Temperature dependence of density profiles for a cloud of non-interacting fermions moving inside a harmonic trap in one dimension

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We extend to finite temperature a Green’s function method that was previously proposed to evaluate ground-state properties of mesoscopic clouds of non-interacting fermions moving under harmonic confinement in one dimension. By calculations of the particle and kinetic energy density profiles we illustrate the role of thermal excitations in smoothing out the quantum shell structure of the cloud and in spreading the particle spill-out from quantum tunnel at the edges. We also discuss the approach of the exact density profiles to the predictions of a semiclassical model often used in the theory of confined atomic gases at finite temperature.

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I. INTRODUCTION

The achievement of Bose-Einstein condensation in ultracold gases of bosonic atoms has given great impulse to the study of dilute quantum gases inside magnetic or optical traps \footnote{1}. Similar cooling and trapping techniques are being used to drive gases of fermionic alkali atoms into the quantum degeneracy regime \footnote{2}. It is also possible to experimentally generate and study strongly anisotropic atomic fluids effectively approaching dimensionality \(D = 2\) or \(D = 1\), at very low temperature and with very high purity, inside magnetic traps where the transverse and the longitudinal confinement are vastly different \footnote{3}.

In the relevant conditions of temperature and dilution the atomic interactions become negligible in a gas of fermions placed in a single Zeeman sublevel inside a magnetic trap \footnote{4}. One can obtain in this way a close laboratory realization of an inhomogeneous, non-interacting Fermi gas, which has special significance in regard to the foundations of density functional theory and to tests of the Thomas-Fermi approximation \footnote{5}. In the quasi-one-dimensional (1D) case the ground state and the excitation spectrum of such an ideal gas of spin-polarized (or ”spinless”) fermions can be mapped into those of a gas of hard-core impenetrable bosons \footnote{6}. The latter is known as the Tonks gas, from the early work of Tonks \footnote{7} on the equation of state of hard-object adsorbates. Advances in atom waveguide technology, with potential applications to atom interferometry and integrated atom optics, especially motivate theoretical studies of dilute gases in a regime where the dynamics becomes essentially 1D \footnote{8}.

The wave functions of a cloud of spinless fermions under harmonic confinement are, of course, Slater determinants of harmonic-oscillator single-particle orbitals. Their representation in terms of Hermite polynomials has, however, limited usefulness for numerical calculations on mesoscopic clouds \footnote{9}. Brack and van Zyl \footnote{10} have developed a more powerful method for non-interacting fermions occupying a set of closed shells under isotropic harmonic confinement in \(D\) dimensions, leading to analytical expressions for the particle and kinetic energy densities at temperature \(T = 0\) in terms of Laguerre polynomials. These expressions are especially useful for numerical calculations on isotropic systems in \(D = 2\) and \(D = 3\). A Green’s function method, which altogether avoids the use of wave functions in favor of the matrix elements of the position and momentum operators, has been developed for similar purposes \footnote{11} and extended to calculations of the pair distribution function in the ground state for the 1D ideal Fermi gas \footnote{12}. This method has also been extended to the ground state of ideal Fermi gases under harmonic confinement of arbitrary anisotropy in higher dimensionalities \footnote{13}.

The purpose of the present paper is to extend the Green’s function method to an inhomogeneous 1D cloud of non-interacting fermions at finite temperature and to illustrate its usefulness by numerical calculations of the particle and kinetic energy density profiles as functions of temperature in the case of harmonic confinement. Analytical expressions have been derived by Wang \footnote{14} for the same system at high temperature, where the chemical potential is lower than the single-particle ground-state energy. The case of non-interacting fermions under 3D harmonic confinement has been treated by Schneider and Wallis \footnote{15} through the use of Laguerre polynomials. The emphasis of our numerical calculations will be to illustrate how the characteristic quantum features of the fermion cloud, i.e. its shell structure and the spill-out of particles at the boundaries beyond the Thomas-Fermi radius, evolve with increasing temperature as a semiclassical regime is being approached.
The chemical potential is again determined by normalization to the average number of fermions.

and

The zero temperature limit of Eq. (1) leads to the Dirac density matrix for fermions, momentum and position operators, and the chemical potential

