Exact Particle and Kinetic-Energy Densities for One-Dimensional Confined Gases of Noninteracting Fermions

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We propose a new method for the evaluation of the particle density and kinetic pressure profiles in inhomogeneous one-dimensional systems of noninteracting fermions, and apply it to harmonically confined systems of up to $N = 1000$ fermions. The method invokes a Green's function operator in coordinate space, which is handled by techniques originally developed for the calculation of the density of single-particle states from Green's functions in the energy domain. In contrast to the Thomas-Fermi approximation, the exact profiles show negative local pressure in the tails and a prominent shell structure which may become accessible to observation in magnetically trapped gases of fermionic alkali atoms.

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The techniques which have led to the achievement of Bose-Einstein condensation in vapors of bosonic atoms [1–4] are currently being used to trap and cool dilute gases of fermionic alkali atoms [5]. Under magnetic confinement the s-wave collisions between pairs of fermions in a single hyperfine level are suppressed by the Pauli principle, and the geometry of the trap can be adapted to have cylindrical symmetry with a transverse confinement which may be hundreds of times stronger than the longitudinal one. It is thus possible to experimentally realize quasi-one-dimensional (quasi-1D) inhomogeneous systems of almost noninteracting fermions at very low temperature and high purity.

A number of one-dimensional (1D) physical models can be solved exactly [6] and their solution serves as a test of approximate theories and contributes to the understanding of real systems. Some important examples are the determination of the ground state and excitation spectrum of a hard-core Bose gas in 1D [7] and the solution of the Kronig-Penney model for the electron energy bands in a 1D crystal lattice [8]. The spectral and transport properties of other 1D systems of noninteracting electrons have been studied as models for polymers and quantum wires, using Green's function methods [9–12] for which ingenuous techniques such as a decimation/renormalization procedure [13,14] have been developed.

In this paper we present a new method for the exact evaluation of the ground-state particle density profile in a spin-polarized 1D system of up to large numbers of noninteracting fermions in arbitrary spatial confinement. In essence we show that, just as the single-particle density of states in the energy domain can be obtained by powerful Green's function methods, similar techniques yield the particle density in the 1D space domain. In fact, our method also allows the evaluation of higher moments of the one-body density matrix: we focus here on its second moment, which is simply proportional to the kinetic-energy density and to the kinetic pressure.

As an application of the general method we give results for the particle density and kinetic pressure profiles of a degenerate Fermi gas in harmonic confinement. This model is directly relevant to the current experiments on atomic Fermi gases and we show that the shell structure noticed for the particle density in earlier theoretical studies in 3D [15,16] is greatly enhanced in 1D. We also use our exact results to test the Thomas-Fermi (local density) approximation in dependence of the number of fermions in the confined gas.

General formulation.—The one-body Dirac density matrix for a system of N noninteracting fermions at zero temperature can be expanded on the single-particle wave functions $\psi_i(x) = \langle x \,|\, \psi_i \rangle$ as $\rho(x_1, x_2) = \sum_{i=1}^{N} \psi_i^*(x_1) \times \psi_i(x_2)$. By using the representation of the translation operator, this becomes

$$\rho(x_1, x_2) = \sum_{i=1}^{N} \psi_i^*(x_1) e^{-i\hat{p}(x_1 - x_2)} \psi_i(x_1)\,, \qquad (1)$$

showing how distant points are correlated through the momentum operator $\hat{p}$. Expansion in powers of the relative coordinate $r = x_1 - x_2$ yields physical observables such as the particle density profile $n(x)$,

$$n(x) = \rho(x + r/2, x - r/2)|_{r=0} = \sum_{i=1}^{N} \langle \psi_i | \delta(x - x_i) \, | \psi_i \rangle \qquad (2)$$

and the kinetic pressure $P(x)$,

$$P(x) = -\frac{\hbar^2}{m} \frac{\partial^2}{\partial r^2} \rho(x + r/2, x - r/2)|_{r=0}$$

$$= \frac{1}{2m} \sum_{i=1}^{N} \langle \psi_i | p_i^2 \delta(x - x_i) + \delta(x - x_i) p_i^2 | \psi_i \rangle\,. \qquad (3)$$

This is twice the kinetic-energy density.

