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Harmonically trapped fermion gases: exact and asymptotic results in arbitrary dimensions

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Abstract

We investigate the particle and kinetic energy densities of harmonically trapped fermion gases at zero temperature in arbitrary dimensions. We derive differential equations connecting these densities, which so far have been proved only in one or two dimensions, and give other interesting relations involving several densities or the particle density alone. We show that in the asymptotic limit of large particle numbers, the densities go over into the semi-classical Thomas–Fermi (TF) densities. Hereby the Fermi energy to be used in the TF densities is uniquely identified. We derive an analytical expansion for the remaining oscillating parts and obtain very simple closed forms for the leading-order oscillating densities. Finally, we show that the simple TF functional relation $\tau_{\text{TF}}[\rho]$ between kinetic and particle densities is also fulfilled for the asymptotic quantum densities $\tau(r)$ and $\rho(r)$ including their leading-order oscillating terms.

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1. Introduction

The recent experimental success in confining degenerate Fermi gases in magnetic traps [1] has triggered a renewed interest in the theoretical description of the particle and kinetic energy densities of harmonically trapped fermions, both at zero [2–8] and finite temperatures [9, 10]. Whereas most of these investigations were limited to $d = 1, 2$ or 3 dimensional systems, general analytical expressions for the particle and kinetic energy densities valid for any dimension d were given in [4, 10]. This paper is devoted to a discussion of exact and asymptotic results for particle and kinetic energy densities in arbitrary dimensions. We put an emphasis on separating their smooth and oscillating parts, identifying analytically the smooth parts with those obtained in the semi-classical Thomas–Fermi (TF) limit, and finding simple closed expressions for the asymptotically leading oscillating parts. Using the latter, we find that the TF functional relation $\tau_{\text{TF}}[\rho]$ between kinetic and particle densities also holds for

the densities including the leading-order quantum oscillations, confirming a recent numerical observation [4] of this surprising result.

We start by recapitulating some basic definitions given in [4]. We consider a system of N spin-1/2 fermions, trapped in a spherical harmonic potential in d dimensions

$$V(r) = \frac{m\omega^2}{2}r^2 \quad r^2 = x_1^2 + x_2^2 + \cdots + x_d^2. \quad (1)$$

We assume that the lowest $M + 1$ shells are filled, so that the ground state is non-degenerate. The local density then depends only on the radial variable r and is given in terms of the wavefunctions $\phi_i(\mathbf{r})$ by

$$\rho(r) = 2 \sum_{\epsilon_i \leq E_F} |\phi_i(\mathbf{r})|^2 \quad (2)$$

where the Fermi energy E_F can be identified with the highest filled level, $E_F = \epsilon_M = M + d/2$, and a spin degeneracy factor of 2 has been included. For the kinetic energy density, we consider the two equivalent expressions

$$\tau(r) = -\frac{\hbar^2}{2m} 2 \sum_{\epsilon_i \leq E_F} \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) \quad (3)$$

$$\tau_1(r) = \frac{\hbar^2}{2m} 2 \sum_{\epsilon_i \leq E_F} |\nabla \phi_i(\mathbf{r})|^2. \quad (4)$$

(Note that in the standard literature on density functional theory, $\tau(r)$ sometimes denotes the quantity which we call here $\tau_1(r)$.) In the presence of time-reversal symmetry (which implies the particle number N to be even), they are simply related by

$$\tau(r) = \tau_1(r) - \frac{1}{2} \frac{\hbar^2}{2m} \nabla^2 \rho(r). \quad (5)$$

A convenient quantity is their average

$$\xi(r) = \frac{1}{2} [\tau(r) + \tau_1(r)] \quad (6)$$

which is numerically known [4, 11] to be a smooth function whereas $\tau(r)$ and $\tau_1(r)$ have oscillations that are opposite in phase (see also figure 2). We can then express $\tau(r)$ and $\tau_1(r)$ in terms of $\xi(r)$ and $\nabla^2 \rho(r)$:

$$\tau(r) = \xi(r) - \frac{1}{4} \frac{\hbar^2}{2m} \nabla^2 \rho(r) \quad \tau_1(r) = \xi(r) + \frac{1}{4} \frac{\hbar^2}{2m} \nabla^2 \rho(r). \quad (7)$$

Equations (2)–(7) are exact expressions; for a given number of particles or filled shells in any dimension they can be computed exactly using the known quantum-mechanical wavefunctions.

It is well-known numerically that for large particle numbers, the exact densities go over to the smooth TF densities, as also demonstrated in the following two figures. In figure 1, we compare exact particle densities $\rho(r)$ with those of the TF model (see section 4 for their precise definition) for two particular cases in two and three dimensions. In figure 2, we show a comparison between the three forms (3), (4) and (6) of the kinetic energy density, along with that of the TF model. In all cases, the exact quantum-mechanical densities oscillate around the TF densities except near the turning points where the latter go to zero by definition. In particular, the two densities $\tau(r)$ and $\tau_1(r)$ have oscillations with exactly opposite phase, which renders their average $\xi(r)$ smooth, following very closely the TF kinetic energy density.

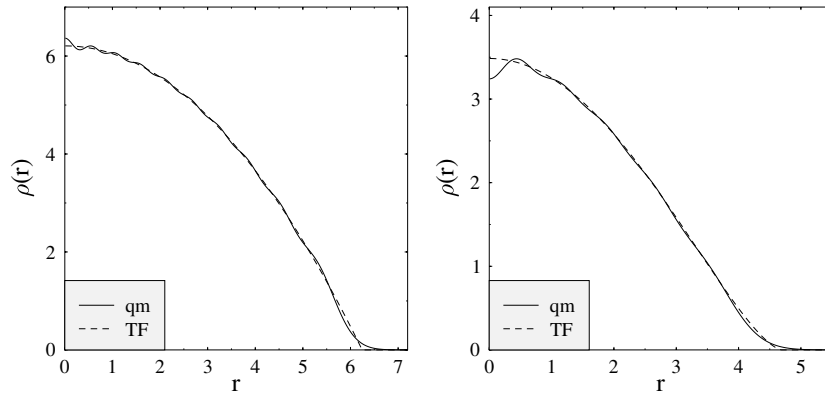


Figure 1. Particle densities of fermions in harmonic traps. The left panel shows $N = 380$ particles filling 19 shells ($M = 18$) in 2D and the right panel $N = 440$ particles filling 10 shells ($M = 9$) in 3D. The solid lines give exact quantum-mechanical densities $\rho(r)$, and the dashed lines Thomas–Fermi densities $\rho_{\text{TF}}(r)$.

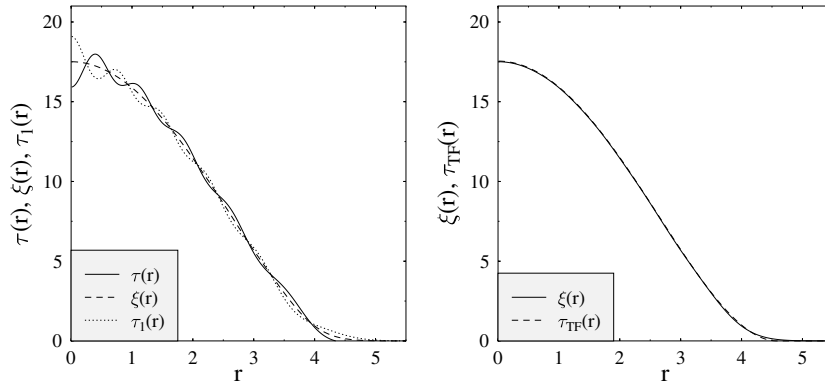


Figure 2. Kinetic energy densities of $N = 110$ fermions ($M = 9$) in a 2D harmonic trap. Left panel: three equivalent quantum-mechanical densities integrating to the exact kinetic energy. Right panel: $\xi(r)$ and Thomas–Fermi density $\tau_{\text{TF}}(r)$.

This paper is devoted to examining various issues related to the correspondence between the exact quantum-mechanical densities and their TF limits, which in the framework of density functional theory correspond to the local density approximation (LDA). We first derive a homogeneous differential equation for the particle density $\rho(r)$, linking it to the kinetic energy density $\xi(r)$ in arbitrary dimensions. This has been one of the challenges in the density functional theory and has only been proved recently [5] in $d = 2$. An interesting consequence of this equation is that the Fermi energy to be used in the TF model is given analytically in terms of the number M of the highest filled shell.

The surprising success of the TF or LDA formalism in reproducing the averaged quantum-mechanical results nearly all the way down to the turning point raises an important question about the domain of validity of the TF approximation. We examine this question in detail. Using a Taylor expansion of the exact densities we show that the leading-order terms in the limit of large particle numbers or, equivalently, large Fermi energies reproduce exactly the TF densities. Furthermore, both smooth and oscillating corrections to the TF limits can be

gleaned from the Taylor expansions. We also use a calculation of the moments of the densities to buttress our conclusions. While the smooth parts may easily be given exactly for even dimensions, they are harder to obtain in odd dimensions, necessitating the asymptotic Stirling expansion of Gamma functions. Nevertheless, the leading-order results and their corrections provide clear pointers to an understanding of the numerical results. In particular, we succeed in extracting the asymptotically leading-order oscillating terms of the densities in a very simple closed analytical form valid for any dimension. The limitations of these asymptotic terms, and interesting relations between them, are investigated numerically.

