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2002 J. Phys. A: Math. Gen. 35 4985

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# The determination of the Dirac density matrix of the $d$ -dimensional harmonic oscillator for an arbitrary number of closed shells

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Received 25 February 2002, in final form 22 April 2002

Published 7 June 2002

Online at [stacks.iop.org/JPhysA/35/4985](http://stacks.iop.org/JPhysA/35/4985)

## Abstract

In 1959, March and Young (*Nucl. Phys.* **12** 237) rewrote the equation of motion for the Dirac density matrix  $\gamma(x, x_0)$  in terms of sum and difference variables. Here,  $\gamma(\vec{r}, \vec{r}_0)$  for the  $d$ -dimensional isotropic harmonic oscillator for an arbitrary number of closed shells is shown to satisfy, using the variables  $|\vec{r} + \vec{r}_0|/2$  and  $|\vec{r} - \vec{r}_0|/2$ , a generalized partial differential equation embracing the March–Young equation for  $d = 1$ . As applications, we take in turn the cases  $d = 1, 2, 3$  and  $4$ , and obtain both the density matrix  $\gamma(\vec{r}, \vec{r}_0)$  and the diagonal density  $\varrho(r) = \gamma(\vec{r}, \vec{r}_0)|_{\vec{r}_0=\vec{r}}$ , this diagonal element already being known to satisfy a third-order linear homogeneous differential equation for  $d = 1$  through  $3$ . Some comments are finally made on the  $d$ -dimensional kinetic energy density, which is important for first-principles density functional theory in allowing one to bypass one-particle Schrödinger equations (the so-called Slater–Kohn–Sham equations).

PACS numbers: 05.30.Fk, 71.10.Ca, 31.15.Ew, 03.75.Fi

## 1. Introduction

Considerable impetus has been given to the theoretical study of many-fermion systems which are harmonically confined, and essentially non-interacting, by the experimental study of DeMarco and Jin [1]. These researchers achieved the evaporative cooling of dilute, and hence almost non-interacting, fermions, following the earlier experimental studies of the Bose–Einstein condensation in ultracold trapped Bose gases. The further experimental studies in [2–5] add to the motivation for further theoretical study. In the above experiments, the focus was on ultracold vapours of the <sup>40</sup>K and <sup>6</sup>Li fermionic isotopes populating hyperfine states

inside magnetic traps. s-wave collisions between fermions in the same hyperfine state are inhibited by the Pauli principle. p-wave scattering and dipole–dipole magnetic interactions are very weak at extremely low temperatures [6, 7]. Thus, a one-component vapour of Fermi atoms in a fully spin-polarized state inside a magnetic trap is a close experimental representation of an ideal non-interacting many-body assembly of fermions.

In current experimental techniques based on axially symmetric magnetic traps, it proves possible to range from a quasi-one-dimensional (1D) trap to a quasi-2D trap [8], and to a fully spherical 3D trap. These possibilities motivated the computer study of Vignolo, Minguzzi and Tosi involving the Green's operator [9, 10] and the analytical work of March and Nieto [11] in 1D, and the generalization to obtain differential equations for the fermion density  $\varrho(r)$  in 2D [12] and 3D [13, 14] isotropic harmonic confinement, for an arbitrary number of closed shells. Throughout all these studies, it is appropriate to focus on singly filled levels, due to the experimental setups dealing with spin-polarized fermions.

The above combination of experimental and theoretical studies made it natural to take the basic development of independent fermion theory of many-particle assemblies further. Then it is worth emphasizing that Dirac [15] already in 1930 introduced his density matrix (DM), called the 1DM  $\gamma(\vec{r}, \vec{r}_0)$  below, which gave a complete description of an assembly of non-interacting fermions described by a single Slater determinant. The quite recent study of Holas and March [16], in which the force  $-\partial V_{xc}/\partial \vec{r}$  in a truly many-body situation,  $V_{xc}(\vec{r})$  being the exchange-correlation potential central to current use of the density functional theory, is related exactly to the 1DM and second-order density matrix, makes further investigation of the Dirac 1DM in relation to the fermion density  $\varrho(\vec{r})$  an important area for further theoretical work. This provides additional motivation for the present study.