Here \( \beta = 1/k_B T \) and \( \mu \) is the chemical potential, while \( \psi_i \) and \( E_i \) are the single-particle orbitals and the corresponding energy eigenvalues. The zero temperature limit of Eq. (1) leads to the Dirac density matrix for \( N \) ideal spinless fermions,

\[
\rho(x_1, x) = \sum_{i=1}^{N} \psi_i^*(x_1) e^{i \hat{p}(x-x_1)} \psi_i(x_1). \tag{2}
\]

The particle density profile \( n(x) \) of the gas at temperature \( T \) and chemical potential \( \mu \) is the zero-order moment of the matrix \( D(x, x_1) \),

\[
n(x) = D(x_1, x; \beta, \mu)|_{x_1=x} = \sum_{i=1}^{\infty} \frac{1}{1 + \exp \left[ \beta (E_i - \mu) \right]} \langle \psi_i | \delta(x - \hat{x}) | \psi_i \rangle. \tag{3}
\]

The kinetic pressure \( P(x) \) is given by a specific second-order moment of \( D(x, x_1) \),

\[
P(x) = \frac{\hbar^2}{m} \frac{\partial^2}{\partial x_1^2} D(x_1, x; \beta, \mu)|_{x_1=x} = \frac{1}{2m} \sum_{i=1}^{\infty} \frac{1}{1 + \exp \left[ \beta (E_i - \mu) \right]} \langle \psi_i | \hat{p}^2 \delta(x - \hat{x}) + \delta(x - \hat{x}) \hat{p}^2 | \psi_i \rangle. \tag{4}
\]

The kinetic pressure \( P(x) \) is twice the kinetic energy density of the fermion cloud. In these equations \( \hat{p} \) and \( \hat{x} \) are the momentum and position operators, and the chemical potential \( \mu \) is determined from the condition

\[
\int n(x; \beta, \mu) dx = N \tag{5}
\]

where \( N \) is the average number of particles.

In the semiclassical regime the particle density and the kinetic pressure of an ideal Fermi gas confined by a 1D potential \( V(x) \) can be calculated by treating the energy levels as a continuum. The appropriate condition of validity is that the level spacing \( \Delta E \) is sufficiently smaller than the thermal energy \( k_B T \). The appropriate expressions in the grand-canonical ensemble are

\[
n_{sc}(x) = \int dE \int \frac{dp}{2\pi \hbar} \delta \left( E - \frac{p^2}{2m} - V(x) \right) \frac{1}{1 + \exp \left[ \beta (E - \mu) \right]} \tag{6}
\]

and

\[
P_{sc}(x) = \int \frac{dp}{2\pi \hbar} \frac{p^2}{m} \left\{ \exp \left[ \beta \left( \frac{p^2}{2m} + V(x) - \mu \right) \right] + 1 \right\}^{-1}. \tag{7}
\]

The chemical potential is again determined by normalization to the average number of fermions.

II. ESSENTIAL DEFINITIONS AND THE SEMICLASSICAL LIMIT

The generalized grand-canonical density matrix for fermions \([16]\) can be written as

\[
D(x_1, x; \beta, \mu) = \sum_{i=1}^{N} \frac{1}{1 + \exp \left[ \beta (E_i - \mu) \right]} \psi_i^*(x_1) e^{i \hat{p}(x-x_1)} \psi_i(x_1). \tag{1}
\]
III. THE GREEN’S FUNCTION METHOD

Equations (3) and (4) can be rewritten in terms of the Green’s function \( \hat{G}(x) = \lim_{\varepsilon \to 0^+} (x - \hat{x} + i\varepsilon)^{-1} \) in coordinate space,

\[
n(x) = -\frac{1}{\pi} \lim_{\varepsilon \to 0^+} \text{Im} \sum_{i=1}^{\infty} \frac{1}{1 + \exp \left[ \beta(E_i - \mu) \right]} \langle \psi_i | \hat{G}(x) | \psi_i \rangle
\]

\[
= -\frac{1}{\pi} \lim_{\varepsilon \to 0^+} \text{Im} \text{Tr} \left( \hat{T} \cdot \hat{G}(x) \right)
\]

and

\[
P(x) = -\frac{1}{\pi m} \lim_{\varepsilon \to 0^+} \text{Im} \sum_{i=1}^{\infty} \frac{1}{1 + \exp \left[ \beta(E_i - \mu) \right]} \langle \psi_i | \hat{p}^2 G(x) | \psi_i \rangle
\]

\[
= -\frac{1}{\pi m} \lim_{\varepsilon \to 0^+} \text{Im} \text{Tr} \left( \hat{T} \cdot \hat{p}^2 \cdot \hat{G}(x) \right).
\]

Here we have used a matrix formalism, by introducing the temperature matrix \( \hat{T} \) whose diagonal elements \( [\hat{T}]_{j,j} = 1/(1 + \exp[\beta(E_j - \mu)])^{-1} \) contain the statistical Fermi factors, while the off-diagonal elements \( [\hat{T}]_{i,j} \) with \( i \neq j \) are null.