The rest of this paper is organized as follows. In section 2, we give explicit expressions for the densities using the definitions given above. Some of the results are already contained in [4] but are simplified here and given explicitly, in order to make further analytical calculations more transparent. Section 3 is devoted to the derivation of exact differential equations, valid in arbitrary dimensions, that connect the kinetic energy and particle densities, and of an equivalent integro-differential equation for the particle density that has the form of a Schrödinger-type eigenvalue equation. In section 4, we discuss the asymptotic limits of the exact densities for large Fermi energies λ and discuss their precise relation with the TF densities. What emerges clearly from this analysis is that the densities can be uniquely separated into smooth and oscillating parts. The two leading-order terms in λ of the smooth parts constitute analytically the TF densities, whereas the oscillating parts are of relative order $1/\lambda$ (or lower), so that they vanish in the asymptotic limit. In section 5, we discuss the oscillating parts of the exact densities. In particular, we show that their leading-order contributions, which for any dimension can be given analytically in terms of Bessel functions, are eigenfunctions of the radial Laplace operator. The TF functional $\tau_{\text{TF}}[\rho]$ is shown to hold for the asymptotic densities including the leading-order oscillating terms. The full oscillating parts of the densities can be expanded as series of higher-order Bessel functions, which we exhibit analytically for even dimensions. Some numerical tests of our asymptotic relations are presented in section 5.4. In section 6, we finally present a summary of all the new results obtained in this paper. Some technical details are given in three appendices.

2. Analytical densities for filled spherical shells

Following the general definitions given in the previous section, we quote here the exact expressions for the densities derived in [4] and give some new and more general analytical expressions which serve as starting points for the following investigations. In the remainder of this paper, we work throughout with dimensionless units corresponding to the choice $m = \omega = \hbar = 1$. The exact quantum-mechanical densities $\rho(r)$ and $\xi(r)$ can be written [4], for a given number M of the last filled shell, in the simple form

$$\rho(r, M) = \frac{1}{\pi^{d/2}} 2 \sum_{\mu=0}^M F_{M-\mu}^{(d)} (-1)^\mu L_\mu(2x) e^{-x} \quad (8)$$

$$\xi(r, M) = \frac{1}{\pi^{d/2}} \frac{d}{2} \sum_{\mu=0}^M G_{M-\mu}^{(d)} (-1)^\mu L_\mu(2x) e^{-x} \quad (9)$$

where $x = r^2$ and $L_\mu(2x)$ are Laguerre polynomials. The coefficients $F_\nu^{(d)}$, $G_\nu^{(d)}$ are given by

$$F_\nu^{(d)} = \nu + 1 + \sum_{m=1}^{[\nu/2]} (\nu + 1 - 2m) g_m^{(d)} \quad G_\nu^{(d)} = (\nu + 1)^2 + \sum_{m=1}^{[\nu/2]} (\nu + 1 - 2m)^2 g_m^{(d)} \quad (10)$$

where $[v/2] \equiv \text{integer}(v/2)$. The factors $g_m^{(d)}$ are defined through

$$(1-x)^{(1-d/2)} = 1 + \sum_{m=1}^{\infty} g_m^{(d)} x^m \implies g_m^{(d)} = \frac{1}{m!} \frac{\Gamma(d/2 + m - 1)}{\Gamma(d/2 - 1)}. \quad (11)$$

The results are particularly simple for $d = 2$, where all the $g_m^{(2)}$ are identically zero:

$$F_v^{(2)} = v + 1 \quad G_v^{(2)} = (v + 1)^2. \quad (12)$$

In [4] it was stated that $F_v^{(d)}$ and $G_v^{(d)}$ can be given in closed analytical form only for even dimensions. We have now found³ that this actually can be done in any dimension d , albeit separately for even and odd indices:

$$F_{2n}^{(d)} = (d/2 + 2n) \frac{\Gamma(d/2 + n)}{n! \Gamma(d/2 + 1)} \quad F_{2n+1}^{(d)} = 2 \frac{\Gamma(d/2 + n + 1)}{n! \Gamma(d/2 + 1)} \quad (13)$$

$$G_{2n}^{(d)} = \frac{1}{4} (32n^2 + d^2 + 16nd + 2d) \frac{\Gamma(d/2 + n)}{n! \Gamma(d/2 + 2)} \quad G_{2n+1}^{(d)} = 2(4n + d + 2) \frac{\Gamma(d/2 + n + 1)}{n! \Gamma(d/2 + 2)}. \quad (14)$$

From (13) one finds that the $F_v^{(d)}$ obey the following summation relations:

$$2 \sum_{\nu=0}^M (-1)^{M-\nu} F_{\nu}^{(d)} = F_{M+1}^{(d)} \quad (M \text{ even}) \quad 2 \sum_{\nu=0}^M (-1)^{M-\nu} F_{\nu}^{(d)} = F_M^{(d)} \quad (M \text{ odd}). \quad (15)$$

Using the above formulae, we can readily give closed expressions for the densities at $r = 0$. For even and odd M , respectively, we get for the particle densities

$$\begin{aligned} \rho_{\text{even}}(0, M) &= \frac{2}{\pi^{d/2}} \frac{\Gamma(M/2 + d/2 + 1)}{\Gamma(d/2 + 1) \Gamma(M/2 + 1)} = \frac{2}{\pi^{d/2}} \frac{(M+d)!!}{d!! M!!} \quad (M \text{ even}) \\ \rho_{\text{odd}}(0, M) &= \frac{2}{\pi^{d/2}} \frac{\Gamma(M/2 + d/2 + 1/2)}{\Gamma(d/2 + 1) \Gamma(M/2 + 1/2)} = \frac{2}{\pi^{d/2}} \frac{(M-1+d)!!}{d!! (M-1)!!} \quad (M \text{ odd}) \end{aligned} \quad (16)$$

and for the kinetic energy densities

$$\begin{aligned} \xi_{\text{even}}(0, M) &= \frac{(4M + d + 2)}{(d + 2)} \rho_{\text{even}}(0, M) \\ \xi_{\text{odd}}(0, M) &= \frac{(4M + 3d + 2)}{(d + 2)} \rho_{\text{odd}}(0, M). \end{aligned} \quad (17)$$

On the right-hand sides in (16), which are easier to evaluate manually, we have used the double factorials defined (for integer n) by

$$\begin{aligned} (2n)!! &= 2n(2n-2) \cdots 2 = \sqrt{\pi} \Gamma(2n+1)/2^n \Gamma(n+1/2) & 0!! &= 1 \\ (2n-1)!! &= (2n-1)(2n-3) \cdots 1 = 2^n \Gamma(n+1/2)/\sqrt{\pi} & (-1)!! &= 1. \end{aligned} \quad (18)$$

Note that the densities (16) for any even M and the next odd $M + 1$ are identical. This is due to the alternating parities of the quantum states in successive shells. While filling a shell with odd parity (i.e. odd $M + 1$), no contribution is added to the density $\rho_{\text{even}}(r, M)$ at $r = 0$. For even dimensions d , expressions (16) and (17) reduce to polynomials of order $d/2$ and $d/2 + 1$ in M , respectively. For odd d , they can be simplified only in the large- M limit discussed in section 4.

³ We have used the mathematical software package Maple[®].

For later reference, we give here also the total particle number N and energy E as functions of the shell number M , making use of the fact that the degeneracy of the m th level $\epsilon_m = m + d/2$ is given by the binomial coefficient $\binom{m+d-1}{d-1}$:

$$N(M) = 2 \sum_{m=0}^M \binom{m+d-1}{d-1} = 2 \binom{M+d}{M} = 2 \frac{(M+d)!}{d!M!} \quad (19)$$

$$E(M) = 2 \sum_{m=0}^M \binom{m+d-1}{d-1} (m+d/2) = d(2M+d+1) \frac{(M+d)!}{(d+1)!M!}. \quad (20)$$

3. Exact differential equations for densities in arbitrary dimensions

As stated by Minguzzi *et al* [5], one of the challenges in density functional theory is to be able to directly calculate the particle density, given the potential energy, without recourse to solving the Schrödinger equation for the wavefunctions. They have achieved this aim for harmonic confinement of independent fermions in $d = 2$. The central result of their paper [5] is the following differential equation for the density

$$\xi(r) = \frac{1}{2} \left[\frac{1}{8} \Delta \rho(r) + \rho(r) \left(M + \frac{3}{2} - \frac{1}{2} r^2 \right) \right] \quad (21)$$

where Δ is the Laplacian operator $\Delta = \nabla^2$ in two dimensions.

Indeed, we now prove that such a differential equation may be derived in arbitrary dimension d . Furthermore, using a ‘differential virial theorem’ derived recently [10] for any d , we show that a linear, homogeneous third-order differential equation for the particle density may be established in arbitrary dimensions, as has been done [5] in the case of $d = 2$.

In order to proceed, we note that the radial part of the Laplacian in d dimensions is given by

$$\Delta = \frac{d^2}{dr^2} + \frac{(d-1)}{r} \frac{d}{dr}. \quad (22)$$

For the following derivation it is useful to express it in terms of the variable $x = r^2$:

$$\Delta = 4x \frac{d^2}{dx^2} + 2d \frac{d}{dx}. \quad (23)$$

The Laplacian acting on the particle density (8) is given by

$$\Delta \rho(x) = \frac{1}{\pi^{d/2}} 2 \sum_{\mu=0}^M F_{M-\mu}^{(d)} (-1)^\mu [(4x - 2d - 8\mu)L_\mu(2x) + (4d - 8)L'_\mu(2x)] e^{-x} \quad (24)$$

where we have made use of the differential equation for the Laguerre polynomials [12]

$$yL''_\mu(y) + (1-y)L'_\mu(y) + \mu L_\mu(y) = 0 \quad (25)$$

and the primes denote the derivatives with respect to the full argument of a function. Manipulating the sums in (24), we obtain

$$\frac{1}{8} \Delta \rho(x) + (M + 1 + d/4 - x/2) \rho(x) = \frac{4}{d} \xi(x) + \mathcal{R}(x) \quad (26)$$

where $\mathcal{R}(x)$ is given by

$$\mathcal{R}(x) = \frac{2}{\pi^{d/2}} \sum_{\mu=0}^M (-1)^\mu \left\{ [(M+1-\mu)F_{M-\mu}^{(d)} - G_{M-\mu}^{(d)}]L_\mu(2x) + (d/2-1)F_{M-\mu}^{(d)}L'_\mu(2x) \right\} e^{-x}. \quad (27)$$

Note that $\mathcal{R}(x)$ is identically zero for $d=2$, due to (12), so that (26) reduces readily to (21). For arbitrary dimensions d , now, $\mathcal{R}(x)$ can be cast into the following form (see appendix A for details):

$$\mathcal{R}(x) = \frac{(d-2)}{d}\xi(x) - \frac{(d-2)}{4}\rho(x). \quad (28)$$

Substituting this into (26), we arrive at the differential equation

$$\xi(r) = \frac{d}{(d+2)} \left[\frac{1}{8}\Delta\rho(r) + \rho(r) \left(\lambda_M - \frac{1}{2}r^2 \right) \right] \quad (29)$$

which is valid for any d and obviously reduces to (21) for $d=2$ as given in [5]. Here λ_M is given by

$$\lambda_M = M + (d+1)/2 \quad (30)$$

which corresponds to the average of the highest filled and the lowest unfilled level and will be identified as the Fermi energy of the smooth densities in the large- M limit (see section 4).

