One-Particle Density Matrix for a Quantum Gas in the Box Geometry

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We have analytically obtained 1-particle density matrices for ideal Bose and Fermi gases in 3-D box geometries for the entire range of temperature. We also have obtained quantum cluster expansions of the grand free energies in closed forms for the same systems in the restricted geometries. We also have considered short ranged interactions in our analyses for the quasi 1-D cases of Bose and Fermi gases in the box geometries. Our results are exact and are directly useful for a postgraduate course on statistical mechanics or that on many-body physics.

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I. INTRODUCTION

Density matrix is of very high interest in physics [1–4]. It maps equilibrium statistical mechanics to quantum dynamics and vice versa with the application of Wick rotation \((1/k_B T \mapsto it/\hbar)\) which maps inverse temperate \((1/T)\) to imaginary time \((it)\) [4, 5]. Density matrix elements, which physically represents spatial correlations in a thermodynamic or mechanical system, are nothing but the propagators in the position representation [4]. Density matrix elements are thus useful to get path integrals in statistical field theory and quantum field theory [4].

Density matrix is often introduced in several postgraduate courses on physics such as statistical mechanics, many-body physics, quantum mechanics, quantum field theory, quantum optics, etc [4, 6]. Density matrix elements (and 1-particle density matrix elements for many-body systems [7, 8]) are often calculated in position representation in the class for systems having no boundaries at all, e.g. a free particle, a harmonic oscillator, a free Bose gas at a temperature \(T\), a free Fermi gas at a temperature \(T\), etc [4, 9]. There have been many discussions on in the frontiers level in connection with the 1-particle density matrices or cluster expansions or spatial correlations in quantum gases [10–14]. However, hardly any discussions are found on the finite size effects on the density matrices in the graduate-course text-books or even in the research articles. Practically all the thermodynamic systems which come to equilibrium with the respective heat (and in some occasions particle) reservoirs are bounded. Hence we are interested in calculating 1-particle density matrix [8] for ideal Bose and Fermi gases in 3-D box geometries at a temperature \(T\). We are also interested to explore the same interacting Bose and Fermi gases confined at least in quasi 1-D boxes. We also want to have quantum cluster expansions [15, 16] of the grand free energies for these systems in connection with the density matrices. Thermodynamic properties of the systems and the finite-size effects on them can be easily obtained from the quantum cluster expansions of the grand free energies.

Study of ultracold quantum gases has been a topic of high experimental and theoretical interest [17–19] after the observation of Bose-Einstein condensation of alkali atoms in 3-D magneto-optical harmonic traps in 1995 [20–22]. Bose-Einstein condensation of a dilute Bose gas of \(^{87}\text{Rb}\) atoms has also been observed recently in a 3-D magneto-optical box trap with quasi-uniform potential in it [23]. Thus studying 1-particle density matrix for ideal Bose and Fermi gases in 3-D box geometries and that of quantum cluster expansions of these systems would be relevant in the current context not only from science-education point of view but also from research point of view.

Calculations of this article begin with the introduction of the statistical mechanical density matrix and the equation for its matrix-element in position-space representation for a single particle in equilibrium with a heat bath at an absolute temperature \(T\). Then solve the equation for the density matrix-element for a particle in 1-D box. Then we generalize the solution for 3-D box. Then we generalize the 3-D case of the single particle to the ideal gases of many-particles (i.e. for identical bosons and fermions) with 1-particle density matrix within grand-canonical ensemble. Then we obtain quantum cluster expansions for grand free energies for these systems. Then we consider short ranged interactions in our analyses for the quasi 1-D cases of Bose and Fermi gases in the box geometries. We conclude finally.

II. STATISTICAL MECHANICAL DENSITY MATRIX

Let us consider a thermodynamic system in equilibrium with a heat bath at an absolute temperature \(T\). Statistical mechanical density matrix is defined for the

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The definition leads to the equation for the density matrix-element as
$$\frac{\partial}{\partial \beta} \rho(x, x'; \beta) = -\hat{H}_x \rho(x, x'; \beta) = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \rho(x, x'; \beta),$$
(4)
where $\hat{H}_x = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$ is the position representation of the Hamiltonian of the system in the nonrelativistic domain, and $m$ is the mass of the system. By sending $\beta \to 0$ in Eqn. (3) we get $\rho(x, x'; 0) = \delta(x - x')$. This can be considered as an inhomogeneous boundary condition for the solution to the diffusion Eqn. (4). The solution for $L \to \infty$, i.e. for the case of free particle,
$$\rho_f(x, x'; \beta) = \sqrt{\frac{m}{2\pi \hbar^2 \beta}} e^{-\frac{m(x' - x)^2}{2\hbar^2 \beta}},$$
(5)
is well known in the literature [4].

