Noninteracting fermions in a one-dimensional harmonic atom trap: Exact one-particle properties at zero temperature

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One-particle properties of noninteracting fermions in a one-dimensional harmonic trap and at zero temperature are studied. Exact expressions and asymptotic results for a large fermion number N are given for the particle density distribution $n_0(z,N)$. For large N and near the classical boundary at the Fermi energy, the density displays increasing fluctuations. A simple scaling of these tails of the density distribution with respect to N is established. The Fourier transform of the density distribution is calculated exactly. It displays a small but characteristic hump near $2k_F$, with k_F being a properly defined Fermi wave number. This is due to Friedel oscillations, which are identified and discussed. These quantum effects are missing in the semiclassical approximation. Momentum distributions are also evaluated and discussed. As an example of a time-dependent one-particle problem, we calculate exactly the evolution of the particle density when the trap is suddenly switched off, and find a simple scaling behavior, in agreement with recent general results.

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I. INTRODUCTION

Recent years brought about spectacular successes in the study of dilute bosonic quantum gases confined to atomic traps at extremely low temperatures. These and experimental details were reviewed in Ref. [1].

The next stage of investigations will incorporate fermionic quantum gases. Fermi degeneracy of potassium atoms (^{40}K) was recently observed in Ref. [2]. The effects of interactions between neutral atoms are of particular interest. They can give rise to collective ground states like superfluid phases.

Another development regards the construction of highly anisotropic traps, e.g., the microtraps in Refs. [3–7]. Magnetic trapping fields can be tailored so as to make the confining potential harmonic. If the longitudinal confinement frequency ω_ℓ is smaller than the radial frequency ω_r by a factor λ, it is possible to fill the first N longitudinal states, while the radial wave functions of the fermions are still those of the ground state, provided $N<1/\lambda$ holds.

From the semiclassical theory or local-density approximation (LDA), it is well known (cf., e.g., [8]), that a Fermi wave number $k_F=\sqrt{(2N-1)m\omega_\ell/\hbar}$ can be associated with a one-dimensional Fermi gas of atomic mass m in a harmonic trap. It is noted that the condition $N<1/\lambda$ is roughly in line with the standard estimate $k_F<1/l_t$ for a Fermi system which is confined to a transverse width l_t to be quasi-one-dimensional, provided the length l_t is identified with the extension $l_r=\sqrt{\hbar/m\omega_r}$ of the radial ground state wave function in the trap.

Noninteracting fermions in anisotropic harmonic traps were studied recently [8–10] using exact and semiclassical methods. The thermodynamics of harmonically confined spin-polarized fermions in any spatial dimension, including a harmonic two-particle interaction, was studied in Ref. [11] using a general approach [12]. The latter results are not available in closed form, and require numerical evaluation. A finite series representation for the free energy of one-dimensional noninteracting spin-polarized Fermions confined by a harmonic potential was given in Ref. [13].

In view of the feasibility of realizing one-dimensional fermions at ultralow temperatures, it seems worthwhile to supplement these works by studying the strictly one-dimensional case of noninteracting fermions at zero temperature when a number of exact explicit results can be obtained. Interactions between spin-polarized identical fermions are weak, because the Pauli principle forbids s-wave scattering. On the other hand, the theory of Luttinger liquids (cf., e.g., Ref. [14] for a review) shows that even small interactions change a one-dimensional Fermi system substantially. Nevertheless, it is useful to have results for the noninteracting case with which to compare the effect of interactions. The results that we present below show features specific for one spatial dimension.

In existing microtraps magnetic gradients of up to 30 T/cm were already realized [3] resulting in a periodic motion of the trapped atoms on a time scale of microseconds. Versions of microtraps based on microfabricated current conductors achieve even higher gradients, with an expected radial atomic oscillation frequency of above 1 MHz [6]. For the longitudinal oscillation a frequency of 1 Hz appears to be a reasonable lower limit, because time scales longer than 1 sec give rise to experimental difficulties due to seismic and acoustic noise. Thus the maximum value which is currently feasible for λ is 10^{-6}, and would limit the number of atoms inside the trap to about 1 000 000. The main experimental difficulty, however, is to fill the 10^6 states of the microtrap with a substantial number of atoms. Starting from an optically cooled sample of atoms with a phase-space density of typically 10^{-6} [15], a phase-space compression of six orders of magnitude is required to completely fill up the wave guide. Such a compression is possible with state-of-the-art techniques of evaporative cooling [16]. Thus a conservative estimation for realistic experimental conditions would assume a one-component fully spin-polarized Fermigas with a radial frequency inside the microtrap of 10^5 Hz. The longitudinal frequency can be set at 10 Hz, giving $\lambda = 10^{-4}$. Thus $N = 10^4$ quasi-one-dimensional fermions can be accommodated inside the trap. Assuming ^{6}Li atoms (in the hyperfine state $|m_s = 1/2, m_i = 1\rangle$ the inverse harmonic-oscillator length α according to

$$\alpha = \sqrt{m\omega_{\ell}/\hbar} \tag{1}$$

is estimated as $\alpha \approx 8 \times 10^2$ cm^{-1}, leading to a Fermi wave number $k_F \approx 10^5$ cm^{-1}.

Obviously the quasi-one-dimensional Fermi energy ϵ_F, i.e., the energy of the highest occupied state without the radial contribution, is

$$\epsilon_F = \hbar\omega_{\ell}\left(N - \frac{1}{2}\right). \tag{2}$$

Under the above assumptions ϵ_F corresponds to about 5 μK, and this temperature must be larger than the physical temperature in order to achieve degeneracy of the Fermi gas.

Another relevant quantity is the spatial extension of the inhomogeneous Fermi gas. The appropriate measure is twice that later given in Eq. (14), and leads to a characteristic extension of 0.4 cm and to an average Fermion density of about 3×10^4 atoms per cm. The radial width $2l_r$ is about 3×10^{-5} cm. Thus the tonks gas limit [17] is avoided and the fermionic atoms can be treated as point particles.

