}{Z_N N!} \sum_{C_1,\ldots,C_N} M(C_r) \sum_{q=1}^N \frac{2\hbar^2 e^{-\beta \hbar \omega_\perp}}{(1 - e^{-\beta \hbar \omega_\perp})^2} q^2 C_q \prod_{r=1}^N Z_1(r\beta)^{C_r},
\]

(24)

where

\[
M(C_1,\ldots,C_N) = \frac{N!}{\prod_q q! C_q}
\]

(25)

is the number of permutations with \( C_1 \) 1-cycles, \( C_2 \) 2-cycles etc (see [18, above Eq. (2.154)]). By using this and Eqs. (8) and (14)

\[
I_{qm} = \beta \langle L_z^2 \rangle = 2\hbar^2 \sum_{q=1}^N \frac{q\beta e^{-q\beta \hbar \omega_\perp}}{(1 - e^{-q\beta \hbar \omega_\perp})^2} (qC_q).
\]

(26)

So we can calculate the quantum mechanical value of the momentum of inertia by using the cycle occupations in [10].

Now we turn to the classical moment of inertia. One can do the analogous analysis as before for \( I_{qm} \). Here, one meets terms like

\[
\langle ij | (x_j^2 + y_j^2) e^{-q\beta H} | ij \rangle = \frac{\hbar}{m\omega_\perp} \frac{1 + e^{-q\beta \hbar \omega_\perp}}{1 - e^{-q\beta \hbar \omega_\perp}} Z_1(q\beta)
\]

(27)

in analogy to (23) or (24). Eq. (27) is most easily computed using the eigenstates \( |n_x,n_y,n_z\rangle \) of the harmonic trap Hamiltonian.

Finally, \( I_{\text{class}} \) can be written as

\[
I_{\text{class}} = \frac{\hbar}{\omega_\perp} \sum_{q=1}^N \frac{1 + e^{-q\beta \hbar \omega_\perp}}{1 - e^{-q\beta \hbar \omega_\perp}} (qC_q),
\]

(28)

which again depends on the cycle occupation numbers. Eqs. (24) and (28) constitute the main result of the present work, they allow the computation of the superfluid fraction from Eqs. (11), (12) totally based on the cycle occupation numbers in (10).

IV. NUMERICAL RESULTS AND COMPARISON TO PATH INTEGRAL MONTE-CARLO RESULTS

We now turn to the comparison of the cycle approach with results from other methods for the description of the trapped Bose gas.

In Fig. 1 we show the superfluid fraction as a function of temperature for \( N = 25 \) particles in a spherical trap. The full line shows the result originating from our cycle analysis. It is obtained by using (11, 12, 26, 28). \( \langle qC_q \rangle \) has been calculated from the recursion relations for \( Z_N(\beta) \).

![FIG. 1. Superfluid density for \( N = 25 \) (a) resp. \( N = 100 \) (b) particles in a spherically symmetric harmonic trap as a function of temperature (\( T_c \) is the usual critical temperature for Bose condensation in a harmonic trap). The full line denotes our results using the cycle analysis. The short dashed line shows the results of Stringari’s considerations based on the grand canonical ensemble [6]. The long dashed curve stems from the modified two-fluid model (Eq. (23)). The crosses with error bars are from a Monte-Carlo calculation based on path integrals.]

The first comparison is with the model of Stringari [6] who has given a formula for \( \rho_s/\rho \) based on grand canonical considerations. This result is plotted with short dashes in Fig. 1. The difference between the canonical and grand canonical values is clearly visible both for \( N = 25 \) particles and for \( N = 100 \). The two chosen examples already illustrate that the difference between the two ensembles will vanish in the limit \( N \to \infty \).

It is interesting that by using the canonical expectation
values we can also reconcile the cycle analysis given above with a simple two-fluid model of the inhomogeneous Bose gas [21, 22]. In that model the superfluid fraction is totally made up of the condensed part of the system and the normal fluid is identical to the non-condensed part. We here modify the two-fluid model by inserting the number of condensed particles \(\langle N_0 \rangle\) (see [3]) from the canonical averages. For the case of the harmonic trap, \(\langle N_0 \rangle\) can be written as

\[
\langle N_0 \rangle = \sum_{q=1}^{N} (1 - e^{-q\beta\hbar \omega_{\perp}})^2 (1 - e^{-q\beta\hbar \omega_{\parallel}}) \langle qC_q \rangle. \tag{29}
\]