The main idea of this Letter is to rewrite Eqs. (2) and (3) as the imaginary part of the ground-state average of suitable operators related to the Green's function in coordinate space $G(x) = (x - \hat{x} + i\varepsilon)^{-1}$. We have

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$$n(x) = -\frac{1}{\pi} \lim_{\varepsilon \to 0^+} \mathrm{Im} \sum_{i=1}^{N} \langle \psi_i | G(x) | \psi_i \rangle \qquad (4)$$

and

$$P(x) = -\frac{1}{\pi} \lim_{\varepsilon \to 0^+} \mathrm{Im} \sum_{i=1}^{N} \langle \psi_i | \frac{\hat{p}^2}{m} G(x) | \psi_i \rangle . \qquad (5)$$

$G(x)$ can then be treated by methods analogous to those used for treating Green's functions in the energy domain.

The equivalence between expressions (2) and (4) is easily proved in the coordinate representation, where the density profile in Eq. (4) reads

$$n(x) = -\frac{1}{\pi} \lim_{\varepsilon \to 0^+} \mathrm{Im} \sum_{i=1}^{N} \int dx_i \, |\psi_i(x_i)|^2 \, \frac{1}{x - x_i + i\varepsilon} , \qquad (6)$$

yielding Eq. (2) when one takes the limit $\varepsilon \to 0^+$. The equivalence between expressions (3) and (5) for $P(x)$ is similarly proved.

Evidently, this method can be applied to all 1D systems which may be described by single-particle orbitals: one only needs to know the representation of the position and momentum operators on such a basis. Hence, interactions could also be included in evaluating the particle density through the use of Kohn-Sham single-particle orbitals. Models of displacement fields (such as those induced by impurities) may also be studied directly without previous evaluation of orbitals.

Noninteracting fermi gas in harmonic trap.—As already noted, a 1D Fermi model is relevant to the spin-polarized fermionic vapors in magnetic confinement [5], where it is possible to realize experimentally a 1D configuration by making use of very anisotropic axially symmetric traps. At low temperature, only the transverse ground state of the trap is populated and the vapor can be described by an effective 1D harmonic Hamiltonian.

An analytic expression for the particle density of this system has been given by Husimi [17,18] in terms of the wave function of the Nth fermion in the trap. However, a calculation of the density profile and the kinetic pressure by his approach is limited to small values of N and has been reported only for $N = 1$ and 2 [18]. Our method allows us to efficiently evaluate these ground-state properties even for quite large numbers of particles. Of course, the simplicity of the representation of the position and momentum operators in this system makes it a favorable example.

A. Particle density profile: We start with the calculation of the particle density. For a linear harmonic oscillator the position operator is represented as $\hat{x} = (a + a^\dagger)/\sqrt{2}$ on the basis $\{|\psi_i\rangle\}$ of the eigenvectors of the Hamiltonian. As usual, the creation and destruction operators satisfy the relations $a|\psi_i\rangle = \sqrt{i-1}\,|\psi_{i-1}\rangle$ and $a^\dagger|\psi_i\rangle = \sqrt{i}\,|\psi_{i+1}\rangle$. A straightforward procedure for evaluating the profile (4) is to invert the matrix $(x - \hat{x} + i\varepsilon)$ and to calculate its trace on the submatrix of its first $N \times N$ block (Tr_N). We employ the relation $\mathrm{Tr}_N Q = \partial[\ln \det(Q^{-1} + \lambda \mathbb{I}_N)]/\partial\lambda|_{\lambda=0}$, where $\mathbb{I}_N$ is a diagonal semi-infinite matrix with its first N eigenvalues equal to 1 and null elsewhere [19], to obtain

$$n(x) = -\frac{1}{\pi} \lim_{\varepsilon \to 0^+} \mathrm{Im} \frac{\partial}{\partial \lambda} \left[\ln \det(x - \hat{x} + i\varepsilon + \lambda \mathbb{I}_N) \right]_{\lambda=0} . \qquad (7)$$

The calculation of the determinant in Eq. (7) is conveniently performed by the recursive algorithm developed in [20]. Renormalization of the tridiagonal operator $\hat{R} = \hat{x} - \lambda \mathbb{I}_N$ allows us to write

$$\det(x - \hat{R} + i\varepsilon) = \prod_{k=1}^{\infty} (x - \tilde{a}_k + i\varepsilon) \qquad (8)$$

with $\tilde{a}_1 = -\lambda$, $\tilde{a}_{k+1} = -\lambda + \frac{1}{2} k (x - \tilde{a}_k + i\varepsilon)^{-1}$ for $1 < k < N$ and $\tilde{a}_{k+1} = \frac{1}{2} k (x - \tilde{a}_k + i\varepsilon)^{-1}$ for $k \geq N$.