Having established equation (29), we now proceed to derive equations for the particle density alone by eliminating the kinetic energy density $\xi(r)$. To this end we use an integral equation which has recently been derived in [10] for arbitrary dimensions d , and its equivalent differential form:

$$\xi(r) = \frac{d}{2} \int_r^\infty r' \rho(r') dr' \iff \frac{d}{dr}\xi(r) = -\frac{d}{2}r\rho(r) \iff \frac{d}{dx}\xi(x) = -\frac{d}{4}\rho(x). \quad (31)$$

The differential form had earlier been derived for $d=2$ in [5] and termed ‘differential virial theorem’. Its version for $d=3$ had been correctly guessed in [6]. Inserting the integral form of $\xi(r)$ into (29), we obtain the following integro-differential equation for $\rho(r)$ with eigenvalue λ_M :

$$-\frac{1}{8}\Delta\rho(r) + \frac{1}{2}r^2\rho(r) + \frac{(d+2)}{2} \int_r^\infty r' \rho(r') dr' = \lambda_M\rho(r). \quad (32)$$

This has the form of a Schrödinger equation for $\rho(r)$ with an additional non-local potential. Differentiating both sides of (32), we can write it as a third-order differential equation for $\rho(r)$:

$$\frac{1}{8} \frac{d}{dr} \Delta\rho(r) + \left(\lambda_M - \frac{1}{2}r^2 \right) \frac{d}{dr} \rho(r) + \frac{d}{2}r\rho(r) = 0. \quad (33)$$

This equation has been previously derived for $d=1$ in [13] and for $d=2$ in [5]. Its form for $d=3$ has been surmised and numerically tested in [6], and general solutions for $\rho(r)$ in the case $d=3$ were discussed in [8].

Using relation (7), we may eliminate the Laplacian term in (29) in favour of the kinetic energy density $\tau(r)$ to obtain the following exact relation between the three densities:

$$\tau(r) = \rho(r) \left(\lambda_M - \frac{1}{2}r^2 \right) - \frac{2}{d}\xi(r) \quad (34)$$

which will prove useful in the discussion of section 5.

Integrating the differential equation (29) over the whole space, using the measure

$$\int d^d r(\dots) = \frac{\pi^{d/2}}{\Gamma(d/2)} \int_0^\infty x^{d/2-1} dx(\dots) \quad (35)$$

and exploiting the virial theorem, we find

$$\lambda_M N(M) = \frac{d+1}{d} E(M) \quad (36)$$

which using (19) and (20) unambiguously confirms the choice of the Fermi energy (30).

4. Large- M limits and relation with the Thomas–Fermi densities

We next address the question as to how the well-known Thomas–Fermi (TF) results are obtained from the exact densities (8), (9) in the limit of large particle numbers or, equivalently, in the large- M limit. The TF densities are given by (see e.g. chapter 4 in [15])

$$\rho_{\text{TF}}(r, \lambda) = \frac{1}{(2\pi)^{d/2}} \frac{4}{d} \frac{1}{\Gamma(\frac{d}{2})} (\lambda - r^2/2)^{d/2} \Theta(\lambda - r^2/2) \quad (37)$$

$$\xi_{\text{TF}}(r, \lambda) = \tau_{\text{TF}}(r, \lambda) = \frac{1}{(2\pi)^{d/2}} \frac{4}{(d+2)} \frac{1}{\Gamma(\frac{d}{2})} (\lambda - r^2/2)^{d/2+1} \Theta(\lambda - r^2/2) \quad (38)$$

where λ is a Fermi energy that is usually determined by normalizing $\rho_{\text{TF}}(r, \lambda)$ to the exact particle number N . The Heaviside step function $\Theta(\lambda - r^2/2)$ ensures that these densities are identically zero outside the classical turning point $r_0 = \sqrt{2\lambda}$.

The proof that the above TF densities can be obtained from the exact quantum-mechanical densities in the large- M limit is by no means trivial, since the summations in (8) and (9) cannot be done analytically in closed form. To our knowledge, a rigorous proof for $d = 2$ has been given only very recently in [10], whereby λ was found to be $\lambda = M + 3/2$. In [3] it was shown for $d = 1$ that the exact density at $r = 0$ is asymptotically given by $\rho_{\text{TF}}(0)$ for large particle numbers, and an expression for the leading-order oscillating part $\delta\rho(x) = \rho(x) - \rho_{\text{TF}}(x)$, valid for small enough x , was given.

We first observe that the differential equation (29) is also satisfied by the corresponding TF densities in the limit of large M , and hence of large λ_M , since the Laplacian acting on the TF density produces terms of lower order in λ_M . In the following we shall show, indeed, that for any dimension d the exact densities given in (8) and (9) in the large- M limit go over into the TF functions (37) and (38), plus smooth corrections of order $1/M^2$ relative to the leading-order TF terms, plus oscillating terms that are of relative order $1/M$ or lower and will be discussed in section 5. Hereby it is essential that the Fermi energy λ be identified with the λ_M given in (30). Whereas the proof given in [10] for $d = 2$ can easily be generalized to any even d (see section 5 and appendix C), the cases with odd d turn out to be more difficult to handle. We will first discuss the separation of smooth and oscillating parts in general. In the two ensuing subsections, we shall then use Taylor expansions of the exact densities and a calculation of their moments in order to prove our claims.

4.1. Separation of smooth and oscillating terms

For the following discussions, it is useful to separate the densities into average and oscillating parts:

$$\rho(r) = \bar{\rho}(r) + \delta\rho(r) \quad \xi(r) = \bar{\xi}(r) + \delta\xi(r). \quad (39)$$

This can be achieved using the following trick. We define the smooth parts by

$$\begin{aligned}\bar{\rho}(r, M) &= \frac{1}{2}[\rho_{\text{even}}(r, M) + \rho_{\text{odd}}(r, M)] \\ \bar{\xi}(r, M) &= \frac{1}{2}[\xi_{\text{even}}(r, M) + \xi_{\text{odd}}(r, M)]\end{aligned}\quad (40)$$

whereby the formal expressions obtained from (8) and (9) for even and odd M must be taken at the same fixed value of M and inserted on the right-hand sides above, irrespective of M being odd or even. In the same fashion, the oscillating parts are defined by

$$\begin{aligned}\delta\rho(r, M) &= (-1)^M \frac{1}{2}[\rho_{\text{even}}(r, M) - \rho_{\text{odd}}(r, M)] \\ \delta\xi(r, M) &= (-1)^M \frac{1}{2}[\xi_{\text{even}}(r, M) - \xi_{\text{odd}}(r, M)].\end{aligned}\quad (41)$$

The resulting expressions are then valid for either even or odd M . The sign $(-1)^M$ in front of the oscillating terms is easy to understand due to the alternating parities of successive oscillator shells, as discussed in section 2 after equations (16) for the density at $r = 0$. The alternating sign of $\delta\rho(0, M)$ for successive shell numbers M is intimately connected with the oscillating behaviour of $\delta\rho(r, M)$ as a function of r . For even M , it must have a maximum at $r = 0$ since an even shell always contains an s (zero angular momentum) state. After filling the next (odd) shell, it has acquired a minimum, and so on. This is also illustrated in the numerical examples shown in figure 1.

From the explicit results given below it can be verified that inserting (39) into (29), the smooth parts cancel identically and the following differential equation holds for the oscillating parts alone:

$$\delta\xi(r) = \frac{d}{(d+2)} \left[\frac{1}{8} \Delta \delta\rho(r) + \delta\rho(r) \left(\lambda_M - \frac{1}{2} r^2 \right) \right]. \quad (42)$$

Similarly, all smooth terms cancel also from (34), so that we have the equation:

$$\delta\tau(r) = \delta\rho(r) \left(\lambda_M - \frac{1}{2} r^2 \right) - \frac{2}{d} \delta\xi(r). \quad (43)$$

We finally note that the differential equation given in (31) for the full densities holds separately for their smooth and oscillating parts as well as for the TF densities alone:

$$\frac{d}{dr} \bar{\xi}(r) = -\frac{d}{2} r \bar{\rho}(r) \quad \frac{d}{dr} \delta\xi(r) = -\frac{d}{2} r \delta\rho(r) \quad \frac{d}{dr} \xi_{\text{TF}}(r) = -\frac{d}{2} r \rho_{\text{TF}}(r). \quad (44)$$