The exact quantum-mechanical results usually give only small corrections to the corresponding LDA predictions. Some of them are, however, of qualitative nature, and worth pointing out. Among these are diverging density oscillations near the classical boundary of the trap for large fermion numbers, and the general feature of Friedel oscillations [18] of the density. The paper is organized as follows. Section II presents the basic theory. Sec. III discusses the relevant lengths and energy scales of the one-dimensional Fermi gas in the harmonic trap. In Section IV we compile results for the zero-temperature one-particle density distribution. Section V is concerned with the Fourier transform of the density distribution. Section VI discusses momentum distributions, and in Sec. VII we calculate the expansion of the particle density distribution when the trap is suddenly switched off. An Appendix summarizes the mathematical formulas used in our calculations.

II. BASIC THEORY

We consider a gas of spinless noninteracting fermions in one spatial dimension and trapped in a harmonic potential

$$V(z) = \frac{1}{2} m\omega_{\ell}^2 z^2. \tag{3}$$

The Hamiltonian in second quantization and for the grand canonical ensemble is

$$\hat{H}_0 = \sum_{n=0}^{\infty} (\hbar\omega_n - \mu)\hat{c}_n^\dagger \hat{c}_n \tag{4}$$

with one-particle energies $\hbar\omega_n = \hbar\omega_{\ell}(n+1/2), n = 0,1, \ldots$. The chemical potential is denoted μ. The fermion creation operators $\hat{c}^+$ and destruction operators $\hat{c}$ obey the fermionic algebra $\hat{c}_m\hat{c}_n^\dagger + \hat{c}_n^\dagger\hat{c}_m = \delta_{m,n}$. This ensures that each (nondegenerate) energy level $\epsilon_n = \hbar\omega_n$, with a (real) single-particle wave function

$$\psi_n(z) = \sqrt{\frac{\alpha}{2^n n! \pi^{1/2}}} e^{-\alpha^2 z^2/2} H_n(\alpha z) \tag{5}$$

(normalized according to $\langle m|n\rangle = \delta_{m,n}$) is at most singly occupied. The intrinsic length scale of the system is the oscillator length $l = \alpha^{-1}$, where α is defined by Eq. (1). H_n denotes a Hermite polynomial.

We consider the spatial density of one-dimensional fermions in the harmonic trap, i.e., the one-particle distribution function

$$n(z;T,\mu) = \mathrm{Tr}\,\hat{\rho}\,\hat{\psi}^\dagger(z)\hat{\psi}(z). \tag{6}$$

In Eq. (6) the operator $\hat{\psi}(z)$ destroys a fermion at position z. It can be expanded as

$$\hat{\psi}(z) = \sum_{n=0}^{\infty} \psi_n(z)\hat{c}_n. \tag{7}$$

The density operator is

$$\hat{\rho} = Z^{-1} e^{-\beta\hat{H}_0}, \tag{8}$$

with $Z = \mathrm{Tr}\exp[-\beta\hat{H}_0]$. A standard textbook exercise then gives

$$n_0(z;T,\mu) = \sum_{m=0}^{\infty} \psi_m^2(z) p_m(T,\mu), \tag{9}$$

where

$$p_m(T,\mu) = \{e^{\beta(\hbar\omega_m - \mu)} + 1\}^{-1} \tag{10}$$

is the thermal occupation number of the single-particle state ψ_m.

The present paper deals with the case $T \to 0$, when a number of analytical results are available. The important simplification results from the fact that for $T \to 0$ the first N levels are completely filled while all others are empty, i.e.,

$$p_m(T \to 0, \mu) \to \Theta(N - 1 - m) \tag{11}$$

and μ becomes the Fermi energy ϵ_F:

$$\mu \to \epsilon_F = \hbar\omega_{\ell}\left(N - \frac{1}{2}\right). \tag{12}$$

The density $n_0(z;T \to 0,\mu)$, which we henceforth denote $n_0(z,N)$, takes the form

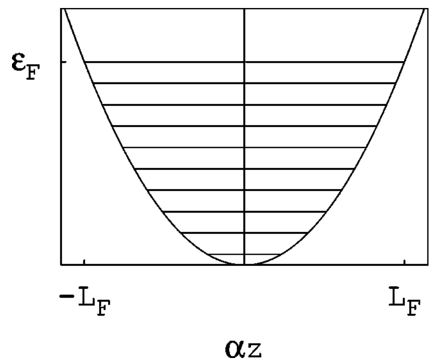

FIG. 1. $N=10$ noninteracting spinless fermions filling the lowest single-particle levels in the harmonic trap at zero temperature. ϵ_F denotes the Fermi energy, and L_F the half-width of the Fermi system.

$$n_0(z,N)=\sum_{n=0}^{N-1}\psi_n^2(z). \tag{13}$$

The zero-temperature case is depicted in Fig. 1. Equation (13) is the main object of the present study. Under the condition $k_BT\ll\epsilon_F$ it correctly describes the density of noninteracting Fermions in a harmonic trap. Figure 2 shows the density profile with the characteristic ripples on top. This is in contrast to an infinite Fermi gas (or one with periodic boundary conditions), where the density is homogeneous. The ripples appear here as a finite-size effect. In the center of the trap they will be identified below as Friedel oscillations [18].

III. LENGTHS AND ENERGY SCALES

In this section we summarize the relevant scales of a one-dimensional fermion gas in a harmonic trap. They are expressed in terms of the basic quantities m, ω_ℓ, and N. One of them is clearly the Fermi energy ϵ_F according to Eq. (12). At the Fermi energy the filled Fermi sea has a spatial extension $2L_F$ according to $m\omega_l^2L_F^2/2=\hbar\omega_\ell(N-1/2)$ or

$$L_F=\frac{1}{\alpha}\sqrt{2N-1}\equiv L_{n=N-1}, \tag{14}$$

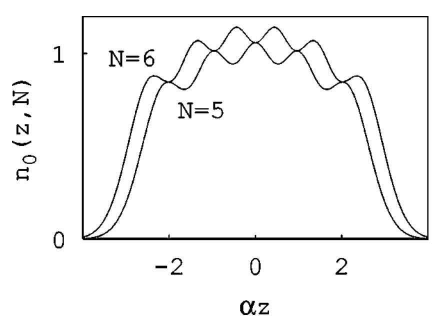

FIG. 2. Particle density distribution functions in units of the inverse oscillator length α for $N=5$ and $N=6$ fermions in a one-dimensional harmonic trap and at zero temperature. The added fermion resides in the area between the two curves. The density oscillations near the center can be identified as Friedel oscillations.

a quantity frequently appearing later. The positions $z=\pm L_F$ are classical turning points for a fermion with energy ϵ_F. The length L_F is the largest length of the problem followed by α^{-1}, which is associated with the zero point energy.