The solution to the Eqn. (4) for finite $L$, however, is not known in the literature in compact form. Dirichlet boundary conditions on the energy eigenstates in Eqn. (3) leads to take the form of the solution, for finite $L$, as
$$\rho(x, x'; \beta) = \sum_{j=1}^{\infty} \tilde{\rho}(j, x'; \beta) \sin \left( \frac{j \pi x}{L} \right)$$
(6)
where $\sin \left( \frac{j \pi x}{L} \right) = \sqrt{\frac{2}{j}} \psi_j(x) = \sqrt{\frac{2}{j}} |\psi_j\rangle$ is $\sqrt{\frac{2}{j}}$ times the normalized energy eigenstate for the particle in the box, and the Fourier series expansion-coefficient, $\tilde{\rho}(j, x'; \beta)$, is to be determined from Eqn. (4) by performing the inverse transformation for the same inhomogeneous boundary condition. Thus, the expansion-coefficient takes the form $\tilde{\rho}(j, x'; \beta) = \sqrt{\frac{2}{j}} \sin \left( \frac{j \pi x}{L} \right) e^{-\frac{m \pi^2 j^2}{2 \hbar^2 \beta}}$ so that the solution becomes
$$\rho(x, x'; \beta) = \sum_{j=1}^{\infty} \frac{2}{L} e^{-\frac{m \pi^2 j^2}{\hbar^2 \beta}} \sin \left( \frac{j \pi x}{L} \right) \sin \left( \frac{j \pi x'}{L} \right)$$
$$= \sum_{j=1}^{\infty} e^{-\frac{m \pi^2 j^2}{\hbar^2 \beta}} \left[ \cos \left( \frac{j \pi [x' - x]}{L} \right) - \cos \left( \frac{j \pi [x' + x]}{L} \right) \right].$$
(7)
This form of solution also directly follows from Eqn. (3) as the energy eigenvalues are $E_j = \frac{\pi^2 j^2}{2mL^2}$ for all $j$ for the particle in the 1-D box. However, by performing the summation over $j$ in Eqn. (7) we get an exact result in compact form as
$$\rho(x, x'; \beta) = \frac{1}{2L} \left[ \partial_3 \left( \pi [x' - x] \right) e^{-\frac{m \pi^2 j^2}{2 \hbar^2 \beta}} \right]$$
$$- \partial_3 \left( \pi [x' + x] \right) e^{-\frac{m \pi^2 j^2}{2 \hbar^2 \beta}} \right]$$
(8)
where $\partial_3$ represents a Jacobi (elliptic) theta function in the usual notation [31]. The second term in the right hand

### A. Density matrix for a single particle in a 1-D box

If the points $x$ and $x'$ be any two arbitrary points inside a 1-D box of length $L$ which confines a point-particle such that $0 < x < L$, then the density matrix element of the system can be defined in position representation as
$$\rho(x, x'; \beta) = \langle x | \hat{\rho} | x' \rangle = \langle x | e^{-\beta \hat{H}} | x' \rangle$$
$$= \sum_{j=1}^{\infty} e^{-\beta E_j} \psi_j(x) \psi_j^\dagger (x')$$
(3)
side of Eqn.(8) breaks the translational symmetry in the density matrix-element, as before, the density matrix-element no longer depends on separation of the points x and x′ for finite L. We plot the density matrix-element (Eqn. (8)) and also compare it with the one with the free-boundary (Eqn.(5)) in FIG. 1. Eqn.(8) is significantly different from Eqn.(5) in the low temperature regime when thermal de Broglie wavelength, $\lambda_T = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$, becomes comparable to or bigger than the system size (L). It is also clear from the dashed line of the figure, that, the density matrix-element is not being maximized at $x' = x$ unless $x = L/2[32]$, as the translation symmetry is broken for the finite size (L) of the system.

### B. Density matrix for a single particle in a 3-D box

Let us now consider the particle to be in a 3-D box of lengths $L_1$, $L_2$, $L_3$ along the x, y, z axes respectively. Position of the particle is now given by $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$ (or $\vec{r}' = x'\hat{i} + y'\hat{j} + z'\hat{k}$) such that $0 < x < L_1$, $0 < y < L_2$, $0 < z < L_3$. Since the system is linear, as there are no inter particle interactions, motions of the particle along x, y and z axes would be independent of each other. Thus, we can generalize the result for the density matrix-element in Eqn.(8) for the 3-D as product of the density matrix elements for the individual axes:

$$
\rho(\vec{r}, \vec{r}'; \beta) = \Pi_{l=1}^{3} \frac{1}{2L_l} \left[ \vartheta(3) \left( \frac{\pi [x'_l - x_l]}{2L_l}, e^{-\beta \frac{2\pi^2}{mL_l^2}} \right) 
- \vartheta(3) \left( \frac{\pi [x'_l + x_l]}{2L_l}, e^{-\beta \frac{2\pi^2}{mL_l^2}} \right) \right]
$$

where $x_1 = x$, $x_2 = y$, $x_3 = y$, and so as for the primed coordinates.