The evaluation of the expressions in Eqs. (3) and (4) is carried out by an immediate extension of the procedure developed in [11] for the case of zero temperature. The trace of a generic matrix \( A \) is connected to the elements of the inverse matrix \( A^{-1} \) by the relation

\[
\text{Tr} A = \frac{\partial}{\partial \lambda} \left[ \ln \det(A^{-1} + \lambda I) \right]_{\lambda=0}.
\]

We get from Eqs. (3) and (4)

\[
n(x) = -\frac{1}{\pi} \lim_{\varepsilon \to 0^+} \text{Im} \frac{\partial}{\partial \lambda} \left[ \ln \det(x - \hat{x} + \lambda \hat{T} + i\varepsilon) \right]_{\lambda=0}
\]

and

\[
P(x) = -\frac{1}{\pi m} \lim_{\varepsilon \to 0^+} \text{Im} \frac{\partial}{\partial \lambda} \left[ \ln \det(x - \hat{x} + i\varepsilon + \lambda \hat{T} \cdot \hat{p}^2) \right]_{\lambda=0}.
\]

In the specific case of harmonic confinement we make use of the representation of the position and the momentum operators in the basis of the eigenstates of the harmonic oscillator with energy \( E_n = (n - 1/2)\hbar \omega \) : that is, \( \hat{x} = (a + a^\dagger)/\sqrt{2} \) and \( \hat{p} = i(a^\dagger - a)/\sqrt{2} \) with \( a | \psi_n \rangle = \sqrt{n - 1/2} | \psi_{n-1} \rangle \) and \( a^\dagger | \psi_n \rangle = \sqrt{n} | \psi_{n+1} \rangle \). The tridiagonal form of the matrices representing \( \hat{x} \) and \( \hat{p} \) allows us to express the determinants in Eqs. (11) and (12) by a recursive algorithm [11, 15] as products of an infinite number of matrices having dimension \( 1 \times 1 \) for the particle density and \( 2 \times 2 \) for the kinetic pressure. If we write the matrix \( \mathcal{K}^\nu = \hat{x} - \lambda \hat{T} \cdot \hat{p}^2 \) in the tridiagonal form

\[
\mathcal{K}^\nu = \begin{pmatrix}
A_1 & B_{1,2} & \cdots & B_{1,\nu} \\
B_{2,1} & A_2 & \cdots & B_{2,\nu} \\
\vdots & \vdots & \ddots & \vdots \\
B_{\nu,1} & B_{\nu,2} & \cdots & A_\nu
\end{pmatrix}
\]

where the indices refer to blocs of dimension \( 1 \times 1 \) if \( \nu = 0 \) and \( 2 \times 2 \) if \( \nu = 2 \), we obtain

\[
\det(x - \mathcal{K}^\nu + i\varepsilon) = \prod_{j=1}^{\nu} \det(x - \tilde{\mathbf{A}}_j + i\varepsilon).
\]

Here \( \tilde{\mathbf{A}}_1 = \mathbf{A}_1 \) while the renormalized blocs \( \tilde{\mathbf{A}}_j \) for \( j > 1 \) are given by the recursive formula

\[
\tilde{\mathbf{A}}_j = \mathbf{A}_j + \mathbf{B}_{j,j-1}(x - \tilde{\mathbf{A}}_{j-1} + i\varepsilon)^{-1}\mathbf{B}_{j-1,j}.
\]

As in the calculation of density profiles at \( T = 0 \) [11], the evaluation of the determinant in Eq. (14) converges quite rapidly, yielding accurate results for mesoscopic fermion clouds with a moderate amount of numerical effort.
IV. NUMERICAL RESULTS

We report in this section some numerical results for the particle density and the kinetic pressure that we have obtained by the Green’s function method. Our main purpose is to illustrate the approach of the profiles to their semiclassical expressions and we consider for clarity clouds containing rather small average numbers of particles, i.e. $N = 4$ and $N = 20$. Some sharpening of the structures in the profiles should be expected in a canonical ensemble viewpoint, where fluctuations in the particle number are suppressed.