Equation (A8) of the Appendix shows that a wave function ψ_n behaves as a standing wave with wave vector $k_n=\alpha\sqrt{2n+1}$ in the middle of the trap, provided that $n\gg1$. At the Fermi energy the wave number becomes $k_F=\alpha\sqrt{2N-1}$. Together with Eq. (12) this leads to $\epsilon_F=\hbar^2k_F^2/2m$, as suggested in Ref. [8] for the three-dimensional anisotropic case. The Fermi wave number k_F^{-1} is the shortest length scale of the problem, and the Fermi energy the largest energy.

What is the relation between k_F and the particle density? In a one-dimensional fermion gas of spatial extension $2L_F$, with periodic or open (infinite potential well) boundary conditions, the relation in both cases is

$$k_F^{(0)}=\pi n_0=\pi\frac{N}{2L_F}. \tag{15}$$

In the present inhomogeneous situation k_F increases as $N^{1/2}$, because the width $2L_F$ of the trap also increases as $N^{1/2}$. However, we can discuss the peak density $n_0^{(p)}$ and average density $\overline{n_0}$ [or even higher moments of $n_0(z,N)$]. The peak density is clearly found near $z=0$. Using the asymptotic result [Eq. (A9)]

$$n_0(z,N)=\frac{k_F}{\pi}+\frac{1}{2\pi L_F}[1-(-1)^N\cos 2k_Fz] \tag{16}$$

gives

$$n_0^{(p)}\sim\frac{k_F}{\pi}. \tag{17}$$

The sign $\sim$ here and further on denotes an asymptotic correspondence for $N\gg1$. Note that this asymptotic limit does not imply a semiclassical approximation.

From (17) it is seen that the usual relation [Eq. (15)] between k_F and the one-dimensional particle density refers here to its peak value near the center. It is more difficult to discuss the average density $\overline{n_0}$, since an averaging length is needed. Equations (20) or (21) only give the obvious sum rule

$$\int_{-\infty}^{\infty}dz\, n_0(z,N)=N. \tag{18}$$

We thus resort to the semiclassical approximation, where the local density is given [8] by

$$n_{sc}(z,N)\equiv\frac{k_F(z)}{\pi}=\frac{k_F}{\pi}\sqrt{1-\left(\frac{z}{L_F}\right)^2}, \tag{19}$$

which is zero outside $|z|\leqslant L_F$. The corresponding average density clearly is $\overline{n}_0=k_F/4$, and is only slightly smaller than the peak density.

The sum rule for n_{sc} gives $N-1/2$, i.e., half a fermion is missing under the curve n_{sc}. This is due to the neglect of the fermion density leaking out of the classical region $|z|\leqslant L_F$ by tunneling. One might conclude that the number of fermions in the oscillations is about one-half. This is not correct for a large fermion number N when the difference between $n_0(z,N)$ and $n_{sc}(z,N)$ near the boundaries becomes significant due to increasing oscillations in the exact density, as detailed in the next Sec. IV.

Finally, using formula (A9) immediately allows the identification of the ripples in $n_0(z,N)$ near the center with the well-known Friedel oscillations [18] of wave number $2k_F$ around an impurity in the degenerate Fermi sea. In a naive interpretation these oscillations result from the superposition of incoming and reflected parts of the uppermost wave function, which both have a wave number k_F near the center of the trap. A more subtle interpretation refers to the inherent instability of the degenerate free Fermi gas toward static longitudinal perturbations of the wave number $q=2k_F$. A well-studied example are free electrons (cf., e.g., Ref. [19]). While in three dimensions only a logarithmic singularity in the derivative with respect to q appears in the susceptibility, it becomes a logarithmic singularity in one dimension due to perfect nesting. This causes charge- and spin-density-wave instabilities when backscattering interactions are present. In bounded Luttinger liquids (cf. Refs. [20,21]) the interactions modify the divergence of the density oscillation near the boundary.

But even without interactions, breaking of translational invariance by inhomogeneities like impurities and boundaries triggers density oscillations of the wave vector $2k_F$. In one dimension this effect is well known for noninteracting fermions with open boundary conditions. While in one dimension the effect is most pronounced it is, nevertheless, possible to identify the oscillations in the isotropic density calculated in Ref. [9] as three-dimensional Friedel oscillations. Since the one-dimensional Friedel oscillations contain only about one atom, it will be difficult to detect this effect experimentally. However, it is conceivable to use an array of shorter microtraps, each filled with a reduced number of atoms. The oscillations within each trap then add up, and lead to a total effect that is enhanced by the number of traps. Using microfabrication techniques it should be possible to combine 100 traps on one substrate, leading to a signal that may become within reach of advanced imaging techniques. Friedel oscillations though difficult to observe are a fundamental property of the degenerate Fermi gas which eludes the semiclassical approximation.

IV. ONE-PARTICLE DENSITY DISTRIBUTION

With the help of Eq. (A3) the summation in Eq. (13) can be performed for any z and N, with the result

$$n_0(z,N)=N\psi_N^2(z)-\sqrt{N(N+1)}\,\psi_{N+1}(z)\,\psi_{N-1}(z). \tag{20}$$

Using the recurrence relations for the wave functions ψ_n (cf. the Appendix), this expression can be brought into another useful form:

$$n_0(z,N)=N\psi_{N-1}^2(z)-\sqrt{N(N-1)}\,\psi_N(z)\,\psi_{N-2}(z). \tag{21}$$

This shows that the density distribution must be a polynomial of order $N-1$ in α^2z^2 times the exponential $\exp\{-\alpha^2z^2\}$, since the density is an even function of z.