The scheme given in Eqs. (7) and (8) is easily implemented numerically. In practice we have performed the calculation of the determinant (8) up to the product of its first M terms, which corresponds to inverting an $M \times M$ matrix. We have checked the convergence of this approximation by increasing the dimension M and correspondingly decreasing the value of ε.

In Fig. 1 we report the density profile $n(x)$ for $N = 5$, 10, and 20 fermions, with $M = 10^5$ and $\varepsilon = 0.01$. The exact profiles are also compared with those given by the Thomas-Fermi approximation (equivalent to the local density operator, or LDA),

$$n_{\mathrm{LDA}}(x) = \frac{1}{\pi} (2N - x^2)^{1/2} \qquad (9)$$

(in units such that $\hbar = 1$, $m = 1$, and $\omega = 1$). The exact profiles contain N oscillations, which become smaller in

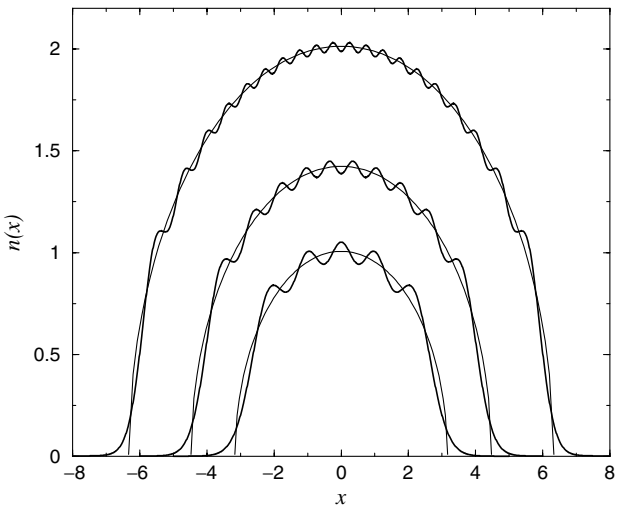

FIG. 1. Exact particle density profile (bold lines) for $N = 5$, 10, and 20 harmonically confined fermions, compared with the corresponding profiles evaluated in the local density approximation. Positions are in units of the characteristic length of the harmonic oscillator $a_{\mathrm{ho}} = \sqrt{\hbar/(m\omega)}$ and the particle density in units of a_{ho}^{-1}.

relative amplitude as N increases. Without any special numerical efforts we have evaluated the exact density profile up to $N = 1000$: this would otherwise require the calculation of Hermite polynomials up to the 1000th degree. For large N the oscillations are so small in relative amplitude that their smoothing in the LDA profile becomes reasonably accurate, except for the region of the tails.

B. Kinetic pressure profile: The particle density profile that we have evaluated above is the analog of the density of single-particle states in the energy domain. In the space domain other single-particle quantities acquire physical interest, as is the case for the kinetic pressure in Eq. (3). We also show for this function how one can profitably resort to a renormalization technique.

Taking $Q = \hat{p}^2 G(x)$, Eq. (5) can be written as

$$P(x) = -\frac{1}{\pi} \lim_{\varepsilon \to 0^+} \mathrm{Im} \frac{\partial}{\partial \lambda} [\ln \det(x - \hat{x} + i\varepsilon + \lambda \mathbb{I}_N \hat{p}^2)]_{\lambda=0} . \tag{10}$$

