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On the density profile in Fourier space of harmonically confined ideal quantum gases in *d* dimensions

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Abstract

Closed-form analytical expressions and asymptotic results are obtained for the density distribution in Fourier space of harmonically trapped fermion gases at zero and nonzero temperatures in d dimensions. The result is applied to weakly interacting Fermi gases and to the elastic scattering from atomic nuclei. The Fourier transform of the momentum density for a d-dimensional harmonic confinement is also found.

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1. Introduction

The experimental realization of trapped and cooled quantum gases [1, 2], to the regime where the quantum effects of quantum statistics such as the shell structure in the single particle density profile can be observed, has motivated a series of theoretical studies [3-10]. In this work we shall limit ourselves to the case of the harmonic oscillator confining potential, since most experiments are performed in harmonic traps [11].

Let us recall some basic concepts, in an arbitrary dimension d, concerning a degenerate system of N independent particles in a potential $V(r) = \frac{1}{2}m\omega^2 r^2$, with $r^2 = x_1^2 + \cdots + x_d^2$. The one-particle state is specified by a set of quantum numbers $\{n_1, \ldots, n_d\}$, its energy being $\epsilon_n = \hbar\omega(n + d/2)$ with $n = n_1 + \cdots + n_d$. The spatial wavefunction $\Phi(x_1, \ldots, x_d) = \varphi_{n_1}(x_1)\varphi_{n_2}(x_2)\cdots\varphi_{n_d}(x_d)$ is the product of the one-dimensional normalized wavefunctions $\varphi_n(x) = \exp(-\alpha^2 x^2/2)H_n(\alpha x)(\alpha/(2^n n!\sqrt{\pi}))^{1/2}$, where H_n are Hermite polynomials and $\alpha = (m\omega/\hbar)^{1/2}$. At zero temperature, and if the particles completely fill (M + 1) oscillator shells, the spatial one-particle density is defined as

$$\rho^{(d)}(\mathbf{r}, M) = 2 \sum_{n=0}^{M} \sum_{n_1 + \dots + n_d = n} \left| \varphi_{n_1}(x_1) \cdots \varphi_{n_d}(x_d) \right|^2.$$
(1)

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From now on, the superscript (d) stands for the dimensionality of the space. Here the factor 2 accounts for a spin degeneracy but note that, in the case of spin polarized fermions or spinless bosons, such a factor should be dropped. In the ground state the number N of particles is related to the quantum number M by

$$N = 2 \begin{pmatrix} M+d \\ d \end{pmatrix}.$$
 (2)

For the density $\rho^{(d)}(r, M)$ given in equation (1), several authors have obtained exact closed analytical expressions at zero temperature in one dimension [3, 4, 6, 12] and at higher dimensions [5, 7]. Note that, in the asymptotic limit of large particle numbers, analytical results have also been found [5, 10]. In the present work we shall be concerned with the Fourier transform of the particle density distribution in a *d*-dimensional harmonic trap, a problem that may find application in optical detection [13]. In the one-dimensional case, the analytical expression of the Fourier transform of the particle density has been shown by Gleisberg *et al* [4] to have a very simple analytical form. In the next section we shall derive an exact analytical expression as well as the asymptotic result for the density profile in Fourier space in arbitrary dimensions. Then, in section 3, we will extend our analysis to finite temperature. Two physical applications will be presented in section 4: the case of a weakly interacting Fermi gas and the elastic scattering from atomic nuclei. In section 5, the Fourier transform of the momentum density is also examined. Finally, the summary puts an end to the paper.