Formulas (20) and (21) admit a number of exact conclusions as well as some remarkable asymptotic results with respect to the fermion number N. Differentiating Eqs. (20) and (21) with respect to z, and using the recurrence relations (A1) and (A2), gives

$$\frac{\partial n_0(z,N)}{\partial z}=-\alpha\sqrt{2N}\,\psi_N(z)\,\psi_{N-1}(z),$$

$$\frac{\partial^2 n_0(z,N)}{\partial z^2}=2\alpha^2N[\psi_N^2(z)-\psi_{N-1}^2(z)]. \tag{22}$$

This shows that the density distribution $n_0(z,N)$ has (i) N maxima at the N zeros $z_\nu^{(N)}$ of $\psi_N(z)$, $(\nu=1,\ldots,N)$, and (ii) $N-1$ minima at the $N-1$ zeros $z_\nu^{(N-1)}$ of $\psi_{N-1}(z)$, $(\nu=1,\ldots,N-1)$. As a consequence the minima of $n_0(z,N+1)$ touch the maxima of $n_0(z,N)$ at the points $z_\nu^{(N)}$. This is shown in Fig. 2 for $N=5$. The area between $n_0(z,6)$ and $n_0(z,5)$ contains precisely one fermion. In this way the Pauli exclusion principle is optimally implemented. The above considerations also show that about half a fermion is contained in the ripples of the density distribution. The density at the maxima is given by

$$n_0(z_\nu^{(N)},N)=N\,\psi_{N-1}^2(z_\nu^{(N)}), \tag{23}$$

and at the minima it is

$$n_0(z_\nu^{(N-1)},N)=(N-1)\,\psi_{N-2}^2(z_\nu^{(N-1)}). \tag{24}$$

Due to the knot theorems [22] the topological features inherent in the above statements carry over to arbitrary concave potentials. Thus counting the number of maxima of the density distribution gives the number of Fermions in any concave trap.

We now come to asymptotic results for $N\gg1$. In practice, $N\approx20$ is a good lower bound. In the asymptotic region the powerful formula (A4) is available for the full range $|z|\leqslant L_F$. Inserting Eq. (A4) into Eq. (21) gives

$$n_0(z,N)\sim k_F\left\{\left(1+\frac{3}{4N}\right)\frac{(-t_{N-1})^{1/2}}{\sin\phi_{N-1}}\mathrm{Ai}^2(t_{N-1})-\left(1+\frac{1}{4N}\right)\right.$$
$$\left.\times\frac{(t_Nt_{N-2})^{1/4}}{\sqrt{\sin\phi_N\sin\phi_{N-2}}}\mathrm{Ai}(t_N)\mathrm{Ai}(t_{N-2})\right\}. \tag{25}$$

The functions $t_n(z)$ and $\phi_n(z)$ are defined in Eq. (A5) and Eq. (A6). The advantage of this formula lies in the fact that the indices of the wave functions moved into the arguments of the Airy functions.

Evidently, the positions $z_\nu^{(N)}$ of the maxima are now found from

$$\mathrm{Ai}(t_N(z_\nu^{(N)}))=0. \tag{26}$$

We are interested in the positions of the last maximum, i.e., those lying in the neighborhood of L_F. The asymptotic expansion of t_N in the region $z \leqslant L_F \sim (2N)^{1/2}$ is

$$-t_N \sim 2\,N^{2/3}\left(1-\frac{z}{L_F}\right). \tag{27}$$

One also finds

$$t_{(N-1)\pm 1} \sim t_{N-1} \mp N^{-1/3}. \tag{28}$$

Provided $N^{1/3}$ is much larger than unity, this leads to (the prime means the derivative)

$$\begin{aligned} n_0(z_\nu^{(N)},N) &\sim \alpha\sqrt{2}\,N^{5/6}\mathrm{Ai}^2(t_{N-1}(z_\nu^{(N)})) \\ &\sim \alpha\sqrt{2}\,N^{1/6}\mathrm{Ai}'(t_N(z_\nu^{(N)}))^2. \end{aligned} \tag{29}$$

Specifically, we consider the last maximum at $z_N^{(N)}$. It corresponds to the first zero of the Airy function Ai(t) which is at $t_N(z_N^{(N)})=-2{,}33\ldots.$

This gives

$$z_N^{(N)} \sim L_F\left(1-\frac{1.17}{N^{2/3}}\right) \equiv L_F-\Delta x_N. \tag{30}$$

Note that

$$\Delta x_N \sim \frac{1.17}{N^{2/3}}L_F \sim \frac{1.65}{\alpha N^{1/6}}, \tag{31}$$

while the density at the maximum is

$$n_0(z_N^{(N)},N) \sim 0.7\alpha\,N^{1/6}. \tag{32}$$

In the same way the distance $l \equiv z_N^{(N)} - z_{N-1}^{(N)}$ between the last two maxima can be calculated. It determines the smallest local wave number $k^{(min)} \equiv 2\pi/l$, which is found to be

$$k^{(min)} \sim 2\pi\alpha\,0.8\,N^{1/6}. \tag{33}$$

It requires more than $N=50$ fermions to make $k^{(min)}$ less than half the maximal wave number $k^{(max)} \equiv 2k_F$ appropriate for the central part of the trap. When we define a shrinking region $S(N)$ near L_F according to

$$\Delta x \equiv L_F - z = \frac{f}{\alpha N^{1/6}}, \tag{34}$$

with—say—f varying from 1 to 10, then we have

$$-t_{N-1} \sim 2N^{2/3}\frac{f}{\alpha L_F N^{1/6}} \sim \sqrt{2}\,f, \tag{35}$$

which is independent of N.

In $S(N)$ the density [Eq. (25)] can be drastically simplified to read

$$\begin{aligned} n_0(z,N) \sim \alpha\sqrt{2}\,N^{1/6}\{&\mathrm{Ai}'(-t_{N-1}(z))^2 \\ &-\mathrm{Ai}(t_{N-1}(z))\mathrm{Ai}''(t_{N-1}(z))\}. \end{aligned} \tag{36}$$

Thus Eq. (29) leads to a self-similarity of the tails of the density for $z \in S(N)$ defined above: Calling $\tilde{n}_0(\Delta x,N) = n_0(z=L_F-\Delta x,N)$, the graph of $\tilde{n}_0(\Delta x \in S(N_2),N_2)$ maps precisely onto that of $\tilde{n}_0(\Delta x \in S(N_1),N_1)$ when the density is rescaled according to $(N_1/N_2)^{1/6}$ and the position Δx according to $(N_2/N_1)^{1/6}$. Note that $\tilde{n}_{sc}(\Delta x,N)$ also satisfies the scaling in $S(N)$.