Let us now look at the densities at the centre of the system, $r = 0$. As stated at the end of section 2, for even dimensions d expressions (16) and (17) for $\rho(0)$ and $\xi(0)$ are polynomials in M of order $d/2$. It is easy to see that the coefficients of their highest power in M are identical with those of $\rho_{\text{TF}}(0, \lambda_M)$ and $\xi_{\text{TF}}(0, \lambda_M)$, respectively, so that the latter become exact in the large- M limit. For odd d , we have to use the Stirling expansion of the Gamma functions in (16), valid for large M (cf [12], equation (6.1.37)), in order to find the same result. It is even more instructive to look separately at the smooth and oscillating parts. We find that in the large- M limit, the smooth parts reproduce the *two* highest powers of M in the corresponding TF densities at $r = 0$ correctly:

$$\begin{aligned}\bar{\rho}(0, M) &= \frac{1}{(2\pi)^{d/2}} \frac{4}{d} \frac{1}{\Gamma(\frac{d}{2})} \lambda_M^{d/2} [1 + \mathcal{O}(1/M^2) + \dots] \\ \bar{\xi}(0, M) &= \frac{1}{(2\pi)^{d/2}} \frac{4}{(d+2)} \frac{1}{\Gamma(\frac{d}{2})} \lambda_M^{d/2+1} [1 + \mathcal{O}(1/M^2) + \dots]\end{aligned}\quad (45)$$

whereby the series in $1/M$ stop at order M^0 for even d . The oscillating parts are found to be

$$\begin{aligned} \delta\rho(0, M) &= (-1)^M \frac{1}{(2\pi)^{d/2}} \frac{1}{\Gamma(\frac{d}{2})} \lambda_M^{d/2-1} [1 + \mathcal{O}(1/M) + \dots] \\ \delta\xi(0, M) &= (-1)^M \frac{1}{(2\pi)^{d/2}} \frac{d(d-2)}{16\Gamma(\frac{d}{2})} \lambda_M^{d/2-2} [1 + \mathcal{O}(1/M) + \dots]. \end{aligned} \tag{46}$$

We see that $\delta\rho(0)$ is of order $1/\lambda_M$ lower than the leading power in the smooth density, whereas the suppression factor in the $\delta\xi(0)$ is $1/\lambda_M^3$. This hints at the numerically known fact that $\xi(r)$ is much smoother than $\rho(r)$.

4.2. Taylor expansion of the densities

We now want to study how the above results extend to $x > 0$. In appendix B, we give the explicit Taylor expansions of the exact densities (8) and (9) in powers of $x = r^2$:

$$\rho^{(d)}(x, M) = \sum_{m=0}^{\infty} \rho^{(m)}(d, M)x^m \quad \xi^{(d)}(x, M) = \sum_{m=0}^{\infty} \xi^{(m)}(d, M)x^m. \tag{47}$$

The expansion coefficients cannot be given in closed form for any d , but must be evaluated separately for even and odd values of M . From these, one can reconstruct separately the expansion coefficients of the smooth and oscillating parts according to (40) and (41).

As shown in detail in appendix B, we find the following structure of the results for even dimensions d . The smooth parts are finite polynomials in x which have exactly the structure of the TF densities (37) and (38), including the step functions that cut these densities at the classical turning point. However, only the two highest powers of M appearing in the coefficients of each power of x agree with those in the corresponding powers of the Fermi energy $\lambda_M = M + (d + 1)/2$ (30) appearing in the TF densities. In other words, the smooth parts go in the large- M limit over into the TF densities plus smooth terms of order $1/M^2$ and lower relative to the leading TF terms:

$$\begin{aligned} \bar{\rho}(r, M) &= \rho_{\text{TF}}(r, \lambda_M)[1 + \mathcal{O}(M^{-2}) + \dots] \\ \bar{\xi}(r, M) &= \xi_{\text{TF}}(r, \lambda_M)[1 + \mathcal{O}(M^{-2}) + \dots] \end{aligned} \tag{48}$$

which is the straightforward extension of (45). To put this structure into evidence, we list here the complete smooth densities for the lowest even dimensions, re-expressed in terms of the Fermi energy. For $d = 2$ we get, with $\lambda = M + 3/2$:

$$\begin{aligned} \bar{\rho}^{(2)}(r) &= \frac{1}{\pi}(\lambda - r^2/2)\Theta(\lambda - r^2/2) \\ \bar{\xi}^{(2)}(r) &= \frac{1}{2\pi}[(\lambda - r^2/2)^2 - 1/4]\Theta(\lambda - r^2/2). \end{aligned} \tag{49}$$

For $d = 4$ we get, with $\lambda = M + 5/2$:

$$\begin{aligned} \bar{\rho}^{(4)}(r) &= \frac{1}{4\pi^2}[(\lambda - r^2/2)^2 - 3/4]\Theta(\lambda - r^2/2) \\ \bar{\xi}^{(4)}(r) &= \frac{1}{6\pi^2}[(\lambda - r^2/2)^3 - 7\lambda/4 + 9r^2/8]\Theta(\lambda - r^2/2). \end{aligned} \tag{50}$$

The oscillating parts, characterized by the alternating sign $(-1)^M$, contain infinite power series in x that can be resummed into oscillating functions of x , as shown in appendix C and further discussed in section 5. After resummation, they are found to be of order $1/M$ or lower, relative to the leading-order terms of the smooth parts, so that they become negligible in the large- M limit.

The situation is more complicated for odd dimensions d . This becomes evident when we compare the powers of π appearing in the denominators of the exact densities (8), (9) and their TF expressions (37), (38): whereas they are the same for even d , they are different by a factor $\sqrt{\pi}$ for odd d . The reason is that in order to obtain the TF densities in the large- M limit, one has to perform a large- M Stirling expansion of the Γ functions in (16), as seen above for $\rho(0)$. In doing so for specific odd values of d , we find that the resulting densities have the same structure as for even d . Their smooth parts yield the Taylor expansions of the TF densities (37), which here are infinite due to the half-integer power $d/2$:

$$\bar{\rho}^{(d)}(r, M) = \rho_{\text{TF}}^{(d)}(0, \lambda) \left[1 - \frac{d}{2} \frac{x}{2\lambda} + \frac{d(d-2)}{8} \left(\frac{x}{2\lambda} \right)^2 - \dots \right] [1 + \mathcal{O}(M^{-2}) + \dots] \quad (51)$$

with $\lambda = \lambda_M$ given in (30), and analogously for the average kinetic energy densities $\bar{\xi}^{(d)}(r, M)$. The oscillating parts are again at least of order $1/M$ relative to the leading smooth parts and therefore vanish in the large- M limit.

Summarizing up to this point, we find that the densities $\rho(r)$ and $\xi(r)$ can be uniquely decomposed into smooth and oscillating parts. In the large- M limit, the smooth parts $\bar{\rho}(r)$ and $\bar{\xi}(r)$ reach their TF forms (37), (38) in terms of the Fermi energy λ_M given in (30), plus terms of relative order $1/M^2$ and lower at each power of x in their Taylor expansions. The oscillating parts $\delta\rho(r)$ and $\delta\xi(r)$ are of order $1/M$ and $1/M^3$, respectively, compared to the leading-order TF terms, as discussed explicitly in section 5. This clearly establishes the TF densities as the asymptotic large- M limits of the exact quantum-mechanical densities.

4.3. Calculation of moments of the densities

As an alternative way to demonstrate the asymptotic equality of the exact and TF densities, we will now calculate their moments and show that they are all identical to the two leading orders of M . Since the densities are functions only of $x = r^2$, it is sufficient to compute only the even moments of r , i.e., the moments of the variable x . We define them as

$$C^{(m)} = \int d^d r x^m \rho(x) \quad D^{(m)} = \int d^d r x^m \xi(x). \quad (52)$$

Integrating $D^{(m)}$ by parts using (31) and (35), one easily sees that the following relation holds:

$$D^{(m)} = \frac{d}{(4m+2d)} C^{(m+1)}. \quad (53)$$

Note that this relation for $m = 0$ yields the virial theorem, since $D^{(0)}$ is the kinetic energy and $C^{(1)}$ twice the potential energy. The moments of the TF density are readily found to be

$$C_{\text{TF}}^{(m)} = \int d^d r x^m \rho_{\text{TF}}(x, \lambda_M) = \frac{\Gamma(d/2 + m)}{\Gamma(d/2)} \frac{2^{m+1}}{(m+d)!} \lambda_M^{(m+d)}. \quad (54)$$

The corresponding moments of the exact density might be obtained by direct integration of x^m over expression (8) which leads to

$$C_{qm}^{(m)} = \frac{\Gamma(d/2 + m)}{\Gamma(d/2)} 2 \sum_{\mu=0}^M F_{M-\mu}^{(d)} (-1)^\mu F(-\mu, m + d/2; 1; 2) \quad (55)$$

where $F(a, b; c; z)$ is a hypergeometric function. However, we were not able to do the above sums analytically for arbitrary d . We therefore turn to the case $d = 1$, where the moments are more easily obtained from a summation of the corresponding matrix elements. The matrix

Table 1. The lowest moments $C^{(m)}$ of the density of the one-dimensional harmonic oscillator with $M + 1$ filled shells, expressed in terms of the Fermi energy $\lambda = M + 1$. Column 2 contains quantum-mechanical values from (57), column 3 contains TF values from (54). Column 4 contains the quantum-mechanical moments for the two-dimensional oscillator; the TF values (not shown explicitly) are given by the leading term for each m .

m	$C_{TF}^{(m)} (d = 1)$	$C_{qm}^{(m)} (d = 1, \lambda = M + 1)$	$C_{qm}^{(m)} (d = 2, \lambda = M + 3/2)$
0	2λ	2λ	$\lambda^2 - \frac{1}{4}$
1	λ^2	λ^2	$\frac{2}{3}(\lambda^3 - \frac{1}{4}\lambda)$
2	λ^3	$\lambda^3 + \frac{1}{2}\lambda$	$\frac{2}{3}(\lambda^4 + \frac{1}{2}\lambda^2 - \frac{3}{16})$
3	$\frac{5}{4}\lambda^4$	$\frac{5}{4}(\lambda^4 + 2\lambda^2)$	$\frac{4}{5}(\lambda^5 + \frac{5}{2}\lambda^3 - \frac{11}{16}\lambda)$
4	$\frac{7}{4}\lambda^5$	$\frac{7}{4}(\lambda^5 + 5\lambda^3 + \frac{3}{2}\lambda)$	$\frac{16}{15}(\lambda^6 + \frac{25}{4}\lambda^4 + \frac{19}{16}\lambda^2 - \frac{90}{128})$
5	$\frac{21}{8}\lambda^6$	$\frac{21}{8}(\lambda^6 + 10\lambda^4 + \frac{23}{2}\lambda^2)$	$\frac{32}{21}(\lambda^7 + \frac{49}{4}\lambda^5 + \frac{259}{16}\lambda^3 - \frac{309}{64}\lambda)$
6	$\frac{33}{8}\lambda^7$	$\frac{33}{8}(\lambda^7 + \frac{53}{2}\lambda^5 + 49\lambda^3 + \frac{45}{4}\lambda)$	$\frac{16}{7}(\lambda^8 + 21\lambda^6 + \frac{567}{8}\lambda^4 + \frac{89}{16}\lambda^2 - \frac{1575}{256})$

element of x^m in the n th quantum state of the one-dimensional harmonic oscillator is found to be

$$\langle n | x^m | n \rangle = \frac{(2m)!}{2^{2m} m!} (-1)^n F(-n, m + 1; 1; 2). \tag{56}$$