2. The density profile in Fourier space

We start with the definition of the Fourier transform of the one-particle density $\rho^{(d)}(r)$ in d dimensions, that is,

$$n^{(d)}(k) = \int \rho^{(d)}(r) \,\mathrm{e}^{-\mathrm{i}k \cdot r} \,\mathrm{d}r.$$
(3)

The inverse Fourier transform reads

$$o^{(d)}(\mathbf{r}) = \int n^{(d)}(\mathbf{k}) \,\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \frac{\mathrm{d}\mathbf{k}}{(2\pi)^d}.$$
(4)

Note that if the spatial density is normalized such that $N = \int \rho^{(d)}(r) dr$, equation (3) gives

$$n^{(d)}(\mathbf{0}) = N,\tag{5}$$

and from equation (4) we can extract the density at the center of the trap, that is,

$$\rho^{(d)}(\mathbf{0}) = \int n^{(d)}(\mathbf{k}) \frac{\mathrm{d}\mathbf{k}}{(2\pi)^d}.$$
 (6)

In [4] the relation

$$\int_{-\infty}^{\infty} \varphi_m(x)\varphi_n(x) \,\mathrm{e}^{-\mathrm{i}kx} \,\mathrm{d}x = \left(-\frac{k^2}{2\alpha^2}\right)^{(n-m)/2} \sqrt{\frac{m!}{n!}} \exp\left(-\frac{k^2}{4\alpha^2}\right) L_m^{n-m}\left(\frac{k^2}{2\alpha^2}\right),\tag{7}$$

which is satisfied by the wavefunctions $\varphi_n(x)$ of the harmonic oscillator, is used to calculate, in one dimension (d = 1), the integral in equation (3) for the density $\rho^{(d)}(r)$ given in equation (1). The result obtained is

$$n^{(1)}(k,M) = 2\exp\left(-\frac{k^2}{4\alpha^2}\right) \sum_{m=0}^{M} L_m\left(\frac{k^2}{2\alpha^2}\right) = 2\exp\left(-\frac{k^2}{4\alpha^2}\right) L_M^1\left(\frac{k^2}{2\alpha^2}\right),$$
(8)



Figure 1. Plot of the density profile in Fourier space $n^{(d)}(k, M)$ given in equation (12) as a function of $k = |\mathbf{k}|$ for N = 240 particles. Three situations are shown: (a) the one-dimensional case d = 1and M + 1 = 120 closed shells (solid line), (b) the two-dimensional case d = 2 and M + 1 = 15closed shells (dashed line) and (c) the three-dimensional case d = 3 and M + 1 = 8 closed shells (dotted line). Units are chosen such that $\alpha = 1$.

where $L_M^d(x)$ are the well known associated Laguerre polynomials. The summation relation $\sum_{n=0}^{M} L_n^{d-1}(x) = L_M^d(x)$ [14] is used to obtain this equation. Let us now extend this result to higher dimensions, taking into account that the

multidimensional version of equation (7) is

$$\int_{-\infty}^{\infty} e^{-ik_1x_1} |\varphi_{n_1}(x_1)|^2 dx_1 \times \dots \times \int_{-\infty}^{\infty} e^{-ik_dx_d} |\varphi_{n_d}(x_d)|^2 dx_d$$
$$= \exp\left(-\frac{k^2}{4\alpha^2}\right) L_{n_1}\left(\frac{k_1^2}{2\alpha^2}\right) \cdots L_{n_d}\left(\frac{k_d^2}{2\alpha^2}\right)$$
(9)

where $k^2 \equiv k^2 = k_1^2 + \dots + k_d^2$. With the above result, using (1) and (3) the density $n^{(d)}(k, M)$ becomes

$$n^{(d)}(k,M) = 2\exp\left(-\frac{k^2}{4\alpha^2}\right) \sum_{n=0}^{M} \sum_{n_1+\dots+n_d=n} L_{n_1}\left(\frac{k_1^2}{2\alpha^2}\right) \cdots L_{n_d}\left(\frac{k_d^2}{2\alpha^2}\right),$$
(10)

and using the identity [14]

$$\sum_{n_1+\dots+n_d=n} L_{n_1}(x_1)\dots L_{n_d}(x_d) = L_n^{d-1}(x_1+\dots+x_d)$$
(11)