Finally we exploit the approximation [Eq. (A7)] which holds for large values of $(-t)$, i.e., slightly away from the classical turning points $z=\pm L_F$. We are interested in results for $|z|<L_F$ which better the result [Eq. (A9)] valid in the very middle of the trap.

Using the expansion

$$\phi_{(N-1)\pm 1} \sim \phi_{N-1} \pm \frac{1}{2N-1}\,\frac{z}{\sqrt{L_F^2-z^2}}, \tag{37}$$

which requires distances $\Delta x/\alpha$ away from the boundary to be much larger than $N^{-1/6}$, we find

$$\begin{aligned} n_0(z,N) &= n_{sc}(z,N) + \frac{1}{2\pi L_F\sqrt{1-(z/L_F)^2}} - \frac{1}{2\pi L_F} \\ &\quad \times \frac{\sin\{(2N-1)[\sqrt{1-(z/L_F)^2}\,z/L_F - \arccos(z/L_F)]\}}{\sqrt{1-(z/L_F)^2}}. \end{aligned} \tag{38}$$

Equation (38) separates the slowly varying background n_{sc} from an increasing and spatially oscillating part due to quantum effects.

It is also seen that the oscillating part increases toward the boundaries $z=\pm L_F$. A naive extrapolation would give an envelope

$$E(z) \sim \frac{1}{\pi L_F\sqrt{1-(z/L_F)^2}} \tag{39}$$

of these oscillations which formally diverges near L_F as $[1-(z/L_F)^2]^{-1/2}$. In view of the range of validity of Eq. (38) this is, however, unwarranted. Nevertheless, it raises the question of how the oscillating part diverges at the boundaries when N diverges.

N noninteracting fermions in a one-dimensional box of width L confined between $z=0$ and $z=L$, and with infinite barriers (open boundary conditions), have the density distribution (for $N \gg 1$)

$$n_0(z,N) = \frac{k_F^{(0)}}{\pi}\left[1 - \cot\left(\frac{\pi z}{L}\right)\frac{\sin 2k_F^{(0)} z}{2N}\right]. \tag{40}$$

Using Eq. (15), i.e., $k_F^{(0)} = \pi N/L$, this gives an envelope for $z \ll L$ according to

$$E(z) \sim \frac{1}{\pi z} \equiv \frac{1}{\pi z^{\delta}}. \tag{41}$$

We conjecture that in our case of a soft boundary the limiting behavior near the right boundary for very large N is

$$E(z \leqslant L_F) \sim \frac{1}{2\pi L_F (1 - z/L_F)^{\delta(N)}}. \tag{42}$$

There is numerical evidence for $\delta(N \to \infty) \to 1$, though in a very slow approach $[\delta(N) \approx 1 - 1/\ln N]$. This would imply that the integrated absolute fluctuations

$$\delta N = \int_{-LF}^{LF} dz \left| n_0(z,N) - n_{sc}(z,N) \right|,$$

i.e., the number δN of fermions in the density oscillations, diverges logarithmically with N as it does for ideal fermions in a box. The mathematical problem in clarifying this point lies in the enormous difficulty in subtracting out the oscillating part in the boundary region $z \to L_F (N \gg 1)$ which is outside the bounds of approximation (37). In the case of interacting spinless one-dimensional fermions in a box, it is known that the exponent δ is given by the coupling constant K [20].

V. DENSITY PROFILE IN FOURIER SPACE

With possible application to optical detection, we discuss the Fourier transform of $n_0(z,N)$:

$$F[n_0(k,N)] \equiv \int_{-\infty}^{\infty} dz\, e^{ikz} n_0(z,N). \tag{43}$$

It can be evaluated exactly in the following way: The integral in Ref. [23] can be converted to the form

$$\int_{-\infty}^{\infty} dz\, e^{ikz} \psi_m(z) \psi_n(z) = e^{-k^2/4\alpha^2} \left(\frac{-k^2}{2\alpha^2}\right)^{(n-m)/2} \sqrt{\frac{m!}{n!}} L_m^{(n-m)}(k^2/2\alpha^2) \tag{44}$$

$(n \geqslant m)$, where L_n denotes a Laguerre polynomial. Applying Eq. (44) to Eq. (21), and using recursion relations for Laguerre polynomials [31], gives

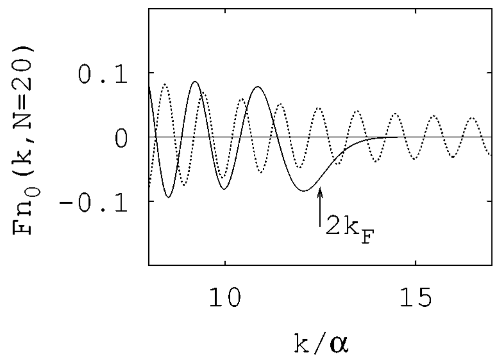

FIG. 3. Part of the Fourier-transformed density distribution function for $N=20$ noninteracting fermions at zero temperature. Note the small hump near the wave number $2k_F$ due to Friedel oscillations which provide the shortest length scale of the problem. The dotted line is the semiclassical approximation lacking that feature.

$$F[n_0(k,N)] = e^{-k^2/4\alpha^2} L_{N-1}^{(1)}(k^2/2\alpha^2). \tag{45}$$

The Fourier transform of the semiclassical expression [Eq. (19)] can also be given in closed form involving a Bessel function:

$$F[n_{sc}(k,N)] = \frac{k_F}{k} J_1(k^2/2\alpha^2). \tag{46}$$

Note the sum rules

$$\int_{-\infty}^{\infty} dk\, F[n_0(k,N)] = 2k_F = \int_{-\infty}^{\infty} dk\, F[n_{sc}(k,N)] \tag{47}$$

and the limits

$$F[n_0(k \to 0,N)] = N, \quad F[n_{sc}(k \to 0,N)] = N - \frac{1}{2}. \tag{48}$$

The basic difference between the exact result [Eq. (45)] which takes care of the ripples in the density profile and the semiclassical form [Eq. (46)] is a hump somewhat below the wave number $2k_F$, as shown in Fig. 3. For larger wave numbers $F[n_0(k,N)]$ drops to zero while $F[n_{sc}(k,N)]$ shows a multitude of oscillations similar to that produced by a slit of spatial width $2L_F$. For $k \ll 2k_F$, however, the exact result and the semiclassical approximation agree very well.