Eqn.(9) is our result for statistical mechanical density matrix element $(\rho(\vec{r}, \vec{r}'; \beta) = \langle \hat{n}_{\vec{r}} \hat{n}_{\vec{r}'} \rangle)$ for a single particle in a 3-D box in equilibrium with a heat bath at a temperature $T$. In the following section, we extend the statistical mechanical density matrix for many-body systems within grandcanonical ensemble.

### III. ONE-PARTICLE DENSITY MATRIX FOR AN IDEAL QUANTUM GAS IN A 3-D BOX

One-particle density matrix for an ideal quantum gas (i.e. Bose or Fermi gas of indistinguishable particles) in equilibrium with a heat (and particle) bath at a temperature $T$ (and chemical potential $\mu$) is defined (by generalizing Eqn.(2)) as [7, 8]

$$
\hat{\rho}^1 = \sum_{j=1}^{\infty} \frac{1}{e^{\beta(E_j - \mu)} + 1} |\psi_j\rangle \langle \psi_j| 
$$

where $\{|\psi_j\rangle\}$ are the orthonormalized and complete set of eigenstates of eigenvalues $\{E_j\}$ for the single-particle Hamiltonian of the many-body system and the prefactor, $\frac{1}{e^{\beta(E_j - \mu)} + 1}$, represents the average occupation number of particles $\langle \hat{n}_j \rangle$ to the single-particle state $|\psi_j\rangle$. Thus we generalize Eqn.(9) to the 1-particle density matrix for the many-body system in the 3-D box as

$$
\rho^1(\vec{r}, \vec{r}'; \beta) = \sum_{j_1=1}^{\infty} \sum_{j_2=1}^{\infty} \Pi_{l=1}^{3} \frac{2}{L_l} \sin \left( \frac{j_l\pi x_l}{L_l} \right) \sin \left( \frac{j_l\pi x'_l}{L_l} \right)
$$

where $E_{j_l} = \frac{\pi^2\hbar^2}{2mL_l^2}$ for $i = 1, 2, 3$, and upper sign represents Bose gas and lower sign represents Fermi gas.

While single-particle ground state energy of the system is given by $E_0 = \frac{\pi^2\hbar^2}{2mL_1^2}$, fugacity of the system is given by $\tilde{z} = e^{\mu/\hbar T}$ which ranges as $0 \leq \tilde{z} \leq e^{E_0/\hbar T}$ for the ideal Bose gas and $0 \leq \tilde{z} \leq \infty$ for the ideal Fermi gas. One-particle density matrix-element (in position representation) catches long-ranged order in the many-body system at least for 3-D free Bose gas [7, 8]. The finite size effect kills the long-ranged order in the many-body system as the density matrix element has to vanish at the boundaries as clear even in FIG. 1. Expansion of the r.h.s. of Eqn.(11) around $\tilde{z} = 0$ leads to

$$
\rho^1(\vec{r}, \vec{r}'; \beta) = \sum_{l=1}^{\infty} (\pm 1)^{l-1} \tilde{z}^l \rho(\vec{r}, \vec{r}'; l\beta).
$$

If boundaries along x and y axes are removed, i.e. if $L_1$ and $L_2$ are sent to $\infty$, then the system would be confined only along the z-axis. The one-particle density matrix in this situation would be

$$
\rho^1(\vec{r}, \vec{r}'; \beta) = \sum_{l=1}^{\infty} (\pm 1)^{l-1} \frac{\tilde{z}^l}{l} \rho_f(\vec{r}_\perp, \vec{r}_\perp'; l\beta) \rho(z, z'; l\beta)
$$

where $\vec{r}_\perp = x\hat{i} + y\hat{j}$, $\vec{r}_\perp' = x'\hat{i} + y'\hat{j}$.

$$
\rho_f(\vec{r}_\perp, \vec{r}_\perp'; l\beta) = \frac{1}{\lambda_T^2} e^{-\frac{\lambda_T^2 \tilde{z}^2}{l^2}}
$$

is the density matrix for a free-particle in the $x-y$ plane [4], and $\rho(z, z'; \beta)$ is the density-matrix of the particle, similar to that in Eqn.(8), for the bounded motion along the z-axis. For 3-D free quantum gas, Eqn.(13) takes the form [7, 8]

$$
\rho^1_f(\vec{r}, \vec{r}'; \beta) = \frac{1}{\lambda_T^2} \sum_{l=1}^{\infty} (\pm)^{l-1} \frac{\tilde{z}^l}{l^2} e^{-\frac{\lambda_T^2 \tilde{z}^2}{l^2}}
$$

The term with the first power of the fugacity $\tilde{z}$ in the density matrix-element in Eqn.(13) corresponds to the classical case. We plot the 1-particle density matrix-element.
that the box-confinement reduces the spatial correlations in the Fermi gas in comparison to that in the Bose gas as clear in the FIG. 2. It is seen from the FIG. 2 that the box-confinement reduces the spatial correlations in the system in comparison to that in the free quantum (Bose or Fermi) gas. The finite size effect kills the long-ranged order in the 3-D ideal Bose gas as the density matrix element has to vanish at the boundaries as clear in the FIG. 2. The dotted line would come arbitrary close to the solid line at \( z = L_3/2 \) for \( \bar{z} \to 0 \).