In the calculations reported below we have approximated the determinant in Eq. (14) by the product of its first $M$ terms with $M = 10^7$ as an upper bound. This choice allows for up to $10^7$ thermally excited states and the corresponding value of the spectral resolution parameter is chosen as $\varepsilon = 10^{-3}$. These two choices evidently limit to some minor extent the accuracy of our numerical results relatively to the formally exact theory given in Sect. III. Of course, for such small numbers of particles one may also approach the same calculations by using directly the expression of the harmonic-oscillator orbitals in Eq. (1). However, the routines that are available to evaluate Hermite polynomials also involve numerical approximations which are increasingly severe for polynomials of high degree, as needed to describe the gas at finite temperature.

The first step in our calculations is to evaluate the chemical potential at fixed $N$ by means of a self-consistent solution of Eqs. (5) and (6) \cite{18}. The resulting semiclassical value of $\mu$ is used in Eqs. (11) and (12) for the evaluation of the particle density and kinetic pressure profiles. The procedure is justified \textit{a posteriori} by the fact that integration of the spatial density $n(x)$ obtained at this stage reproduces the correct average number $N$ of fermions.

In Figures 1 and 2 we report the particle density profiles at various temperatures for $N = 4$ and $N = 20$, respectively. The corresponding profiles of kinetic pressure are given in Figures 3 and 4. In each Figure the left-hand panel shows how the quantum effects, which consist of oscillations from shell structure in the profiles and in particle spill-out and negative kinetic pressure at the edges, are washed away by thermal excitations. The right-hand panels show instead how the profiles approach the semiclassical regime: the latter already holds to a good approximation when $k_B T \simeq \hbar \omega$, although some trace of a negative kinetic pressure in the spill-out region remains in the “exact” profile at this temperature.

V. CONCLUSIONS

In conclusion, in this paper we have extended to finite temperature the Green’s function method that was previously developed for the formally exact evaluation of ground-state properties of an inhomogeneous ideal Fermi gas in 1D. The method dispenses with knowledge of the single-particle orbitals in favour of the single-particle energy levels and of the matrix elements of the position and momentum operators. Our numerical applications to clouds containing small numbers of particles under harmonic confinement have shown that the commonly used semiclassical approach to a thermally excited fermion cloud yields (i) accurate values of the chemical potential except at the lowest temperatures, and (ii) a reliable account of particle and kinetic energy density profiles once their main quantum features become essentially washed out at $k_B T \simeq \hbar \omega$.

Two further comments are in order. Firstly, the profiles shown in Figures 1 and 2 also describe (aside from an immediate rescaling of the units used on the axes) the momentum distribution of the fermion cloud under harmonic confinement. Secondly, the same profiles also refer to the Tonks gas of impenetrable bosons in 1D, as was explicitly shown by Yang and Yang \cite{19}.

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FIG. 1. Particle density profile for $N = 4$ harmonically confined fermions at various values of the temperature. Left panel: “exact” profiles at $T = 0$ (solid curve, calculated by the method of Ref. [1]) and at $T = 0.2k_B/\hbar\omega$ (dashed curve); the other curves refer to $k_BT/\hbar\omega = 0.5, 1.0, 2.0$ and $3.0$, in order of decreasing peak height. Positions are in units of the harmonic oscillator length $a_{ho} = \sqrt{\hbar/(m\omega)}$ and the particle density is in units of $a_{ho}^{-1}$. The right-hand panel reports again the profiles at $k_BT/\hbar\omega = 0.2, 1.0$ and $3.0$, together with those calculated in the semiclassical approximation (light lines); for the latter two values of $k_BT/\hbar\omega$ the “exact” profiles are hardly distinguishable from the semiclassical ones.
FIG. 2. The same as in Figure 1, for $N = 20$ harmonically confined fermions.

FIG. 3. Kinetic pressure profile for $N = 4$ harmonically confined fermions at the same values of the temperature as in Figure 1. Left panel: “exact” profiles; right panel: comparison with the semiclassical profiles for $k_B T/\hbar \omega = 0.2$, 1.0 and 3.0 (light lines). Positions are in units of $a_{ho}$ and the kinetic pressure is in units of $\hbar \omega a_{ho}^{-1}$. 
FIG. 4. The same as in Figure 3, for $N = 20$ harmonically confined fermions.