The matrix $(x - \hat{x} + i\varepsilon + \lambda \mathbb{I}_N \hat{p}^2)$ appearing in Eq. (10) is pentadiagonal on the first N rows, owing to the form of the operators $\hat{x}$ and $\hat{p} = i(a^\dagger - a)/\sqrt{2}$ in the basis of the energy eigenstates $\{|\psi_i\rangle\}$. The calculation of the determinant of such a matrix can again be performed by the recursive algorithm given in [20]. Renormalization of the operator $\hat{K} = \hat{x} - \lambda \mathbb{I}_N \hat{p}^2$ is made on blocks of dimension 2 for the pentadiagonal part and on blocks of dimension 1 for the tridiagonal part. This allows us to write

$$\det(x - \hat{K} + i\varepsilon) = \begin{cases} \prod_{j=1}^{(N+2)/2} \det(x - \tilde{A}_j + i\varepsilon) \prod_{k=N+3}^{\infty} (x - \tilde{a}_k + i\varepsilon) & (\text{even } N), \\ \prod_{j=1}^{(N+3)/2} \det(x - \tilde{A}_j + i\varepsilon) \prod_{k=N+4}^{\infty} (x - \tilde{a}_k + i\varepsilon) & (\text{odd } N). \end{cases} \tag{11}$$

The renormalized 2×2 blocks, $\tilde{A}_j$, satisfy the recursion relation

$$\tilde{A}_j = A_j + B_{j,j-1}(x - \tilde{A}_{j-1} + i\varepsilon)^{-1} B_{j-1,j} \tag{12}$$

for $j > 1$ and $\tilde{A}_1 = A_1$. The matrices A_j, $B_{j,j+1}$, and $B_{j+1,j}$ are submatrices of the operator $\hat{K}$, which are defined as follows:

$$A_j = \begin{pmatrix} -\lambda(2j - 3/2)\theta_{N-2j+1} & \sqrt{(2j-1)/2} \\ \sqrt{(2j-1)/2} & -\lambda(2j - 1/2)\theta_{N-2j} \end{pmatrix}, \tag{13}$$

$$B_{j,j+1} = \begin{pmatrix} \lambda\sqrt{2j(2j-1)}\,\theta_{N-2j+1}/2 & 0 \\ \sqrt{j} & \lambda\sqrt{2j(2j+1)}\,\theta_{N-2j}/2 \end{pmatrix}, \tag{14}$$

and

$$B_{j+1,j} = \begin{pmatrix} \lambda\sqrt{2j(2j-1)}\,\theta_{N-2j-1}/2 & \sqrt{j} \\ 0 & \lambda\sqrt{2j(2j+1)}\,\theta_{N-2j-2}/2 \end{pmatrix}, \tag{15}$$

with $\theta_k = 1$ for $k \geq 0$ and $\theta_k = 0$ otherwise. The recursion relation for the elements $\tilde{a}_k$ is again $\tilde{a}_{k+1} = \frac{1}{2}\, k/(x - \tilde{a}_k + i\varepsilon)$, the first elements being $\tilde{a}_{k+1} = \frac{1}{2} k\{x + i\varepsilon - [\tilde{A}_{k/2}]_{22} - [\tilde{A}_{k/2}]_{21}[\tilde{A}_{k/2}]_{12}/(x + i\varepsilon - [\tilde{A}_{k/2}]_{11})\}^{-1}$ with $k = N + 2$ for even N and $k = N + 3$ for odd N. We have studied the convergence of the determinant in Eq. (11) as for the case of the particle density profile.

In Fig. 2 the kinetic pressure $P(x)$ is plotted for $N = 5$, 10, and 20 with $M = 10^5$ and $\varepsilon = 0.01$, together with the profiles $P_{\mathrm{LDA}}(x)$ evaluated in the Thomas-Fermi approximation,

$$P_{\mathrm{LDA}} = \frac{1}{3\pi} (2N - x^2)^{3/2}. \tag{16}$$

The exact kinetic pressure shows N oscillations and has the peculiarity of being negative in the tails. This microscopic quantum effect, which is missing in the local density description, reflects the fact that in the low density region the kinetic energy decreases with increasing density. We have checked that our results agree with those reported in [18] for $N = 1$ and 2, and carried out the calculation of $P(x)$ up to $N = 1000$. The kinetic pressure profile for $N = 1000$, as shown in Fig. 3, looks almost indistinguishable from