Alternating series expansion in Eqn.(13) further reduces the spatial correlations in the Fermi gas in comparison to that in the Bose gas as clear in the FIG. 2. Eqn.(13), for the Fermi gas, can be recast as

\[
\rho^1(\vec{r}, \vec{r}'; \beta) = \sum_{j_3=1}^{\infty} \left[ \int_{j_3}^{\infty} \frac{e^{\beta(p_\perp^2/2m + F_{j_3}) - \mu}}{e^{\beta(p_\perp^2/2m + F_{j_3}) - \mu} + 1} (2\pi \hbar)^2 \frac{2}{L_3} \sin \left( \frac{j_3 \pi x}{L_3} \right) \sin \left( \frac{j_3 \pi y'}{L_3} \right) \right] \quad \text{d}p_\perp \quad \text{d}p_{\perp'}
\]

\[
= \sum_{j_3=1}^{\infty} \left[ \int_{0}^{\infty} \frac{2 \pi J_0( |\vec{r}_\perp - \vec{r}'_\perp|/p_\perp \hbar) |p_{\perp'}| J_1( |\vec{r}'_\perp - \vec{r}_{\perp'}|/p_{\perp'} \hbar)}{(2\pi \hbar)^2} \right] \quad \text{d}p_\perp \quad \text{d}p_{\perp'}
\]

\[
= \sum_{j_3=1}^{\infty} \left[ \int_{0}^{\infty} \frac{2 \pi J_0( |\vec{r}_\perp - \vec{r}'_\perp|/p_\perp \hbar) |p_{\perp'}| J_1( |\vec{r}'_\perp - \vec{r}_{\perp'}|/p_{\perp'} \hbar)}{(2\pi \hbar)^2} \right] \quad \text{d}p_\perp \quad \text{d}p_{\perp'}
\]

which can be further recast for \( T \to 0 \), for which \( \mu \geq \frac{\pi^2 \hbar^2}{2mL_3^2} \) and \( p_\perp \) ranges from 0 to \( p_{Fj_3} = \sqrt{2m\mu - \frac{\pi^2 \hbar^2}{L_3^2}} \), as

\[
\rho^1(\vec{r}, \vec{r}'; \infty) = \frac{1}{\pi L_3} \sum_{j_3=1}^{\infty} \left[ \int_{0}^{\infty} \frac{2 \pi J_0( |\vec{r}_\perp - \vec{r}'_\perp|/p_\perp \hbar) |p_{\perp'}| J_1( |\vec{r}'_\perp - \vec{r}_{\perp'}|/p_{\perp'} \hbar)}{(2\pi \hbar)^2} \right] \quad \text{d}p_\perp \quad \text{d}p_{\perp'}
\]

\[
= \frac{1}{\pi L_3} \sum_{j_3=1}^{\infty} \left[ \int_{0}^{\infty} \frac{2 \pi J_0( |\vec{r}_\perp - \vec{r}'_\perp|/p_\perp \hbar) |p_{\perp'}| J_1( |\vec{r}'_\perp - \vec{r}_{\perp'}|/p_{\perp'} \hbar)}{(2\pi \hbar)^2} \right] \quad \text{d}p_\perp \quad \text{d}p_{\perp'}
\]

\[
= \frac{1}{\pi L_3} \sum_{j_3=1}^{\infty} \left[ \int_{0}^{\infty} \frac{2 \pi J_0( |\vec{r}_\perp - \vec{r}'_\perp|/p_\perp \hbar) |p_{\perp'}| J_1( |\vec{r}'_\perp - \vec{r}_{\perp'}|/p_{\perp'} \hbar)}{(2\pi \hbar)^2} \right] \quad \text{d}p_\perp \quad \text{d}p_{\perp'}
\]

\[
\rho^1(\vec{r}, \vec{r}'; \beta) = \frac{1}{\pi L_3} \sum_{j_3=1}^{\infty} \left[ \int_{0}^{\infty} \frac{2 \pi J_0( |\vec{r}_\perp - \vec{r}'_\perp|/p_\perp \hbar) |p_{\perp'}| J_1( |\vec{r}'_\perp - \vec{r}_{\perp'}|/p_{\perp'} \hbar)}{(2\pi \hbar)^2} \right] \quad \text{d}p_\perp \quad \text{d}p_{\perp'}
\]