The outline of this paper is as follows. In section 2, the partial differential equation satisfied by the Dirac density matrix  $\gamma(\vec{r}, \vec{r}_0)$  is derived for the  $d$ -dimensional harmonic oscillator in terms of sum and difference variables  $|\vec{r} + \vec{r}_0|$  and  $|\vec{r} - \vec{r}_0|$ . Then, in sections 3 and 4 we take in turn the explicit cases  $d = 1$  and 2 respectively, and in particular in section 4 a form of the 1DM  $\gamma$  is given in which summation over shells is avoided by means of multiple integration. The diagonal element  $\gamma(\vec{r}, \vec{r}_0)|_{\vec{r}_0=\vec{r}} = \varrho(r)$  is shown by example to be readily amenable to numerical computation. Section 5 summarizes, more briefly, some progress on  $d = 3$  and 4 cases. Section 6 is concerned with the  $d$ -dimensional kinetic energy density within the present framework. Finally section 7 constitutes a summary, plus some suggestions for future study.

## 2. Partial differential equation for the Dirac density matrix $\gamma(\vec{r}, \vec{r}_0)$ for the $d$ -dimensional harmonic oscillator for an arbitrary number of closed shells

March and Young [17] in an earlier work considered the equation of motion for the Dirac density matrix  $\gamma(x, x_0)$  for fermions moving independently along the  $x$  axis in a common potential energy  $V(x)$ . The so-called equation of motion  $H\gamma - \gamma H = 0$ , with  $H$  as the one-body Hamiltonian, then reads in coordinate representation

$$\frac{\partial^2 \gamma(x, x_0)}{\partial x^2} - \frac{\partial^2 \gamma(x, x_0)}{\partial x_0^2} = \frac{2m}{\hbar^2} [V(x) - V(x_0)] \gamma(x, x_0). \quad (2.1)$$

Following [17], one next introduces sum and difference variables  $\xi$  and  $\eta$ , defined by

$$\xi = \frac{x + x_0}{2} \quad \eta = \frac{x - x_0}{2}. \quad (2.2)$$

Then, March and Young rewrote equation (2.1) in the form

$$\frac{\partial^2 \gamma(\xi, \eta)}{\partial \xi \partial \eta} = \frac{2m}{\hbar^2} [V(\xi + \eta) - V(\xi - \eta)] \gamma(\xi, \eta). \quad (2.3)$$

Throughout this paper, we shall be concerned with the harmonic potential energy

$$V(x) = \frac{1}{2}m\omega^2x^2 \tag{2.4}$$

generalized below, however, to  $d$  dimensions.

Then, equation (2.3) takes the explicit form

$$\frac{\partial^2\gamma(\xi, \eta)}{\partial\xi\partial\eta} = \frac{2m}{\hbar^2} \frac{1}{2}m\omega^2[(\xi + \eta)^2 - (\xi - \eta)^2]\gamma(\xi, \eta) = \frac{4m^2\omega^2}{\hbar^2}\xi\eta\gamma(\xi, \eta). \tag{2.5}$$

If we now make the change of function (compare, e.g., equation (3.4) below)

$$\gamma(\xi, \eta) = e^{-\frac{m\omega}{\hbar}(\xi^2+\eta^2)} f(\xi, \eta) \tag{2.6}$$

and introduce new independent variables

$$p = \xi^2 \quad q = \eta^2 \tag{2.7}$$

we get a simple partial differential equation with constant coefficients:

$$\frac{\partial^2 f(p, q)}{\partial p \partial q} = \frac{\partial f(p, q)}{\partial p} + \frac{\partial f(p, q)}{\partial q}. \tag{2.8}$$

We shall return to an application of equation (2.8) in section 3.