The exact moments are therefore

$$C_{qm}^{(m)} = \frac{(2m)!}{2^{2m} m!} 2 \sum_{n=0}^M (-1)^n F(-n, m + 1; 1; 2). \tag{57}$$

The above hypergeometric functions are easy to create recursively by the relation

$$(m + 1)\mathcal{F}_{m+1}(n) = (2n + 1)\mathcal{F}_m(n) + m\mathcal{F}_{m-1}(n) \tag{58}$$

where

$$\mathcal{F}_m(n) = (-1)^n F(-n, m + 1; 1; 2) \tag{59}$$

and using $F(-n, 1; 1; 2) = (-1)^n$ (see [14], equation (9.121.1)). This yields

$$\begin{aligned} \mathcal{F}_0(n) &= 1 \\ \mathcal{F}_1(n) &= 2n + 1 \\ \mathcal{F}_2(n) &= 2n^2 + 2n + 1 \\ \mathcal{F}_3(n) &= (2n + 1)(2n^2 + 2n + 3)/3 \end{aligned} \tag{60}$$

and so on, after which the summation in (57) becomes elementary. We give in table 1 (left part) a list of the first few moments, obtained in the TF approximation from (54) and exactly from (57), expressed in terms of the Fermi energy $\lambda = M + 1$. We see that the TF moments reproduce the exact ones up to terms of relative order $1/\lambda^2$ and lower, which are equivalent to terms of order $1/M^2$ and lower.

The same result can, with some more algebraic effort, be found for higher dimensions by manual evaluation of (55). For even d , the moments are more easily obtained from a Taylor expansion of the Laplace transforms $P(s)$ and $X(s)$ of the exact densities, given in appendix C, in powers of s . For $d = 2$, the simplicity of (12) allowed us to derive the recurrence relation

$$C_{qm}^{(m+1)} = \left(\frac{m + 1}{m + 3}\right) [2\lambda C_{qm}^{(m)} + m^2 C_{qm}^{(m-1)}] \quad (d = 2). \tag{61}$$

Table 2. Same as in column 4 of table 1, but for $d = 3$ and $d = 4$.

m	$C_{qm}^{(m)}(d = 3, \lambda = M + 2)$	$C_{qm}^{(m)}(d = 4, \lambda = M + 5/2)$
0	$\frac{1}{3}(\lambda^3 - \lambda)$	$\frac{1}{12}\left(\lambda^4 - \frac{5}{2}\lambda^2 + \frac{9}{16}\right)$
1	$\frac{1}{4}(\lambda^4 - \lambda^2)$	$\frac{1}{15}\left(\lambda^5 - \frac{5}{2}\lambda^3 + \frac{9}{16}\lambda\right)$
2	$\frac{1}{4}(\lambda^5 - \lambda)$	$\frac{1}{15}\left(\lambda^6 - \frac{5}{4}\lambda^4 - \frac{41}{16}\lambda^2 + \frac{45}{64}\right)$
3	$\frac{7}{24}\left(\lambda^6 + \frac{5}{2}\lambda^4 - \frac{7}{2}\lambda^2\right)$	$\frac{8}{105}\left(\lambda^7 + \frac{7}{4}\lambda^5 - \frac{161}{16}\lambda^3 + \frac{153}{64}\lambda\right)$
4	$\frac{3}{8}\left(\lambda^7 + 7\lambda^5 - \frac{7}{2}\lambda^3 - \frac{9}{2}\lambda\right)$	$\frac{2}{21}\left(\lambda^8 + 7\lambda^6 - \frac{133}{8}\lambda^4 - \frac{177}{16}\lambda^2 + \frac{945}{256}\right)$

In the rightmost column of table 1 we give the lowest quantum-mechanical moments for $d = 2$, and in table 2 we give them for $d = 3$ and $d = 4$. Their leading terms reproduce in all cases the TF values (54). Note that the polynomials seen in these tables, translated into polynomials in M , appear exactly in the coefficients of the Taylor expansions of the densities for even d . This can be checked for $d = 2$ and $d = 4$ with the expansions given in appendix B.

This establishes the desired result that in the asymptotic limit, all moments of the quantum-mechanical density $\rho(r, M)$ are identical with those of the TF density $\rho_{\text{TF}}(r, \lambda_M)$ up to relative terms of order $1/M^2$ or $1/\lambda_M^2$. By virtue of (53), the same conclusion can be drawn for the kinetic energy density $\xi(r)$ since the proportionality constant in this equation does not depend on M or λ .

5. Oscillating parts of the densities

In this section, we focus on the oscillating parts $\delta\rho(r)$ and $\delta\xi(r)$ of the densities as defined in (41). We first derive series expansions of these oscillating densities and then exhibit that their asymptotically leading terms are of order $1/M$ and $1/M^3$, respectively, relative to the leading-order terms of their smooth parts.

5.1. Expansions of the exact oscillating parts

We employ here a method proposed recently in [10]. In terms of the variable $t = 2x = 2r^2$, we define the Laplace transforms

$$P(s) = \int_0^\infty e^{-st} \rho(t) dt \quad X(s) = \int_0^\infty e^{-st} \xi(t) dt. \quad (62)$$

For even dimensions d these can be evaluated analytically, as shown in appendix C, and the transforms of the smooth and oscillating parts can be readily identified. Taking the inverse Laplace transforms of the smooth parts yields exactly the results discussed in the previous section and summarized in (48), including the step function which puts the TF densities identically to zero at and beyond the classical turning point. The inverse Laplace transforms of the oscillating parts yield, after a suitable expansion for large M which is shown in appendix C, the following series for $d = 2$:

$$\delta\rho^{(2)}(r) = \frac{(-1)^M}{2\pi} \left\{ \mathcal{J}_0(z) - \frac{1}{4}x^2 \mathcal{J}_2(z) - \frac{\lambda}{9}x^3 \mathcal{J}_3(z) - \frac{1}{192}x^4 \mathcal{J}_4(z) + \dots \right\} \quad (63)$$

$$\delta\xi^{(2)}(r) = \frac{(-1)^M}{8\pi} \left\{ -2x \mathcal{J}_1(z) + \frac{1}{6}x^3 \mathcal{J}_3(z) + \frac{\lambda}{18}x^4 \mathcal{J}_4(z) + \frac{1}{480}x^5 \mathcal{J}_5(z) + \dots \right\} \quad (64)$$

with $\lambda = M + 3/2$ and

$$z = 2\sqrt{2\lambda x} = 2r\sqrt{2\lambda}. \quad (65)$$

Hereby we have defined the functions $\mathcal{J}_\mu(z)$ by

$$\mathcal{J}_\mu(z) = \Gamma(\mu + 1) \left(\frac{2}{z}\right)^\mu J_\mu(z) \quad (\mu > -1) \quad (66)$$

in terms of the standard Bessel functions $J_\mu(z)$. Note that the $\mathcal{J}_\mu(z)$ functions are eigenfunctions of the radial Laplace operator, as discussed further below, and normalized such that $\mathcal{J}_\mu(0) = 1$.

For $d = 4$ we find the results

$$\delta\rho^{(4)}(r) = \frac{(-1)^M}{4\pi^2} \left\{ \lambda \mathcal{J}_1(z) + \frac{3}{4}x \mathcal{J}_1(z) + \frac{\lambda}{6}x^2 \mathcal{J}_2(z) - \frac{1}{32}x^3 \mathcal{J}_3(z) - \frac{\lambda}{80}x^4 \mathcal{J}_4(z) + \dots \right\} \quad (67)$$

$$\delta\xi^{(4)}(r) = \frac{(-1)^M}{8\pi^2} \left\{ \mathcal{J}_0(z) - \frac{3}{4}x^2 \mathcal{J}_2(z) - \frac{\lambda}{9}x^3 \mathcal{J}_3(z) + \frac{1}{64}x^4 \mathcal{J}_4(z) + \frac{\lambda}{200}x^5 \mathcal{J}_5(z) + \dots \right\} \quad (68)$$

with $\lambda = M + 5/2$. It is readily checked that in both cases, the above results satisfy the differential equation in (44) connecting $\delta\xi(r)$ with $\delta\rho(r)$.

Using the known Taylor expansions of the Bessel functions, the above results yield exactly the expansions of the oscillating terms given in appendix B and discussed in the previous section. For the following it is important to note that the two leading powers in M of each Taylor expansion coefficient are correctly reproduced by the leading-order Bessel functions in the above series; the higher-order terms just correct the terms of order $1/M^2$ and lower in each coefficient.

We were not able to find the same expansions of the oscillating densities for odd d , since their Fourier transforms could not be obtained in a tractable analytical form. We have contented ourselves with the observation that the leading-order Bessel functions, given below for arbitrary d , are recovered from the Taylor expansions discussed in the previous section, again up to terms of relative order $1/M^2$ and lower in each Taylor coefficient.

The convergence of the above series is tested numerically in section 5.4 below. They are asymptotic in nature and converge only for sufficiently small values of x , i.e., sufficiently far from the classical turning points. At $x = 0$, only their leading terms (i.e., the first Bessel function in each series) contribute, for which we give some particularly nice closed forms in the following subsection.