we then obtain the very compact form

$$n^{(d)}(\boldsymbol{k}, M) = 2\exp\left(-\frac{\boldsymbol{k}^2}{4\alpha^2}\right) \sum_{n=0}^{M} L_n^{d-1}\left(\frac{\boldsymbol{k}^2}{2\alpha^2}\right) = 2\exp\left(-\frac{\boldsymbol{k}^2}{4\alpha^2}\right) L_M^d\left(\frac{\boldsymbol{k}^2}{2\alpha^2}\right).$$
(12)

A simple test of equation (12) can be done as follows. If we evaluate $n^{(d)}(\mathbf{0}, M)$ and since $L_M^d(0) = \binom{M+d}{d}$ [14], the exact result given in equation (5) is obtained.

A plot of the density profile in Fourier space (12) is shown in figure 1 for N = 240, a number of particles which completely fill M + 1 = 120, 15, 8 oscillator shells for d = 1, 2, 3, 3respectively.

2.1. Asymptotic result for the density profile in Fourier space

In the following we present a simple analytical result for $n^{(d)}(k, M)$ at T = 0 in the limit of large $M \gg 1$, which corresponds to the limit of a large particle number N. Such an asymptotic

limit is easily obtained since in equation (12) appears only one associated Laguerre polynomial, and therefore applying the asymptotic form [14]

$$L_n^a(y) \sim \frac{1}{\sqrt{\pi}} e^{y/2} y^{-a/2 - 1/4} n^{a/2 - 1/4} \cos\left(2\sqrt{ny} - \frac{a\pi}{2} - \frac{\pi}{4}\right),$$
 (13)

with $y = k^2/(2\alpha^2)$, n = M and a = d, to equation (12), one obtains

$$n^{(d)}(k,M) \sim \frac{2^{d/2+5/4} \alpha^{d+1/2} M^{d/2-1/4}}{\sqrt{\pi} k^{d+1/2}} \cos\left(\frac{k}{\alpha} \sqrt{2M} - \left(\frac{d}{2} + \frac{1}{4}\right)\pi\right).$$
(14)

Remark the oscillating behavior of $n^{(d)}(k, M)$, a fact that already appears, although not for big values of k, in the curves of figure 1.

3. The density profile in Fourier space at finite temperature

In the following we shall derive the expression of the Fourier transform of the particle density at nonzero temperatures. Using the grand canonical ensemble, the one-particle density, in coordinate space, of a noninteracting fermion gas in a d-dimensional harmonic trap at temperature T, is simply given by

$$\rho_T^{(d)}(\mathbf{r}) = 2 \sum_{n=0}^{\infty} f(n) \sum_{n_1 + \dots + n_d = n} \left| \varphi_{n_1}(x_1) \varphi_{n_2}(x_2) \cdots \varphi_{n_d}(x_d) \right|^2,$$
(15)

where

$$f(n) = \left[\exp\left(\frac{\epsilon_n - \mu}{k_B T}\right) + 1\right]^{-1}$$
(16)

are the Fermi–Dirac occupation numbers, with $\epsilon_n = \hbar \omega (n + d/2)$ and μ the chemical potential. Equation (15) is the generalization to finite temperature of equation (1). It should be noted that closed analytical expressions for the density (15) have been obtained [8, 9]. Let us now come to the density profile $n_T^{(d)}(k)$ in Fourier space at nonzero temperatures. Its calculation is entirely analogous to the zero temperature case, the main difference here being that we cannot eliminate the summation over the entire energy spectrum. Using obvious notations, one finds

$$n_T^{(d)}(k) = 2 \exp\left(-\frac{k^2}{4\alpha^2}\right) \sum_{n=0}^{\infty} L_n^{d-1}\left(\frac{k^2}{2\alpha^2}\right) \frac{1}{\exp\left(\frac{\epsilon_n - \mu}{k_B T}\right) + 1}.$$
 (17)