VI. ONE-PARTICLE MOMENTUM DISTRIBUTIONS

Even for a confined system one can define a momentum density distribution by

$$p(k) \equiv \langle \hat{c}_k^{\dagger} \hat{c}_k \rangle. \tag{49}$$

The operator $\hat{c}_k$ annihilates a fermion with (continuous) momentum $\hbar k$. It can be decomposed into fermionic annihilation operators for the harmonic oscillator according to

$$\hat{c}_k = \sum_{n=0}^{\infty} (-1)^n f_n^k \hat{c}_n, \tag{50}$$

with the transformation function

$$f_m^k = \frac{i^m}{\alpha} \psi_m(z = k/\alpha^2). \tag{51}$$

The momentum density p_0 of noninteracting fermions in a harmonic trap and at zero temperatures thus becomes

$$p_0(k;N,T=0) = \sum_{m=0}^{\infty} (f_m^k)^* f_m^k \Theta(N-1-m)$$
$$= \sum_{m=0}^{N-1} (-1)^m (f_m^k)^2, \tag{52}$$

leading to the remarkable result

$$p_0(k;N,T=0) = \frac{1}{\alpha^2} \sum_{m=0}^{N-1} \psi_m^2(z = k/\alpha^2)$$
$$\equiv \frac{1}{\alpha^2} n_0(z = k/\alpha^2; N, T=0). \tag{53}$$

The momentum density is isomorphic to the particle density with k_F replacing L_F. Obviously, it satisfies the general sum rule

$$\int_{-\infty}^{\infty} dk\, p(k;N,T) = N. \tag{54}$$

Alternatively, we can study the momentum probability

$$P(k;N,T=0) \equiv \int_{-\infty}^{\infty} dz\, e^{ikz} \langle \hat{\psi}^\dagger(z) \hat{\psi}(0) \rangle^{(N)}, \tag{55}$$

which is also appropriate for symmetric confining potentials centered at $z=0$.

For noninteracting fermions at zero temperature in the harmonic trap, we can use Eq. (A3) to find

$$\langle \hat{\psi}^\dagger(z) \hat{\psi}(0) \rangle_0^{(N)} = \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 z^2/2} \sum_M \{ \delta_{N,2M+1} L_M^{(1/2)}(\alpha^2 z^2)$$
$$+ \delta_{N,2M} L_{M-1}^{(1/2)}(\alpha^2 z^2) \}. \tag{56}$$

In the limit $N \gg 1$, this reduces to the simple expression

$$\langle \hat{\psi}^\dagger(z) \hat{\psi}(0) \rangle_0^{(N)} \sim \frac{\sin k_F z}{\pi z} + 0\left(\frac{1}{\sqrt{N}} \right). \tag{57}$$

The corresponding discrete momentum distribution for the harmonic oscillator is the well known step function

$$P_0(k; N \gg 1, T=0) = \Theta(k_F - k), \tag{58}$$

with $k = k_n = \alpha\sqrt{2n+1}$.

Some general remarks may be useful: The centered momentum distribution [Eq. (55)] can be expressed as

$$P(k;N,T) = \int_{-\infty}^{\infty} dk' \langle \hat{c}_k^\dagger \hat{c}_{k'} \rangle. \tag{59}$$

In the case of translational invariance, the integrand in Eq. (59) becomes

$$\langle \hat{c}_k^\dagger \hat{c}_{k'} \rangle = P(k;N,T)\, \delta(k-k'). \tag{60}$$

Under periodic boundary conditions both definitions (49) and (55) coincide.

VII. FREE EXPANSION OF PARTICLE DENSITY

Expansion of a particle cloud is an important tool to investigate Bose-Einstein condensates (cf. Refs. [24,1]). Detailed theories are available for this expansion based on the Gross-Pitaevskii equation [24–28]. In the simplest case the trap is suddenly switched off and the condensate expands freely. Non-interacting boson condensates display universal length scaling [25] in all spatial dimensions. The same has also been shown recently for non-interacting fermions [10].

When particle interactions dominate the kinetic energy, the transverse scaling function in a highly anisotropic trap is

$$b_r(t) = \sqrt{1 + \omega_r^2 t^2}, \tag{61}$$

while the longitudinal expansion is more complicated [26]. This was confirmed experimentally in full detail in Refs [29,30].

In accord with Ref. [10], we find that a freely expanding degenerate one-dimensional gas of noninteracting fermions behaves according to Eq. (61), with ω_ℓ replacing ω_r. The calculation is fully quantum mechanical, and supplements the approach in Ref. [10].

The quantity to be calculated is

$$n(z,t) = \mathrm{Tr}\, \hat{\rho}(t) \hat{\psi}^\dagger(z) \hat{\psi}(z). \tag{62}$$

where $\hat{\rho}(t)$ is the density operator of the freely expanding gas. It is given in terms of the statistical operator $\hat{\rho}(0)$ immediately before the trap is opened at time $t=0$ by

$$\hat{\rho}(t) = e^{-i\hat{H}_{00}t/\hbar} \hat{\rho}(0) e^{i\hat{H}_{00}t/\hbar}. \tag{63}$$

The free expansion of noninteracting one-dimensional fermions is governed by the Hamiltonian

$$\hat{H}_{00} = \int_{-\infty}^{\infty} dk \frac{\hbar^2 k^2}{2m} \hat{c}_k^\dagger \hat{c}_k. \tag{64}$$