We plot r.h.s. of Eqn.(17) in FIG. 3. The oscillations in the density matrix-element in Eqn.(17) are coming from the alternation of the sign of \( \hat{z}^2 \) in Eqn.(13). Amplitude of the partial oscillations along \( x \) and \( y \) axes, however, is dying out hyperbolically as the system is not bounded along these two axes. The amplitude of the partial oscillations along the \( z \)-axis, however, are oscillating, as expected, as the system is bounded along this axis. The oscillatory amplitude oscillates rapidly except at around \( z = z' \) if the Fermi energy (i.e. \( \mu \) for \( T \to 0 \)) of the system increases; which further causes increase of the principal maximum of the density matrix-element of the system.

Spatial density correlation in the many-body system can be represented in terms of the 1-particle density matrix as \( \nu(\vec{r}, \vec{r}'; \beta) = \pm \frac{\rho^1(\vec{r}, \vec{r}'; \beta)}{\rho^1(\vec{r}, \vec{r}'; \infty)} \) [24]. All the results we have got in this sections are thus useful to get the spatial density correlations in the many-body systems. These results can also be useful to get the quantum cluster expansions for the grand free energies of the many-body systems confined in the box geometries.
IV. QUANTUM CLUSTER EXPANSION FOR AN IDEAL QUANTUM GAS IN 3-D BOX

Quantum cluster expansion of the grand free energy for a 3-D ideal quantum gas is given by [15, 16]

\[ \Omega = -k_B T \sum_{\nu=1}^{\infty} (\pm 1)^{\nu-1} \frac{h_{\nu}}{\nu} \]  

(18)

where

\[ h_{\nu} = \int_{-\infty}^{\infty} \rho(\vec{r}_1, \vec{r}_2; \beta) \rho(\vec{r}_2, \vec{r}_3; \beta) \ldots \rho(\vec{r}_\nu, \vec{r}_1; \beta) d^3\vec{r}_1 \ldots d^3\vec{r}_\nu \]  

(19)

is the cluster integral for \( \nu \) indistinguishable particles in the system and \( \vec{r}_i \) (\( i = 1, 2, 3, \ldots, \nu \)) is the position vector for a particle in the cluster, and \( \rho(\vec{r}_i, \vec{r}_j; \beta) \) is the single-particle density matrix element for the two positions \( \vec{r}_i \) and \( \vec{r}_j \) as defined in Eqn. (9). Eqn. (9) leads to take the simplest form for the cluster integral \( h_1 \) as

\[ h_1 = \int_0^{L_1} \int_0^{L_2} \int_0^{L_3} \frac{1}{2L_i} \left[ \frac{\pi}{2L_i} e^{-\beta \frac{x_i^2 + x_j^2}{2mL_i^2}} \left( \frac{\pi}{2L_i} e^{-\beta \frac{x_i^2 + x_j^2}{2mL_i^2}} \right) \right] dx_i dx_j \]

\[ = \sum_{j_1, j_2, j_3 = 1}^{\infty, \infty, \infty} e^{-\frac{\beta}{2mL_i} \left( \frac{j_1^2}{L_1^2} + \frac{j_2^2}{L_2^2} + \frac{j_3^2}{L_3^2} \right)} \]  

(20)

Fourier series expansion of the Jacobi (elliptic) theta functions, as was as the Fourier series expansion shown in Eqn. (7) for the density matrix-element for a particle in 1-D box, has been used to get the final expression of \( h_1 \) which by definition is the partition function for a single particle in the 3-D box. It can be shown from the orthonormality of the single-particle energy eigenstates that, two indistinguishable particles in the different energy eigenstates do not contribute to the cluster integral. Thus, by the definition, cluster integral for the two or any number of indistinguishable particles would be the partition function for the same number of particles always in the same single-particle energy eigenstate. Thus we get

\[ h_{\nu} = \sum_{j_1, j_2, j_3 = 1}^{\infty, \infty, \infty} (\pm 1)^{\nu-1} e^{-\nu^2 \frac{\beta}{2mL_i} \left( \frac{j_1^2}{L_1^2} + \frac{j_2^2}{L_2^2} + \frac{j_3^2}{L_3^2} \right)} \]  

(21)

for \( \nu = 1, 2, 3, \ldots \). Now we get the quantum cluster expansion of the ideal quantum (Bose or Fas) gas in a 3-D box, by recasting Eqn. (18), as

\[ \Omega = -k_B T \sum_{\nu=1}^{\infty} (\pm 1)^{\nu-1} \frac{\nu^2}{\nu} \sum_{j_1, j_2, j_3 = 1}^{\infty, \infty, \infty} e^{-\nu^2 \frac{\beta}{2mL_i} \left( \frac{j_1^2}{L_1^2} + \frac{j_2^2}{L_2^2} + \frac{j_3^2}{L_3^2} \right)} \]  