Putting k = 0 in equation (17) and using the fact that $n_T^{(d)}(0) = N$, we obtain the normalization condition from which the chemical potential μ can be obtained, that is,

$$N = 2\sum_{n=0}^{\infty} \frac{L_n^{d-1}(0)}{\exp\left(\frac{\epsilon_n - \mu}{k_B T}\right) + 1}.$$
(18)

Here, the physical meaning of $L_n^{d-1}(0) = \binom{n+d-1}{d-1}$ is nothing but the degeneracy of the *n*th energy level.

Although the derivations of equations (12) and (17) for arbitrary dimensions are simple, to our knowledge, they seem not to have been reported before in the literature except, as previously mentioned, the result given in equation (8) for the case d = 1 at T = 0. In what follows, we will show that the Fourier transform of the particle density has a relevant role in some physical applications.

4. Applications

4.1. Weakly-interacting Fermi gas

A nearly ideal Fermi gas composed of atoms cooled down to a fraction of the Fermi temperature has been achieved experimentally [1, 11]. Such ultracold atomic gas constitutes a dilute system in which the interparticle interactions are weak and readily treated theoretically. Here, we propose to calculate, to the first order of perturbation theory, the total interaction energy term of a very dilute, weakly-interacting Fermi gas. Such a cloud is supposed to be confined by a spherical harmonic trap in *d* dimensions and the atoms are supposed to interact via a two-body attractive delta interaction.

Let us consider the Hamiltonian of the N fermion atoms of mass m of the form

$$H = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 r_i^2 \right) + V_{\text{int}},$$
(19)

where

$$V_{\text{int}} = g \sum_{i < j} \delta(\mathbf{r}_i - \mathbf{r}_j).$$
⁽²⁰⁾

Here the index *i* labels the particles and *g* is the coupling constant of the two-body zero range interaction. In the following we will calculate the total interaction energy in the mean-field Hartree–Fock theory. Let $|\Phi\rangle$ denote the ground state wavefunction of the hamiltonian *H*. The expectation value, $\Delta E_{T=0}^{(d)} = \langle \Phi | V_{\text{int}} | \Phi \rangle$ of V_{int} , represents the total interaction energy. In the mean-field Hartree–Fock theory [15], where the state $|\Phi\rangle$ is a Slater determinant, one has

$$\Delta E_{T=0}^{(d)} = \frac{g}{4} \int \left| \rho_{\text{int}}^{(d)}(r) \right|^2 \mathrm{d}r = \frac{g}{4} \int \left| n_{\text{int}}^{(d)}(k) \right|^2 \frac{\mathrm{d}k}{(2\pi)^d}$$
(21)

where we have used the Parseval theorem. Here, $\rho_{\text{int}}^{(d)}$ and $n_{\text{int}}^{(d)}$ refer to the densities of the full Hamiltonian (19). But if the system is very dilute ($g \ll 1$), we may use for these latter densities the unperturbed expressions (the noninteracting ones) given in the previous sections. Therefore, upon inserting equation (12) into (21), one obtains at zero temperature

$$\Delta E_{T=0}^{(d)} = g \int \exp\left(-\frac{k^2}{2\alpha^2}\right) \left[L_M^d\left(\frac{k^2}{2\alpha^2}\right)\right]^2 \frac{\mathrm{d}k}{(2\pi)^d}.$$
(22)