The operators $\hat{c}_k^\dagger$ and $\hat{c}_k$ were introduced in conjunction with Eq. (49). Equation (62) can also be written as

$$n(z,t) = \mathrm{Tr}\, \hat{\rho}(0) \hat{\psi}^\dagger(z,t) \hat{\psi}(z,t), \tag{65}$$

with

$$\hat{\psi}(z,t)=e^{i\hat{H}_{00}t/\hbar}\hat{\psi}(z)e^{-i\hat{H}_{00}t/\hbar}=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk\,e^{i(kz-\omega_k t)}\hat{c}_k \tag{66}$$

and

$$\omega_k=\frac{\hbar k^2}{2m}. \tag{67}$$

We now use Eqs. (50) and (51) to find

$$n_0(z,t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\,dk'\,e^{-iz(k-k')+i(\omega_k-\omega_{k'})t}\times\sum_{m,n=0}^{\infty}(-1)^{m+n}(f_m^k)^*f_n^{k'}\,\mathrm{Tr}\,\hat{\rho}(0)\hat{c}_m^\dagger\hat{c}_n. \tag{68}$$

For a harmonic trap which is initially in thermal equilibrium, the statistical operator $\hat{\rho}(0)$ is Eq. (8), and, at zero temperature,

$$\mathrm{Tr}\,\hat{\rho}\,\hat{c}_m^\dagger\hat{c}_n=\delta_{m,n}\Theta(N-1-m) \tag{69}$$

holds. We thus find

$$n_0(z,t;T=0)=\frac{1}{2\pi\alpha^2}\int_{-\infty}^{\infty}dk\,dk'\times e^{-iz(k-k')+i(\omega_k-\omega_{k'})t}\times\left\{\sum_{m=0}^{N-1}\psi_m(k/\alpha^2)\,\psi_m(k'/\alpha^2)\right\}. \tag{70}$$

The summation in curly brackets can be performed using Eq. (A3). In order to proceed it is convenient to go over to the Fourier transform and write out the oscillator eigenfunctions in terms of Hermite polynomials. This leads to

$$\begin{aligned}Fn_0(k1,t;T=0)&\equiv\int_{-\infty}^{\infty}dz\,e^{ik_1z}n_0(z,t;T=0)\\&=\sqrt{\frac{1}{\pi}}\frac{1}{2^Nk_1(N-1)!}e^{-k_1^2(1-i\omega_{\parallel}t)/2\alpha^2}\\&\quad\times\int_{-\infty}^{\infty}dk'\,e^{-(k'^2+k'k_1)(1-i\omega_{\parallel}t)/\alpha^2}\\&\quad\times[H_N((k_1+k')/\alpha)H_{N-1}(k'/\alpha)\\&\quad-(N\leftrightarrow(N-1))].\end{aligned} \tag{71}$$

Using Ref. [32], the integration can be performed, giving

$$F[n_0(k,t;T=0)]=e^{-k^2(1+\omega_{\parallel}^2t^2)/4\alpha^2}L_{N-1}^{(1)}\times(k^2(1+\omega_{\parallel}^2t^2)/2\alpha^2)). \tag{72}$$

This formula is isomorphic to Eq. (45) with the inverse length α being replaced by the rescaled value

$$\alpha\rightarrow(1+\omega_{\parallel}^2t^2)^{-1/2}\alpha\equiv\alpha/b(t). \tag{73}$$

Since $F[n_0(k,t)]$ and $n_0(z,t)$ are related via a Fourier transformation, the final result is

$$n_0(z,t;T=0)=\frac{1}{b(t)}n_0(z/b(t),N). \tag{74}$$

Thus a free longitudinal expansion proceeds via a simple length rescaling involving the factor $b(t)$. In the course of time the initial density distribution (Fig. 2) decreases and broadens according to the factor $b(t)$, but preserves its topology including the Friedel oscillations, which correspondingly increase their wave length.

In this picture it is assumed that the fermions remain one dimensional during the expansion. If the transverse confining fields are also removed, transverse expansion in any of the two equivalent transverse directions will also proceed according to Eq. (74) taken for $N=1$ and with the scaling function [Eq. (61)]. This follows simply from the observation that each of the two ground-state wave functions for the transverse directions correspond to a single one dimensionally confined Fermion, with ω_r in place of $\omega_{\parallel}$.

VIII. SUMMARY

We have exactly calculated one-particle properties of noninteracting one-dimensional fermions in a harmonic trap. These are the particle density distribution, including its free expansion when the trap is switched off, and also two momentum distribution functions. The exact calculability can be traced back to two specific mathematical features of the eigenfunctions of the harmonic oscillator, namely that finite sums of bilinear expressions can be performed, and that Fourier transformation essentially reproduces an eigenfunction. Friedel oscillations in the particle density and its analog in the momentum distribution, as well as diverging density oscillations near the classical boundary are basic features of the degenerate one-dimensional ideal fermi gas.

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APPENDIX

The appendix is a compilation of some mathematical formulas used in the derivation of the results given in the main part of the paper. An important role is played by the recurrence relations for Hermite polynomials (cf., e.g., Ref. [31]). Here they are given as recurrence relations for the complete harmonic oscillator wave functions $\psi_n(z)$. These are

$$\sqrt{n+1}\,\psi_{n+1}(z)-\alpha z\sqrt{2}\,\psi_n(z)+\sqrt{n}\,\psi_{n-1}(z)=0, \tag{A1}$$

$$\frac{d}{dz}\psi_n(z)+\alpha^2z\,\psi_n(z)-\alpha\sqrt{2n}\,\psi_{n-1}(z)=0. \tag{A2}$$

The summation of the finite series [Eq. (13)] is accomplished by means of

$$\sum_{m=0}^{n} \psi_m(z_1)\psi_m(z_2) = \sqrt{\frac{n+1}{2}}\left[\frac{\psi_{n+1}(z_1)\psi_n(z_2)-\psi_n(z_1)\psi_{n+1}(z_2)}{\alpha(z_1-z_2)}\right], \tag{A3}$$

which is a conversion of a formula in Ref. [33]. In (A3) the limit $z_1 \to z_2$ can be performed, and the resulting derivatives converted into harmonic oscillator wave function using Eq. (A2) and (A1). This leads to Eq. (20). An alternative derivation applies induction to Eq. (21) which is obviously true for $N=1$ utilizing the recurrence relation [Eq. (A1)].