5.2. Asymptotically leading oscillating parts

We now limit ourselves to the leading-order terms of the oscillating densities, which we will denote by the subscript 'as' for 'asymptotic' and which are given by the first Bessel functions in each of the above exact expansions. For arbitrary d and M they can be written in the following forms:

$$\delta\rho_{\text{as}}(r) = \frac{(-1)^M}{(2\pi)^{\mu+1}} \left(\frac{2\lambda_M}{z}\right)^\mu J_\mu(z) \quad (69)$$

$$\delta\xi_{\text{as}}(r) = \frac{(-1)^M}{(2\pi)^{\mu+1}} \frac{(\mu + 1)}{4} \left(\frac{2\lambda_M}{z}\right)^{\mu-1} J_{\mu-1}(z) \quad (70)$$

with

$$\mu = d/2 - 1 \quad z = 2r\sqrt{2\lambda_M} \quad \lambda_M = M + (d + 1)/2. \quad (71)$$

Note that the above asymptotic forms fulfil the same differential equation as that given for the full oscillating parts in (44). Comparing to the TF densities in (37), (38), we see that $\delta\rho_{\text{as}}(r)$ and $\delta\xi_{\text{as}}(r)$ are of relative order $1/\lambda_M$ and $1/\lambda_M^3$, respectively. This confirms the numerical finding that even for moderate values of M , the densities $\xi(r)$ appear to be smooth, while the oscillations in $\rho(r)$ are clearly visible (see figures 1 and 2).

It is rather easy to verify that the asymptotic densities (69), (70) are eigenfunctions of the Laplace operator for any μ , and hence for any d , with eigenvalue $-8\lambda_M$:

$$\Delta\delta\rho_{\text{as}}(r) = -8\lambda_M\delta\rho_{\text{as}}(r) \quad \Delta\delta\xi_{\text{as}}(r) = -8\lambda_M\delta\xi_{\text{as}}(r). \quad (72)$$

Note, however, that this is not true for the full oscillating densities given in (63)–(68) above. The equation for $\delta\rho_{\text{as}}(r)$ in (72) can also be obtained from the exact differential equation (29) derived in section 3. Taking the asymptotic limit of (42), retaining only the two leading powers in λ_M , the $\delta\xi(r)$ on the lhs and the potential term on the rhs can be neglected so that the first equation in (72) immediately follows.

Gleisberg *et al* [3] have studied the asymptotic expansion in the case $d = 1$ in which our result for $\delta\rho_{\text{as}}$ becomes

$$\delta\rho_{\text{as}}^{(1)}(x) = \frac{(-1)^M}{\pi\sqrt{2\lambda}} \cos(2x\sqrt{2\lambda}) \quad \lambda = M + 1 \quad (73)$$

where x here is the dimensionless coordinate. This result agrees with the oscillating part of their result (cf [3], equations (16) and (A9)), if we replace our Fermi energy λ by $M + 1/2$ which is that of the exact quantum system. (Note that these authors did not include the spin factor 2 in their density.)

We emphasize that the asymptotic forms (69), (70) give the exact values of the oscillating densities at $r = 0$, since all higher correction terms in the series (63)–(68) are zero at the origin. As shown in the numerical investigations of section 5.4, they describe the quantum oscillations of the exact densities near the origin very precisely, where the densities are largest and perhaps most easily detected experimentally.

Next we derive the leading oscillating part of the kinetic energy densities $\tau(r)$ and $\tau_1(r)$ which are seen in figure 2 to exhibit much stronger oscillations than $\xi(r)$. To derive the asymptotic forms of their oscillating parts, we start from (43) and keep, as above, only the two leading-order terms in λ_M on both sides of this equation. We then find the following simple relation:

$$\delta\tau_{\text{as}}(r) = \lambda_M\delta\rho_{\text{as}}(r) \quad (74)$$

which will be tested numerically in section 5.4. Using relations (5) and (72), we finally obtain

$$\delta\tau_{1,\text{as}}(r) = -\lambda_M\delta\rho_{\text{as}}(r) = -\delta\tau_{\text{as}}(r) \quad (75)$$

which confirms explicitly the numerically known fact (cf figure 2) that the oscillations in $\tau_1(r)$ are opposite in phase to those in $\tau(r)$.

5.3. Validity of the TF kinetic energy density functional

In [4], the surprising observation was made that the TF functional for the kinetic energy density

$$\tau_{\text{TF}}[\rho_{\text{TF}}] = \frac{\hbar^2}{2m} \frac{4\pi d}{(d+2)} \left[\frac{d}{4} \Gamma\left(\frac{d}{2}\right) \right]^{2/d} \rho_{\text{TF}}^{1+2/d} \quad (76)$$

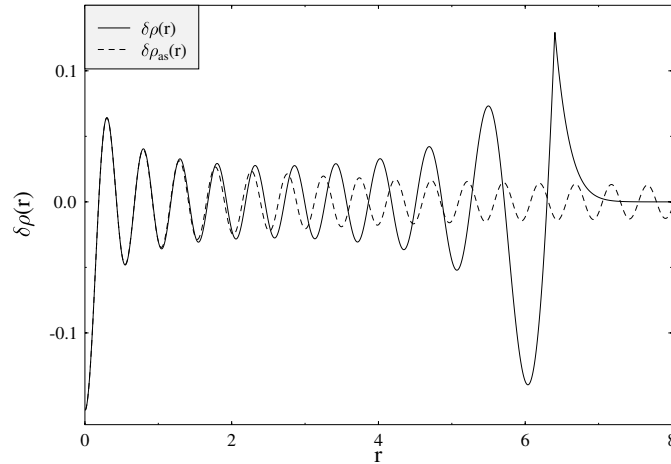


Figure 3. Oscillating part of the density for $N = 420$ particles in a 2D harmonic trap ($M = 20$). The solid line gives the full oscillating part as defined by (41), and the dashed line its asymptotic form given by (69) for $\mu = 0$, $\lambda = 21.5$.

is fulfilled to a high degree of precision also for the exact quantum-mechanical densities $\rho(r)$ and $\tau(r)$, except near the classical turning point and beyond it. Upon integrating, in the case $d = 2$ one even obtains the exact kinetic energy.

Using the above asymptotic results it is easy to prove the validity of the TF functional (76) at the level of the leading-order asymptotic terms. We define the asymptotic total densities by

$$\rho_{\text{as}}(r) = \rho_{\text{TF}}(r) + \delta\rho_{\text{as}} \quad \tau_{\text{as}}(r) = \tau_{\text{TF}}(r) + \delta\tau_{\text{as}} \quad (77)$$

insert these into the TF relation (76), expand the power $[\rho(r)]^{1+2/d}$ up to first order in $\delta\rho_{\text{as}}$, and neglect all terms of relative order $1/\lambda_M^2$ and lower. We then find that the TF functional relation (76) is, indeed, fulfilled also by the total asymptotic densities (77)

$$\tau_{\text{TF}}[\rho_{\text{as}}(r)] = \tau_{\text{as}}(r) + \mathcal{O}(M^{-2}) \quad (78)$$

which explains the results found numerically in [4].

The result (78) is highly nontrivial. In principle, the TF relation $\tau_{\text{TF}}[\rho]$ holds only for systems with constant densities where the LDA is exact. For smoothly varying densities, gradient corrections are known to exist, which may be derived in the so-called extended TF model and have been successfully applied to various fermion systems (see e.g. [15], chapter 4). Nevertheless, our result (78) shows that the simple TF functional applies asymptotically for harmonically trapped fermions also when including the quantum oscillations in both $\rho(r)$ and $\tau(r)$.

5.4. Numerical tests of the asymptotic relations

We first test the asymptotic form (69) of the oscillating part of the density. In figure 3, it is compared to the full oscillating part $\delta\rho(r)$ defined by (41) for $N = 420$ particles in a 2D trap. The cusp in the exact $\delta\rho(r)$ reflects the cut-off of the smooth TF-like density $\bar{\rho}(r)$ in (49) at the classical turning point. We see that $\delta\rho_{\text{as}}$ in (69) is correct only for small distances r from the centre of the system and completely fails near the classical turning point. The situation improves somewhat when we include higher terms of the expansion discussed above. In figure 4 we show the same comparison for $N = 1722$ particles in 2D, with and without

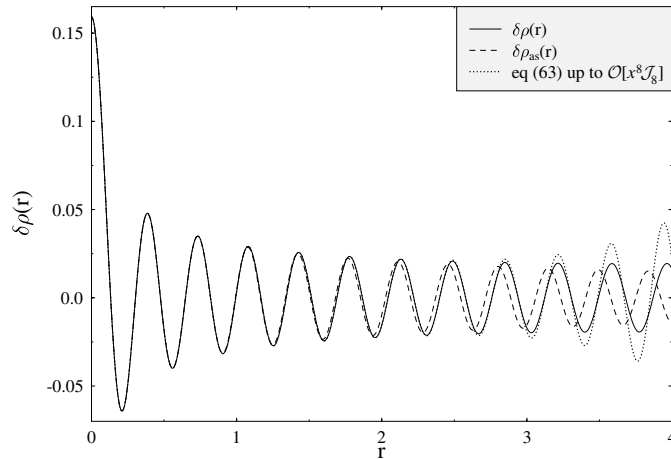


Figure 4. Same as figure 3, but for $N = 1722$ particles ($M = 40$, $\lambda = 41.5$). The dotted line gives the results obtained when including the terms up to $\mathcal{O}[x^8 \mathcal{J}_8]$ in the expansion (63).