Due to the spherical symmetry of the problem, we have $d\mathbf{k} = \frac{2\pi^{d/2}}{\Gamma(d/2)}k^{d-1} dk$, with $k \ge 0$. Then equation (22) becomes

$$\Delta E_{T=0}^{(d)} = g \frac{2\pi^{d/2}}{\Gamma(d/2)} \int_0^\infty \frac{k^{d-1}}{(2\pi)^d} \exp\left(-\frac{k^2}{2\alpha^2}\right) \left[L_M^d\left(\frac{k^2}{2\alpha^2}\right)\right]^2 dk$$
$$= g \frac{\pi^{d/2} \alpha^d 2^{d/2}}{(2\pi)^d \Gamma(d/2)} \int_0^\infty u^{d/2-1} e^{-u} \left[L_M^d(u)\right]^2 du$$
(23)

where we have made the change of the variable $u = k^2/(2\alpha^2)$. If we use [14]

$$L_{M}^{d}(u) = \sum_{n=0}^{M} \frac{\Gamma(d/2+n+1)}{n!\Gamma(d/2+1)} L_{M-n}^{d/2-1}(u),$$
(24)

the integral in (23) can be carried out analytically, to obtain

$$\Delta E_{T=0}^{(d)} = g \frac{4\alpha^d}{d^2 (2\pi)^{d/2} \Gamma^3(d/2)} \sum_{n=0}^M \left(\frac{\Gamma(d/2+n+1)}{n!}\right)^2 \frac{\Gamma(d/2+M-n)}{(M-n)!},\tag{25}$$

where we have used the fact that the crossed terms of the double sum vanish due to the orthogonality property [14]

$$\int_{0}^{\infty} e^{-u} u^{q} L_{n}^{q}(u) L_{m}^{q}(u) du = \frac{\Gamma(q+n+1)}{n!} \delta_{n,m}.$$
 (26)

In two dimensions the analytical expression of equation (25) turns out to be very simple. Indeed, from equation (25), one finds

$$\Delta E_{T=0}^{(2)} = g \frac{\alpha^2}{2\pi} \sum_{n=0}^{M} (n+1)^2 = g \frac{\alpha^2}{12\pi} (M+1)(M+2)(2M+3).$$
(27)

In a similar way to that done for the T = 0 case, if we insert equation (17) into equation (21), we will obtain, after some straightforward calculations, the following finite temperature version of equation (25):

$$\Delta E_T^{(d)} = \frac{g\alpha^d}{(2\pi)^{d/2}\Gamma^3(d/2)} \times \sum_{n=0}^{\infty} \sum_{m=0}^n \sum_{p=n-m}^\infty f(n)f(p) \frac{\Gamma(d/2+m)\Gamma(d/2+p-n+m)\Gamma(d/2+n-m)}{m!(p-n+m)!(n-m)!}, \quad (28)$$

where f(n) is the occupation number given in equation (16). Now, let us write down the above expression in the d = 2 case:

$$\Delta E_T^{(d)} = g \frac{\alpha^2}{2\pi} \sum_{n=0}^{\infty} \sum_{m=0}^n \sum_{p=n-m}^{\infty} f(n) f(p) = g \frac{\alpha^2}{2\pi} \sum_{n=0}^{\infty} \left(\sum_{p=n}^{\infty} f(p) \right)^2.$$
(29)

It can be easily verified that, in the $T \to 0$ limit, equation (29) reduces to its zero temperature limit given in equation (27) since the Fermi distribution f(k) becomes the Heaviside step function $\Theta(\lambda - k - d/2)$, λ being the Fermi energy given for the case of M + 1 filled shells by $\lambda = M + d/2$.

4.2. Elastic particle scattering from atomic nuclei

The Fourier transform defined in equation (3) is nothing but the so-called scattering form factor $F(\mathbf{k}) \equiv n(\mathbf{k})$ and appears in the expression of the elastic differential cross section $(d\sigma/d\Omega)$. For example, in the context of nuclear structure, the elastic scattering of electrons from atomic nuclei are used to probe the nuclear charge distribution. In the Born approximation, and using obvious notations, one has [16]