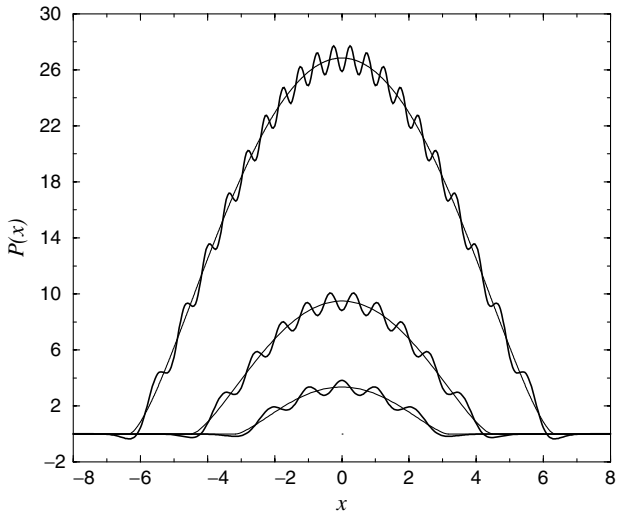

FIG. 2. Exact kinetic pressure profile (bold lines) for $N = 5$, 10, and 20 harmonically confined fermions, compared with the profiles evaluated in the local density approximation. Positions are in units of $a_{\mathrm{ho}} = \sqrt{\hbar/(m\omega)}$ and the kinetic pressure in units of $\hbar\omega a_{\mathrm{ho}}^{-1}$.

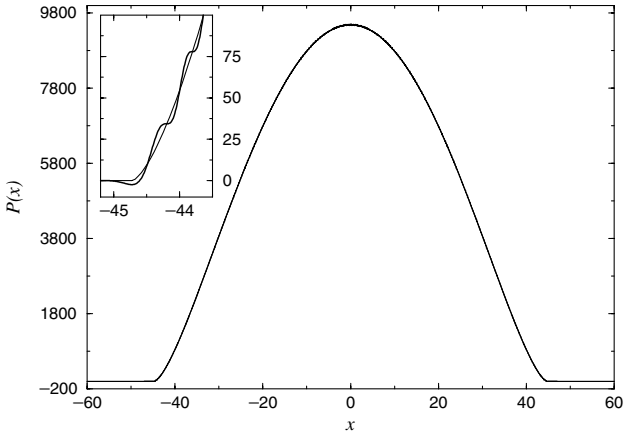

FIG. 3. Exact kinetic pressure profile (bold lines) for $N = 1000$, compared with the profile evaluated in the local density approximation. The inset shows an enlarged view of the tail of the profiles. The units are as in Fig. 2. In this calculation we have employed a matrix of dimension $M = 10^7$ and chosen $\varepsilon = 10^{-3}$ (see notations in the text).

the LDA prediction but still presents a region of negative kinetic pressure in the tails (inset of Fig. 3).

In conclusion, in this Letter we have given a general formula for the exact particle density and kinetic pressure profiles of a 1D many-fermion system in terms of a Green's operator in coordinate space. We have made use of the decimation/renormalization procedure and of other recursive techniques, originally developed to evaluate the spectral properties of quasi-1D systems in solid state physics, to efficiently calculate the exact density profiles of a harmonically confined noninteracting Fermi gas. Within the same general scheme the particle density could also be evaluated by employing a suitable Kirkman-Pendry relation [21], as will be reported elsewhere. We have verified that for large number of atoms ($N = 1000$) the local density approximation reproduces reasonably well the exact profiles except for the region of the tails, where the exact kinetic pressure is negative.

We believe that the present method opens the way for a novel approach to the equilibrium properties of spatially inhomogeneous 1D systems. The expressions here derived can be extended to finite temperature and to calculate partial density profiles for subgroups of atoms. The kinetic-energy density functional can be studied through the calculation of the function $P[x(n)]/2$, where $x(n)$ is obtained by local inversion of the exact profile $n(x)$. Pressure fluctuations will become accessible to study through the evaluation of higher moments of the one-body density matrix. The density profiles of the harmonically trapped Fermi gas in 1D, showing a prominent shell structure as displayed in our calculations, could become observable in experiments on alkali vapors.

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