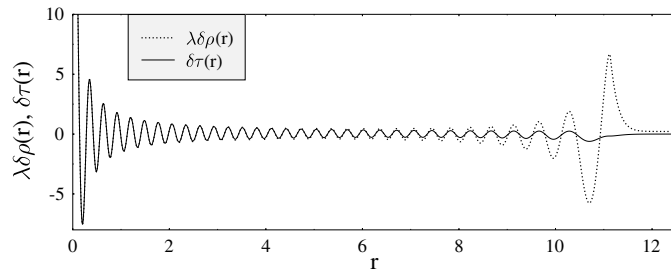


Figure 5. Oscillating parts of densities for $N = 79422$ particles in a 3D harmonic trap ($M = 60$, $\lambda = 62$). The solid line gives $\delta\tau(r)$, and the dotted line the quantity $\lambda\delta\rho(r)$ according to the asymptotic relation (74).

including the terms up to the order $x^8 \mathcal{J}_8(z)$ in the Bessel function expansion (63). Whereas $\delta\rho_{\text{as}}$ is only sufficient up to $r \simeq 1$, the Bessel series truncated at order 8 becomes good up to $r \simeq 2.5$; the phases of the oscillations are correct even further out. But clearly, an infinite number of terms would have to be included before reaching an agreement in the region of the classical turning point.

Whereas this result is not very encouraging, showing that the asymptotic oscillating densities (69) are only useful far away from the classical turning points, a much larger region of validity is found for relation (74) between the asymptotic densities $\delta\tau_{\text{as}}(r)$ and $\delta\rho_{\text{as}}(r)$. This is demonstrated in figure 5, where we have plotted the full quantities $\delta\tau(r)$ and $\lambda\delta\rho(r)$ (with $\lambda = 62$) for $N = 79422$ particles filling 61 shells in a 3D harmonic trap. The agreement is quite good until rather far away from the centre; only near the turning point the proportionality breaks down. The same is shown in figure 6 for $N = 271502$ particles filling 41 shells in a 4D harmonic trap (with $\lambda = 42.5$). To set the scale, the density $\rho(r)$ and its TF limit are also shown in the figure. The particle number is so high here that the oscillations in $\rho(r)$ can only be recognized very close to the centre, which demonstrates once more the excellent approximation provided by the TF density.

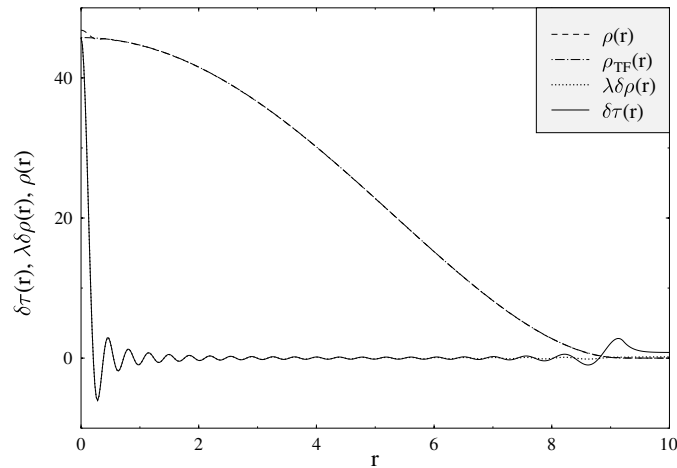


Figure 6. Same as figure 6, but for $N = 271\,502$ particles in a 4D harmonic trap ($M = 40$) with $\lambda = 42.5$. The dashed and dashed-dotted lines give the full density and its TF limit.

Clearly, an appreciable amount of error cancellation must take place on the way to relation (74) between the asymptotic oscillating densities. Its good validity is the basis of the performance of the TF kinetic energy functional $\tau_{\text{TF}}[\rho]$ including the quantum oscillations, as discussed above and established formally through (78).

6. Summary

We have studied the particle densities and several equivalent forms of kinetic energy densities for harmonically trapped fermion gases in arbitrary dimensions d . We established various exact differential equations connecting these densities, and an equivalent integro-differential eigenvalue equation of Schrödinger type for the particle density. Some of these equations have been derived previously, but only in $d = 1$ or 2 dimensions. We have then studied in detail the asymptotic limits of the particle densities $\rho(r)$ and the kinetic energy densities $\xi(r)$ for large particle numbers and Fermi energies λ . Using Taylor expansions, moments and Laplace transforms of these densities, we were able to separate them uniquely into smooth and oscillating parts. The two leading-order powers in λ of the smooth densities $\bar{\rho}(r)$, $\bar{\xi}(r)$ were shown analytically to go over into the well-known Thomas–Fermi (TF) densities, the remaining terms of order $1/\lambda^2$ and lower giving small corrections to the smooth parts. The Fermi energy hereby is given by $\lambda = M + (d + 1)/2$, where M is the quantum number of the highest occupied spherical shell. The oscillating parts $\delta\rho(r)$, $\delta\xi(r)$ are characterized by an oscillating overall sign $(-1)^M$ that reflects the alternating parities of the successive shells. Their asymptotically leading terms could be given in simple closed expressions involving Bessel functions; they are eigenfunctions of the radial Laplace operator with eigenvalue -8λ . They are of order $1/\lambda$ and $1/\lambda^3$ for $\delta\rho(r)$ and $\delta\xi(r)$, respectively, with respect to the leading terms in the smooth densities $\bar{\rho}(r)$ and $\bar{\xi}(r)$. The latter fact—the suppression factor $1/\lambda^3$ —explains the numerical experience that the kinetic energy densities $\xi(r)$ are smooth even for moderate particle numbers. For even dimensions d , we have derived a formally exact expansion of the full oscillating densities in terms of Bessel functions, which was, however, found to converge rather slowly and only sufficiently far away from the classical turning points. Still, these results are useful for expressing the quantum oscillations near the centre of the system in

closed analytical forms. Using our exact differential equations which hold separately for the smooth and oscillating parts of the densities, we could also establish the numerical fact that the kinetic energy densities $\tau(r)$ and $\tau_1(r)$ are oscillating with opposite phases. An interesting proportionality between $\delta\rho(r)$ and $\delta\tau(r)$ was found to hold asymptotically everywhere except near the classical turning points. With our asymptotic relations, we could finally establish analytically the surprising recent observation [4] that the TF functional $\tau_{\text{TF}}[\rho]$ also holds when the quantum-mechanical oscillations are included in both $\tau(r)$ and $\rho(r)$.

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Note added in proof. We are grateful to an anonymous referee for drawing our attention to the recent papers by I A Howard, N H March and L M Nieto in *Phys. Rev. A* **66** 054501 and *J. Phys. A: Math. Gen.* **35** 4955, where our equation (33) for the particle density was independently derived and further relations connecting kinetic and particle densities were discussed.

Appendix A. Evaluation of $\mathcal{R}(x)$

In this appendix, we give details on the evaluation of the quantity $\mathcal{R}(x)$ defined in (27) and used in deriving the differential equation (29). Here we prove the following identity:

$$\begin{aligned} \mathcal{R}(x) &= \frac{2}{\pi^{d/2}} \sum_{\mu=0}^M (-1)^\mu \left\{ [(M+1-\mu)F_{M-\mu}^{(d)} - G_{M-\mu}^{(d)}] L_\mu(2x) + \frac{(d-2)}{2} F_{M-\mu}^{(d)} L'_\mu(2x) \right\} e^{-x} \\ &\equiv \frac{(d-2)}{d} \xi(x) - \frac{(d-2)}{4} \rho(x). \end{aligned} \quad (79)$$

Proof. Using the identity

$$L'_n(2x) = - \sum_{m=0}^{n-1} L_m(2x) \quad (n > 0) \quad (80)$$

which may be derived using equations (8.971.2) and (8.974.3) of [14], noting that $L'_0(2x) = 0$, and inverting the order of summation in the first line of (79), we get

$$\begin{aligned} \mathcal{R}(x) &= \frac{2}{\pi^{d/2}} \sum_{\mu=0}^M (-1)^{M-\mu} \left\{ [(\mu+1)F_\mu^{(d)} - G_\mu^{(d)}] L_{M-\mu}(2x) \right. \\ &\quad \left. - \frac{(d-2)}{2} F_\mu^{(d)} \sum_{m=0}^{M-\mu-1} L_m(2x) \right\} e^{-x}. \end{aligned} \quad (81)$$

(The sum over m above must be put to zero when the upper limit of m takes the value -1 .) We may now reorder the double sum over the last term in such a way that the Laguerre polynomials can be taken out of the inner sum, leading to

$$\mathcal{R}(x) = \frac{2}{\pi^{d/2}} \sum_{\mu=0}^M (-1)^{M-\mu} L_{M-\mu}(2x) H_\mu^{(d)} e^{-x} \quad (82)$$

with the definition

$$H_\mu^{(d)} = (\mu + 1)F_\mu^{(d)} - G_\mu^{(d)} - (-1)^\mu \frac{(d-2)}{2} \sum_{v=0}^{\mu-1} (-1)^v F_v^{(d)}. \quad (83)$$

For the sum over the $F_v^{(d)}$ on the rhs above, we can use formulae (15) given in section 2. Furthermore, from our explicit results (13) and (14) one easily sees that

$$\begin{aligned} (1 + d/2)G_{2n+1}^{(d)} &= (4n + 2 + d)F_{2n+1}^{(d)} \\ (1 + d/2)G_{2n}^{(d)} &= (4n + 1 + d/2)F_{2n}^{(d)} + (d/2 - 1)F_{2n-1}^{(d)}. \end{aligned} \quad (84)$$

Using these identities, it just takes some algebra to find the simple form

$$H_\mu^{(d)} = \frac{(d-2)}{4} [G_\mu^{(d)} - F_\mu^{(d)}] \quad (85)$$

valid for both even and odd μ . Substituting this into (82) we finally obtain the desired result (79).