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right) = \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_0 |F(k)|^2 \tag{30}$$

where $(d\sigma/d\Omega)_0$ is the point-like differential cross section, and $k = k_i - k_f$, with k, k_i and k_f being, respectively, the transferred, the initial and the final momenta of the electron. Despite its limitations the nuclear shell model using the three-dimensional harmonic oscillator wavefunctions has been widely used to describe the light closed shell nuclei. Now, using the result given in equation (12) with equation (30), one obtains

$$\left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right) = 4 \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right)_0 \,\mathrm{e}^{-\frac{k^2}{2\alpha^2}} \left| L_M^3 \left(\frac{k^2}{2\alpha^2}\right) \right|^2. \tag{31}$$

Hence, the differential cross section of the above problem is now expressed in a completely analytical form and this result should be added to the short list of exactly solvable models in scattering theory. From another point of view, this is also an interesting practical quantum mechanical exercise for students.

5. Fourier transform of the momentum density for *d*-dimensional harmonic confinement

In the previous sections we have studied the structure of the Fourier transform $n^{(d)}(k)$ of $\rho^{(d)}(r)$. Another interesting distribution function which has been introduced in [17] is the Fourier transform $\tilde{\rho}^{(d)}(r)$ of the momentum distribution $F^{(d)}(p)$; the latter will be defined below. It has been shown that $\tilde{\rho}^{(d)}(r)$ can be used to obtain the total kinetic energy, which is an important ingredient in density functional theory [15, 18]. Such an alternative route to the total kinetic energy is set out in [17]. Here we are only interested in the analytical form of $\tilde{\rho}^{(d)}(r)$ in the case of harmonic confinement in *d* dimensions and at T = 0. We shall obtain a simple analytical expression for such density which resemble to the form of $n^{(d)}(k)$ given in equation (12). This is due to the symmetry on the interchange of the variables *p* and *r* in the harmonic oscillator Hamiltonian.

For the case of the *d*-dimensional harmonic oscillator, the momentum distribution $F^{(d)}(p)$ is defined by a similar relation to that in equation (1), where one has to convert the normalized r space wavefunctions $\varphi_{n_i}(x_j)$ into their analogues $\phi_{n_i}(p_j)$ in momentum space, that is,

$$F^{(d)}(\boldsymbol{p}, M) = 2 \sum_{n=0}^{M} \sum_{n_1 + \dots + n_d = n} \left| \phi_{n_1}(p_1) \cdots \phi_{n_d}(p_d) \right|^2$$
(32)

with $\varphi_n(p_i) = \exp\left(-\beta^2 p_i^2/2\right) H_n(\beta p_i)(\beta/(2^n n!\sqrt{\pi}))^{1/2}$ is the one-dimensional harmonic oscillator wavefunction in momentum space with $\beta = (\hbar \alpha)^{-1} = 1/(\hbar m \omega)^{1/2}$. Since the analytical form for such a wavefunction is similar to the one in r space, following the same derivation as given in section 1, we then obtain for the Fourier transform $\tilde{\rho}^{(d)}(r)$ of $F^{(d)}(p)$,

$$\widetilde{\rho}^{(d)}(r) = \int F^{(d)}(p) \,\mathrm{e}^{\mathrm{i}\frac{p\,r}{\hbar}} \,\mathrm{d}p,\tag{33}$$

the simple form

$$\widetilde{\rho}^{(d)}(r,M) = 2 \exp\left(-\frac{m\omega r^2}{4\hbar}\right) L_M^d\left(\frac{m\omega r^2}{2\hbar}\right).$$
(34)

6. Summary

In the present work, we have shown that the density profile in Fourier space for a d-dimensional harmonically confined quantum gas has a simple closed form compared to its r-space counterpart at zero and nonzero temperatures. Using such results, we have obtained, to the first order in perturbation theory, a compact analytical expression for the total two-body interaction energy of a very dilute weakly-interacting atom gas. These results may be useful in the study of the radiation light scattered from harmonically confined quantum gases [19]. A simple application to elastic scattering theory is also done, showing an example where the exact result for the differential cross section can be obtained.

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