To compute \(\rho_s/\rho\) we need the moments of inertia \(I_0\) of the condensate and \(I_{nc}\) of the non-condensed part. The condensate particles all reside in the ground state of the trap whose moment of inertia for rotations around the \(z\)-axis is \(\hbar/\omega_{\perp}\), so

\[
I_0 = \langle N_0 \rangle \frac{\hbar}{\omega_{\perp}}, \tag{30}
\]

\(I_{nc}\) is estimated by assuming that the non-condensed particles behave like a Boltzmann gas in the harmonic trap. For the inverse temperature \(\beta\) the moment of inertia then equals \(2/(\beta\omega_{\perp}^2)\) so

\[
I_{nc} = N_{nc} \frac{2}{\beta \omega_{\perp}^2} = N_{nc} \frac{2kT}{\omega_{\perp}^2}, \tag{31}
\]

where \(N_{nc} = N - \langle N_0 \rangle\).

Finally, by noting that the condensate only contributes to the classical moment of inertia \(I_{class}\) but does not take part in the rotation, we can estimate \(\rho_s/\rho\) by

\[
\frac{\rho_s}{\rho} \approx 1 - \frac{I_{nc}}{I_0 + I_{nc}} = \frac{1}{1 + \frac{N - \langle N_0 \rangle}{\langle N_0 \rangle} \frac{2kT}{\hbar \omega_{\perp}}}. \tag{32}
\]

The long dashed lines in Fig. 1 give a plot of this formula. It fits the exact result for the canonical ensemble surprisingly well. The two-fluid model differs from the exact result only due to the small difference between the true non-condensed part and its quasi-classical approximation.

A third way to calculate the superfluid fraction via moments of inertia is the path integral representation of the density matrix [15]. This approach works for both non-interacting and interacting systems. It represents the most important point of comparison as it is a potentially exact method. We have implemented a Path Integral Monte-Carlo (PIMC) code that relies on the bisectioning ideas of Ceperley [16] and on the factorization of the complete density matrix into a non-interacting part and the interaction correction [17].

Here, we will only show that the results discussed in the previous section agree well — as they should — with the data obtained from PIMC calculations without interactions.

The data points (crosses) in Fig. 1 show our results for the superfluid fraction. They have been computed by using the so-called “area formula” [23–13] which is the most appropriate method for our investigations. The superfluid fraction is obtained from

\[
\frac{\rho_s}{\rho} = \frac{4m^2}{h^2 \beta} \langle I_z \rangle. \tag{33}
\]

Here

\[
I_z = \frac{m}{M} \sum_{t=0}^{M-1} \sum_{i=1}^{N} (x_i(t)x_i(t + 1) + y_i(t)y_i(t + 1)) \tag{34}
\]

denotes the PIMC approximation of classical moment of inertia \(m\) is again the mass of the particles, \(x_i(t)\) and \(y_i(t)\) are the coordinates of the \(i\)-th particle on time slice \(t\) of the PIMC simulation and there are \(M\) such time slices. \(I_z\) clearly converges to \(I_{class}\) as \(M \to \infty\).

The expression

\[
A_z = \frac{1}{2} \sum_{t=0}^{M-1} \sum_{i=1}^{N} (x_i(t)y_i(t + 1) - y_i(t)x_i(t + 1)) \tag{35}
\]

is the projected area perpendicular to the rotation axis \(z\). \(\langle A_z^2 \rangle\) is the portion of the moment of inertia that can be traced back to the superfluid fraction \(\rho_s/\rho\).

As Fig. 1 shows, all three methods are in good agreement with each other. We have furthermore calculated the density distribution of the particles in the trap both in the two-fluid model and with PIMC. They also exhibit a nice agreement thus indicating the validity of the empirical two-fluid model.

V. SUMMARY AND CONCLUSION

The main result of our paper is the calculation of the superfluid fraction from the permutation cycles. We have compared this approach to the grand-canonical prediction by Stringari and to PIMC calculations. For small particle numbers our results are in good agreement with the exact (canonical) PIMC results and we were able to reproduce them to a very good accuracy with a two-fluid model which divides the gas into a condensed and a non-condensed part where the latter is treated as a classical Boltzmann gas. For small particle numbers we find a distinct difference between our results and Stringari’s grand canonical approach.

The techniques and results presented in this paper have established a solid starting point of PIMC investigations including interactions. As the calculation of the condensate fraction in PIMC calculations of inhomogeneous Bose gases is still under debate, the role of the permutation cycles deserves further investigations also in the interacting case (see e.g. [24] for a related discussion).
J.S. thanks M. Holzmann for a stimulating discussion on the subject. We gratefully acknowledge financial support by DFG under Grant Nr. SCHE 128/7-1.

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