A very useful asymptotic ($n \gg 1$) expression for the wave functions can be extracted from Ref. [31] (Chap. 19.7):

$$\psi_n(z) \sim \sqrt{\alpha}\left(\frac{2}{n}\right)^{1/4}\left\{\frac{(-t_n)^{1/4}}{\sin^{1/2}\phi_n}\mathrm{Ai}(t_n)\right\}, \tag{A4}$$

with

$$-t_n = \left[\frac{3}{2}\left(\frac{n}{2}+\frac{1}{4}\right)(2\phi_n - \sin 2\phi_n)\right]^{2/3} \tag{A5}$$

and

$$\cos\phi_n = \frac{z}{L_n}. \tag{A6}$$

Ai is the Airy function which oscillates for negative arguments. There is a continuation to positive arguments (the tunneling region) which we will not discuss.

The tilde $\sim$ denotes asymptotic expansion for large n including all prefactors. Inside the trap, i.e., away from the classical borders, the form

$$\psi_n(z) \sim \sqrt{\frac{\alpha}{\pi}}\left(\frac{2}{n}\right)^{1/4}\frac{1}{\sin^{1/2}\phi_n}\cos\left\{\left(\frac{n}{2}+\frac{1}{4}\right)\times(\sin 2\phi_n - 2\phi_n)+\frac{\pi}{4}\right\} \tag{A7}$$

is useful. It results by means of the asymptotic expansion of the Airy function $\mathrm{Ai}(t)$ for $-t \gg 1$. In the limit $|z| \ll L_n$ a further simplification occurs since $\phi_n \to \pi/2 - z/L_n$. This leads to (note that $n \gg 1$)

$$\psi_n \to \left(\frac{2\alpha^2}{n\pi^2}\right)^{1/4}\cos\left(k_n z - \frac{n\pi}{2}\right), \tag{A8}$$

which is used in Sec. IV. The corresponding fermion density well inside the trap is

$$n_0(z,N) = \frac{k_F}{\pi} + \frac{1}{2\pi L_F}[1-(-1)^N \cos 2k_F z]. \tag{A9}$$

Here a small systematic error $1/(2\pi L_F)$ of this approximation for $|z| \ll L_F$ has been subtracted to bring Eq. (A9) into line with the exact result.

[1] W. Ketterle, D.S. Durlee, and D.M. Stamper-Kurn, e-print cond-mat/9904034v2.
[2] B. De Marco and D.S. Jin, Science **285**, 1703 (1999).
[3] V. Vuletic, T. Fischer, M. Praeger, T.W. Hänsch, and C. Zimmermann, Phys. Rev. Lett. **80**, 1634 (1998).
[4] J. Fortagh, A. Grossmann, C. Zimmermann, and T.W. Hänsch, Phys. Rev. Lett. **81**, 5310 (1999).
[5] J. Denschlag, D. Cassettari, and J. Schmiedmayer, Phys. Rev. Lett. **82**, 2014 (1999).
[6] J.H. Thywissen, M. Olshanii, G. Zabow, M. Drndic, K.S. Johnson, R.M. Westervelt, and M. Prentiss, Eur. Phys. J. D **7**, 361 (1999).
[7] J. Reichel, W. Hänsel, and T.W. Hänsch, Phys. Rev. Lett. **83**, 3398 (1999).
[8] D.A. Butts and D.S. Rokhsar, Phys. Rev. A **55**, 4346 (1997).
[9] J. Schneider and H. Wallis, Phys. Rev. A **57**, 1253 (1998).
[10] G.M. Bruun and C.W. Clark, Phys. Rev. A **61**, 061601 (2000).
[11] F. Brosens, J.T. Devreese, and L.F. Lemmens, Phys. Rev. E **57**, 3871 (1998).
[12] F. Brosens, J.T. Devreese, and L.F. Lemmens, Phys. Rev. E **55**, 227 (1997).
[13] M. Takahashi and M. Imada, J. Phys. Soc. Jpn. **53**, 963 (1983).
[14] J. Voit, Rep. Prog. Phys. **58**, 977 (1995).
[15] C.G. Townsend, N.H. Edwards, C.J. Cooper, K.P. Zetie, C. Foot, A.M. Steane, P. Szriftgiser, H. Perin, and J. Dalibard, Phys. Rev. A **52**, 1423 (1995).
[16] O.J. Luiten, M.W. Reynolds, and J.T.M. Walraven, Phys. Rev. A **53**, 381 (1996).
[17] M. Olshanii, Phys. Rev. Lett. **81**, 938 (1998).
[18] J. Friedel, Adv. Phys. **3**, 446 (1995).
[19] D. Pines and P. Nozieres, *The Theory of Quantum Liquids* (Benjamin, New York, 1966).
[20] M. Fabrizio and A.O. Gogolin, Phys. Rev. B **51**, 17 827 (1995).
[21] J. Voit, Yupeng Wang, and M. Grioni, e-print cond-mat/9912392.
[22] G. Szegö, *Orthogonal Polynomials* (American Mathematics Society, Providence, 1987), Chap. 3.
[23] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic Press, New York, 1980), Eq. (7.374/7).
[24] M. Holland and J. Cooper, Phys. Rev. A **53**, R1954 (1996).
[25] Yu. Kagan, E.L. Surkov, and G.V. Shlyapnikov, Phys. Rev. A **54**, R1753 (1996).
[26] Y. Castin and R. Dum, Phys. Rev. Lett. **77**, 5315 (1996).
[27] M.J. Holland, D.S. Jin, M.L. Chiofalo, and J. Cooper, Phys. Rev. Lett. **78**, 3801 (1997).

[28] F. Dalfavo, C. Minniti, S. Stringari, and L. Pitaevskii, Phys. Lett. A **227**, 259 (1997).
[29] U. Ernst, A. Marte, F. Schreck, J. Schuster, and G. Rempe, Europhys. Lett. **41**, 1 (1998).
[30] U. Ernst, J. Schuster, F. Schreck, A. Marte, and G. Rempe, Appl. Phys. B: Lasers Opt. **67**, 719 (1998).
[31] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (Dover, New York, 1970), Chap. 22.
[32] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Ref. [23]), Eq. (7.377).
[33] H. Batemann, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. II, p. 193.