(22)

Average number of particles \( \bar{N} = -\frac{\partial \Omega}{\partial T} \) for \( T, L_1, L_2, L_3 \), on the other hand can be calculated from Eqn. (22) as

\[ \bar{N} = \sum_{\nu=1}^{\infty} (\pm 1)^{\nu-1} \frac{\nu^2}{\nu} \sum_{j_1, j_2, j_3 = 1}^{\infty, \infty, \infty} e^{-\nu^2 \frac{\beta}{2mL_i} \left( \frac{j_1^2}{L_1^2} + \frac{j_2^2}{L_2^2} + \frac{j_3^2}{L_3^2} \right)} \]  

(23)

Let us now define the generalized pressure given by the quantum gas on a wall of the system as \( p = \frac{-\beta}{L_1L_2L_3} \) which would be the true pressure in the thermodynamic limit. Thermodynamic behaviour of the ideal quantum gas can now be extracted from Eqns. (22) and (23).

Let us now remove the boundaries along the \( x \) and \( y \) axes so that \( L_1 \to \infty, L_2 \to \infty \), and the quantum gas remains bounded only along the \( z \) axis. In this situation the summations in Eqns. (22) and (23) over \( j_1 \) and \( j_2 \) can be replaced by integrations from 0 to \( \infty \) without any error by virtue of Poisson summation formula. Thus we get the equation of state of the system, i.e. the pressure given by the quantum gas to either of the walls situated at \( z = 0 \) and \( z = L_3 \), as

\[ p = \frac{k_B T}{L_3^3} \sum_{\nu=1}^{\infty} (\pm 1)^{\nu-1} \frac{\nu^2}{\nu} \sum_{j_1 = 1}^{\infty} e^{-\nu^2 \frac{\beta}{2mL_3} \left( \frac{j_1^2}{L_3^2} \right)} - \frac{1}{2} \]  

(24)

This is quantum cluster expansion of the equation of state for ideal Bose and Fermi gases in the box geometry. As we mentioned before, the upper sign corresponds to the ideal Bose gas and the lower sign corresponds to the ideal Fermi gas. We plot the equation of state in Eqn. (24) for ideal Bose and Fermi gases for fixed fugacity, and compare with the the case of the free Bose gas in FIG. 4.

The solid line approaches the result \( \lambda_1^2 p/k_B T = g_{3/2}(z) \), where \( g_{3/2} \) is the Bose integral [16], for the 3-D free Bose gas as \( L_3/\lambda_T \) tends to \( \infty \). The dashed line approaches the result \( \lambda_1^2 p = f_{3/2}(z) \), where \( f_{3/2} \) is the Fermi integral [16], for the 3-D free Fermi gas as \( L_3/\lambda_T \) tends to \( \infty \). It is clear from the FIG. 4 that, finiteness of system causes less pressure given to the wall with respect to that given by a free gas though finiteness causes more energy.
to the system which is not probabilistic favoured in thermal equilibrium. This pressure is exponentially small for \( \lambda_T \gtrsim L_3 \) as clear from the FIG. 4 too. The finite system effectively behaves like a 2-D system in such a low temperature regime. This pressure, however, is further reduced in Fermi gas for odd permutation effect in clusters of even sizes. Casimir-like effect can also be studied from Eqn. (24) for the finiteness of the system only along the \( z \) axis [25] apart from studying typical finite-size effect on the many-body system.

V. QUANTUM CLUSTER EXPANSION FOR A NON-IDEAL QUANTUM GAS IN A CLOSED RECTANGULAR CYLINDER

Let the Bose gas spin 0 particles be interacting with short-ranged pair-potential energy \( V(|\vec{r}_2 - \vec{r}_1|) \) in a 3-D closed rectangular cylindrical box, so that the many-body Hamiltonian of the system can be written, in usual notation, as [17]

\[
\hat{H} = \int d^3 \vec{r} \hat{\psi}^\dagger(\vec{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \hat{\psi}(\vec{r}) + \frac{1}{2} \int d^3 \vec{r} d^3 \vec{r}' \hat{\psi}^\dagger(\vec{r}) \hat{\psi}^\dagger(\vec{r}') V(|\vec{r} - \vec{r}'|) \hat{\psi}(\vec{r}') \hat{\psi}(\vec{r}) \tag{25}
\]