Appendix B. Taylor expansions of exact densities

We give here some Taylor expansions of the exact densities (8) and (9) in powers of $x = r^2$. Their coefficients, defined in (47), cannot be given in closed form for any d and M , but only separately for even and odd M . The coefficients $\rho^{(0)}(d, M)$ are simply the densities at $r = 0$ given already in (16). For the next three coefficients of the density $\rho(r)$, we find for even M :

$$\rho_{\text{even}}^{(1)}(d, M) = -\rho_{\text{even}}^{(0)}(d, M) \quad (86)$$

$$\rho_{\text{even}}^{(2)}(d, M) = \frac{(2 + d + 4M)}{2(d + 2)} \rho_{\text{even}}^{(0)}(d, M) \quad (87)$$

$$\rho_{\text{even}}^{(3)}(d, M) = -\frac{(d^2 + 6d + 8 + 12dM + 16M + 16M^2)}{6(d + 4)(d + 2)} \rho_{\text{even}}^{(0)}(d, M) \quad (88)$$

and so on. For odd M we find

$$\rho_{\text{odd}}^{(1)}(d, M) = \rho_{\text{odd}}^{(0)}(d, M) \quad (89)$$

$$\rho_{\text{odd}}^{(2)}(d, M) = -\frac{(2 + 3d + 4M)}{2(d + 2)} \rho_{\text{odd}}^{(0)}(d, M) \quad (90)$$

$$\rho_{\text{odd}}^{(3)}(d, M) = \frac{(5d^2 + 10d + 8 + 20dM + 16M + 16M^2)}{6(d + 4)(d + 2)} \rho_{\text{odd}}^{(0)}(d, M) \quad (91)$$

and so forth. Similar expressions are obtained for the coefficients $\xi^{(m)}(d, M)$. We can then reconstruct separately the expansion coefficients of the smooth and oscillating parts defined in (40) and (41). We give here the explicit expansions, valid for both even and odd M , for even dimensions, where the results look more transparent. For $d = 2$ we obtain

$$\begin{aligned} \rho_M^{(2)}(x) &= \frac{1}{\pi} \left[\left(M + \frac{3}{2} \right) - \frac{1}{2}x \right] + \frac{(-1)^M}{2\pi} \left[1 - 2x \left(M + \frac{3}{2} \right) + x^2(M^2 + 3M + 2) \right. \\ &\quad \left. - \frac{2}{9}x^3 \left(M^3 + \frac{9}{2}M^2 + \frac{13}{2}M + 3 \right) + \dots \right]. \end{aligned} \quad (92)$$

$$\begin{aligned} \xi_M^{(2)}(x) = & \frac{1}{2\pi} \left[(M^2 + 3M + 2) - x \left(M + \frac{3}{2} \right) + \frac{1}{4}x^2 \right] - \frac{(-1)^M}{4\pi} \left[x - x^2 \left(M + \frac{3}{2} \right) \right. \\ & + \frac{1}{3}x^3(M^2 + 3M + 2) - \frac{1}{18}x^4 \left(M^3 + \frac{9}{2}M^2 + \frac{13}{2}M + 3 \right) \\ & \left. + \frac{1}{180}x^5(M^4 + 6M^3 + 14M^2 + 15M + 6) + \dots \right]. \end{aligned} \quad (93)$$

For $d = 4$ we get explicitly

$$\begin{aligned} \rho_M^{(4)}(x) = & \frac{1}{4\pi^2} \left[\left(M^2 + 5M + \frac{11}{2} \right) - x \left(M + \frac{5}{2} \right) + \frac{1}{4}x^2 \right] + \frac{(-1)^M}{4\pi^2} \left[\left(M + \frac{5}{2} \right) \right. \\ & - x \left(M^2 + 5M + \frac{11}{2} \right) + \frac{1}{3}x^2 \left(M^3 + \frac{15}{2}M^2 + 17M + \frac{45}{4} \right) \\ & \left. - \frac{1}{18}x^3(M^4 + 10M^3 + 35M^2 + 50M + 24) + \dots \right] \end{aligned} \quad (94)$$

$$\begin{aligned} \xi_M^{(4)}(x) = & \frac{1}{6\pi^2} \left[\left(M^3 + \frac{15}{2}M^2 + 17M + \frac{45}{4} \right) - \frac{3}{2}x \left(M^2 + 5M + \frac{11}{2} \right) \right. \\ & + \frac{3}{4}x^2 \left(M + \frac{5}{2} \right) - \frac{1}{8}x^3 \left. \right] + \frac{(-1)^M}{8\pi^2} \left[1 - 2x \left(M + \frac{5}{2} \right) \right. \\ & + x^2 \left(M^2 + 5M + \frac{11}{2} \right) - \frac{2}{9}x^3 \left(M^3 + \frac{15}{2}M^2 + 17M + \frac{45}{4} \right) \\ & \left. + \frac{1}{36}x^4(M^4 + 10M^3 + 35M^2 + 50M + 24) + \dots \right]. \end{aligned} \quad (95)$$

Note that the smooth and oscillating parts in the above expansions of both densities are readily recognizable, the latter being multiplied by the overall sign $(-1)^M$.

Appendix C. Asymptotic expansion of oscillating parts

We start from the definition of the Laplace transforms (62) of the exact particle and kinetic energy densities (8) and (9). Using the integral (see [14], equation (7.414.2))

$$\int_0^\infty e^{-st} L_n(t) e^{-t/2} dt = \frac{(s - 1/2)^n}{(s + 1/2)^{n+1}} \quad (96)$$

one obtains

$$\begin{aligned} P^{(d)}(s) &= \frac{1}{\pi^{d/2}} 2 \sum_{\mu=0}^M F_{M-\mu}^{(d)} \frac{(1/2 - s)^\mu}{(1/2 + s)^{\mu+1}} \\ X^{(d)}(s) &= \frac{1}{\pi^{d/2}} \frac{d}{2} \sum_{\mu=0}^M G_{M-\mu}^{(d)} \frac{(1/2 - s)^\mu}{(1/2 + s)^{\mu+1}}. \end{aligned} \quad (97)$$

We first discuss the simplest case, $d = 2$, and reproduce the results of [10] in a slightly modified form. Here, as for any even dimension d , the sums in (97) can be done analytically (see footnote 3), with the results

$$P^{(2)}(s) = \frac{1}{\pi s} \left[\left(M + \frac{3}{2} \right) - \frac{1}{4s} \right] + \frac{(-1)^M}{4\pi s} \frac{(1 - 1/2s)^{M+2}}{(1 + 1/2s)^{M+1}} \quad (98)$$

$$X^{(2)}(s) = \frac{1}{2\pi s} \left[(M^2 + 3M + 2) - \frac{1}{2s}(M + 3/2) + \frac{1}{16s^2} \right] + \frac{(-1)^{M+1} (1 - 1/2s)^{M+2}}{8\pi s^2 (1 + 1/2s)^{M+1}}. \tag{99}$$

These expressions fall into two parts which correspond exactly to the Laplace transforms of the smooth and oscillating parts of the densities defined in (39), whereby we recognize the alternating sign $(-1)^M$ in front of the oscillating terms. The smooth parts give after Laplace inversion exactly the results (49).

In the following, we shall concentrate on the oscillating terms. We shall presently show that these terms yield oscillating functions of r (or x) and derive their systematic asymptotic expansion. To this purpose we extract a common factor appearing in both functions above:

$$E(s) = \frac{(1 - 1/2s)^{M+2}}{(1 + 1/2s)^{M+1}} = \left(\frac{1 - 1/2s}{1 + 1/2s} \right)^\lambda \left(1 - \frac{1}{4s^2} \right)^{1/2} \quad \lambda = M + 3/2. \tag{100}$$

Using the substitution $s = \lambda/w$ we rewrite the first factor above and evaluate its asymptotic expansion (see footnote 3) for $\lambda \rightarrow \infty$:

$$\lim_{\lambda \rightarrow \infty} \left(\frac{1 - w/2\lambda}{1 + w/2\lambda} \right)^\lambda = e^{-w} \left[1 - \frac{w^3}{12\lambda^2} - \frac{1}{\lambda^4} \left(\frac{w^5}{80} - \frac{w^6}{288} \right) - \frac{1}{\lambda^6} \left(\frac{w^7}{448} - \frac{w^8}{960} + \frac{w^9}{10368} \right) - \dots \right]. \tag{101}$$

Next we re-insert $w = \lambda/s$ on the rhs above and perform a Taylor expansion of the second factor in (100) in powers of $1/2s$. Note that this expansion converges since we can always deform the contour of the inverse Laplace transform, which is a vertical line to the right of the imaginary axis in the complex s plane, such that $|1/2s| < 1$. As a result, we obtain the following asymptotic expansion of $E(s)$:

$$E(s) = e^{-\lambda/s} \left[1 - \frac{1}{8s^2} - \frac{\lambda}{12s^3} - \frac{1}{128s^4} - \frac{\lambda}{480s^5} + \left(\frac{\lambda^2}{288} - \frac{1}{1024} \right) \frac{1}{s^6} - \frac{\lambda}{53670s^7} + \dots \right]. \tag{102}$$

Together with the prefactors appearing in (98) and (99), we can now Laplace invert the resulting series term by term. Hereby we use the general formula (see [12], equation (29.3.80))

$$\mathcal{L}_t^{-1} \left\{ \frac{1}{s^{\mu+1}} e^{-\lambda/s} \right\} = \left(\frac{t}{\lambda} \right)^{\mu/2} J_\mu(2\sqrt{t\lambda}) \tag{103}$$

where the $J_\mu(z)$ are the cylindrical Bessel functions. Expressing the latter in terms of the $\mathcal{J}_\mu(z)$ defined in (66), we arrive at the results (63), (64) given in section 5.

For the case $d = 4$ we just give here the Fourier transforms of the oscillating parts:

$$\delta P^{(4)}(s) = \frac{(-1)^M}{4\pi^2} \left[1 - \frac{(1 - 1/2s)^{M+4}}{(1 + 1/2s)^{M+1}} \right] \quad \delta X^{(4)}(s) = \frac{(-1)^M (1 - 1/2s)^{M+4}}{8\pi^2 s (1 + 1/2s)^{M+1}} \tag{104}$$

which can again be clearly separated from their smooth parts that yield the results (50) after Laplace inversion. Proceeding exactly as above, but now using $\lambda = M + 5/2$, we arrive at the series (67), (68) of the oscillating densities given in section 5.

Unfortunately, we could not find any tractable analytical expressions after the summations in (97) for odd dimensions d , which yield rather cumbersome combinations of hypergeometric series.

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