where \( V(|\vec{r} - \vec{r}'|) = g_3 \delta^3(|\vec{r} - \vec{r}'|) \) is considered to be a short-ranged pair-potential energy, \( g_3 = \frac{4 \pi \hbar^2 a_s}{m} \) is the coupling constant, and \( a_s \) is the s-wave scattering length which is positive for repulsive interactions. The system would not be stable beyond a critical number of particles for \( g_3 < 0 \) which we are not considering in our analysis [27]. Let us further consider that, \( L_1 \ll L_3 \) and \( L_2 \ll L_3 \) so that low-lying excitations only along \( z \)-direction are probabilistically favoured for low temperatures (for which \( \lambda_T \gg L_1 \) and \( \lambda_T \gg L_2 \)). The system behaves like a quasi 1-D system (0 \( \leq z \leq L_3 \)) in this situation. If the average number of identical bosons in the grandcanonical ensemble (for temperature \( T \) and chemical potential \( \mu \)) be \( \bar{N} \), then the 1-particle (low-lying) excitations \( \psi_j(z); \ j = 1, 2, 3, ... \) follow from the time-independent non-linear Schrodinger equation [28]

\[
\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + g_1 \bar{N} |\psi_j(z)|^2 \right] \psi_j(z) = \bar{E}_j \psi_j(z) \tag{26}
\]

with the 1-particle mean field energy eigenvalue [28]

\[
\bar{E}_j = \frac{\hbar^2 q_j^2}{m L_3^2} (1 + q_j) K^2(q_j), \tag{27}
\]

where \( K(q_j) = \frac{\pi}{2} \left[ 1 + q_j / 4 + 9 q_j^2 / 64 + ... \right] \) is complete elliptic integral of the first kind of the argument \( q_j = 2 \bar{N} q_j^2 / (L_3/2)^2 \) [29], \( g_1 = \frac{2 \pi \hbar^2}{m a_s} \) is the coupling constant for elastic scattering in 1-D, and [28]

\[
\psi_j(z) = \sqrt{\frac{\hbar^2 q_j}{m L_3^2 g_1 N}} \left[ 2 j K(q_j) \right] \sn \left( \frac{2 j K(q_j)}{L_3}, q_j \right) \tag{28}
\]

is the solution (Jacobi elliptic function) to Eqn. (26) for the Dirichlet boundary conditions. One-particle density matrix, for the interacting Bose system, thus takes the form, from the definition, as

\[
\rho^j(z, z'; \beta) = \sum_{j=1}^{\infty} \left[ \frac{\hbar^2 q_j^2 j K^2(q_j)}{m L_3^2 g_1 N} \frac{1}{e^{\beta E_j} - 1} \right] \sn \left( \frac{2 j K(q_j)}{L_3}, q_j \right) \sn \left( \frac{2 j K(q_j)}{L_3}, q_j' \right) \tag{29}
\]

Cluster integral of size \( \nu = 1, 2, 3, ... \) can now be easily written, for the interacting Bose system, by looking at the Eqn. (21), as

\[
h_{\nu} = \sum_{j=1}^{\infty} e^{-\nu E_j}. \tag{30}
\]

It is easy to check, that, all these results are matching with the cases of ideal Bose gas in the 1-D box for \( g_1 \rightarrow 0 \).

Let us now consider the case of interacting Fermi gas of spin 1/2 particles (of 1:1 components of \( s_z = 1/2 \) and \(-1/2\)) in the same situation as above. Pair interactions are now possible between the particles of \( s_z = 1/2 \) and \( s_z = -1/2 \) as effect of other direct pair interactions are cancelled due to that of exchange pair interactions [30]. One-particle density matrix and the cluster integral can now be defined only for one species of the spin component. Thus \( \bar{N} \) in Eqns. (26) - (30) would be replaced by \( \bar{N}/2 \) for the interacting Fermi system. In addition the Bose-Einstein statistics \( (\bar{n}_j = e^{\beta E_j} - 1) \) in Eqn. (29) is to be replaced by the Fermi-Dirac statistics \( (\bar{n}_j = \frac{1}{e^{\beta E_j} + 1}) \) and a phase factor \((-1)^{\nu - 1}\) would be multiplied in the r.h.s. of Eqn. (30).

VI. DISCUSSION AND CONCLUSION

We have analytically obtained statistical mechanics density matrices for a single particle in 1-D and 3-D box. Therefrom we have calculated 1-particle density matrices for 3-D ideal Bose and Fermi gases in the box geometries some times by removing the boundaries along two \( (x - y) \) axes. We also have obtained quantum cluster expansions of the grand free energies in closed forms for the same systems in the restricted geometries. Therefrom we have obtained equations of states for 3-D ideal Bose and Fermi gases in the box geometries. We also have obtained analytic expressions for the 1-particle density matrices for interacting Bose and Fermi gas confined in
quasi 1-D boxes. Thermodynamics of the Bose or Fermi gas in the box geometry can be studied from the cluster expansion obtained by us.

Our results are novel, exact, and are directly useful for a postgraduate course on statistical mechanics or that on many-body physics. All the calculations are done within the scope of undergraduate and postgraduate students. Our result would be relevant in the context of study spatial correlations in ultra-cold systems of dilute Bose and Fermi gases of alkali atoms in 3-D magneto-optical box trap with quasi-uniform potential in it [23].

By density matrix, we mean: statistical mechanical unnormalized density matrix for systems in thermodynamic equilibrium. Replacing $\beta$ by $it/\hbar$, where $t$ is the time taken by a particle in the system to reach $r'$ starting from the position $r$ at $t = 0$, we get the quantum mechanical density matrix-elements for all the cases.

All our results can be generalized for non-ideal cases of 3-D Bose and Fermi systems in box geometries at least within the perturbative formalisms. Our results can also be generalized for $d$-dimensional box geometries. We are keeping these tasks as open problems to the postgraduate students.

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[1] J. von Neumann, Göttinger Nachrichten 1927, 245 (1927)
[2] P.A. M. Dirac, Proc. Cambridge Phil. Soc. 25, 62 (1929); 27, 240 (1931)
[3] R. C. Tolman, The Principles of Statistical Mechanics, p. 327-361 (ch. 9), Clarendon Press, Oxford, Great Britain (1938)
[4] R. P. Feynman, Statistical Mechanics: A Set of Lectures, p. 39-96 (ch. 2-3), Westview Press, Boulder, USA (1972)
[5] G. C. Wick, Phys. Rev. 96, 1124 (1954)
[6] M. Fox, Quantum Optics: An Introduction, p. 171 (ch. 9), Oxford Univ. Press, Oxford, New York, USA (2006)
[7] O. Penrose and L. Onsager, Phys. Rev. 104, 576 (1956)
[8] E. Onofri, Am. J. Phys. 46, 379 (1978)
[9] L. P. Onofri, Am. J. Phys. 46, 379 (1978)
[10] E. Onofri, Am. J. Phys. 46, 379 (1978)
[11] M. T. Batchelor, X. W. Guan, N. Oelkers, and C. Lee, J. Phys. A: Math. Gen. 38, 7787 (2005)
[12] D. M. Gangardt and G. V. Shlyapnikov, New J. Phys. 8, 167 (2006)
[13] J.-S. Caux, P. Calabrese, and N. A. Slavnov, J. Stat. Mech. 2007, P01008 (2007)
[14] M. Kira and S. W. Koch, Phys. Rev. A 78, 022102 (2008)
[15] B. Kahn and G. E. Uhlenbeck, Physica 5, 399 (1938); T. D. Lee and C. N. Yang, Phys. Rev. 117, 22 (1960)
[16] R. K. Pathria, Statistical Mechanics, 2nd edn., p. 254, ch. 9, Butterworth-Heinemann, Oxford, New York, USA
[17] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 71, 463 (1999)
[18] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008)
[19] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. 80, 1215 (2008)
[20] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, E. A. Cornell, Science 269, 198 (1995)
[21] C. C. Bradley, C. A. Sackett, J. J. Tollett, and R. G. Hulet, Phys. Rev. Lett. 75, 1687 (1995)
[22] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. 75, 3969 (1995)
[23] A. L. Gaunt, T. F. Schmidutz, I. Gotlibovsky, R. P. Smith, and Z. Hadzibabic, Phys. Rev. Lett. 110, 200406 (2013); Also see - T. F. Meyrath, F. Schreck, J. L. Hanssen, C.-S. Chuu, and M. G. Raizen, Phys. Rev. A 71, 041604(R) (2005)
[24] L. D. Landau and E. M. Lifshitz, Statistical Physics: part-1, 3rd edn., p. 356 (sec. 117), Butterworth-Heinemann, Oxford, New York, USA (2003)
[25] S. Biswas, J. Phys. A: Math. Theor. 40, 9969 (2007); Eur. Phys. J. D 42, 109 (2007)
[26] A. Bhattacharya, S. Das, and S. Biswas, J. Phys. B: At. Mol. Opt. Phys. 51, 075301 (2018)
[27] S. Biswas, Eur. Phys. J. D 55, 653 (2009)
[28] L. D. Carr, C. W. Clark, and W. P. Reinhardt, Phys. Rev. A 62, 063610 (2000)
[29] S. Biswas, J. K. Bhattacharjee, D. Majumder, K. Saha, and N. Chakravarty, J. Phys. B: At. Mol. Opt. Phys. 43, 085305 (2010)
[30] S. Biswas, D. Jana, and R. K. Manna, Eur. Phys. J. D 66, 217 (2012)
[31] The Jacobi (elliptic) theta function, $\theta_3(u, q)$, is defined as $\theta_3(u, q) = 1 + 2\sum_{j=1}^{\infty} q^{2j} \cos(2ju)$ for $u \in \mathbb{C}$ and $|q| < 1$.
[32] Maximization of the density matrix-element is possible at $x' = x = L/2$ as there is a reflection symmetry about this point.
[33] This is the limiting case of Fermi-Huang potential under Born approximation for low energy scattering [26].