But now we turn to the  $d$ -dimensional equation for the Dirac density matrix  $\gamma$ . Our first objective below is to generalize the result (2.5) to  $d$  dimensions for an isotropic harmonic oscillator with potential energy

$$V(r) = \frac{1}{2}m\omega^2r^2. \tag{2.9}$$

The canonical or Bloch density matrix  $C(\vec{r}, \vec{r}_0, \beta)$  for this problem with  $d = 3$  was solved analytically in the study of Sondheimer and Wilson [18] and is known to depend only on the two scalar variables  $|\vec{r} + \vec{r}_0|$  and  $|\vec{r} - \vec{r}_0|$ . Let us introduce precisely the new  $d$ -dimensional coordinates

$$\vec{\xi} = \frac{\vec{r} + \vec{r}_0}{2} \quad \vec{\eta} = \frac{\vec{r} - \vec{r}_0}{2}. \tag{2.10}$$

The equation to be considered now is the equivalent of (2.1) in  $d$  dimensions for the potential energy (2.9):

$$\nabla_{\vec{r}}^2\gamma(\vec{r}, \vec{r}_0) - \nabla_{\vec{r}_0}^2\gamma(\vec{r}, \vec{r}_0) = \frac{m^2\omega^2}{\hbar^2}(r^2 - r_0^2)\gamma(\vec{r}, \vec{r}_0) \tag{2.11}$$

which is readily transformed into

$$(\nabla_{\vec{\xi}} \cdot \nabla_{\vec{\eta}})\gamma(\vec{\xi}, \vec{\eta}) = \frac{4m^2\omega^2}{\hbar^2}(\vec{\xi} \cdot \vec{\eta})\gamma(\vec{\xi}, \vec{\eta}). \tag{2.12}$$

As we already know that the Dirac density matrix  $\gamma$  depends only on the moduli  $\xi = |\vec{\xi}|$  and  $\eta = |\vec{\eta}|$ , equation (2.12) can be easily seen to reduce to

$$\frac{(\vec{\xi} \cdot \vec{\eta})}{\xi\eta} \frac{\partial^2\gamma(\xi, \eta)}{\partial\xi\partial\eta} = \frac{4m^2\omega^2}{\hbar^2}(\vec{\xi} \cdot \vec{\eta})\gamma(\xi, \eta) \tag{2.13}$$

which is precisely the same equation (2.5) that we displayed in the one-dimensional case.

### 3. Explicit form of density matrix $\gamma(\xi, \eta)$ for $d = 1$ and for $N$ singly occupied levels

In deriving a differential equation for the fermion density  $\varrho(x)$  for fermions occupying singly  $N$ -levels of the potential energy (2.4), Lawes and March [19] appealed to the result of Husimi [20] for the Dirac density matrix  $\gamma(x, x_0)$ , namely

$$\gamma(x, x_0) = \frac{1}{2}\psi_N(x)\psi_N(x_0) + \frac{1}{2(x-x_0)}[\psi_N(x)\psi'_N(x_0) - \psi_N(x_0)\psi'_N(x)] \quad (3.1)$$

where  $\psi_N(x)$  is the normalized wavefunction for the  $N$ th state, the lowest level corresponding to  $N = 1$ .

The completeness theorem for eigenfunctions  $\psi_i(x)$ , namely

$$\gamma(x, x_0) = \sum_{\text{all } i} \psi_i^*(x)\psi_i(x_0) = \delta(x - x_0) \quad (3.2)$$

evidently tells us that in the limit  $N \rightarrow \infty$  the exact result (3.1), which is valid for all  $N$ , must become independent of the variable  $\xi$  in equation (2.2).

The other simple case is, of course,  $N = 1$ , for which

$$\gamma(x, x_0) = \psi_1(x)\psi_1(x_0) = \frac{1}{\sqrt{\pi}} \exp\left(-\frac{x^2 + x_0^2}{2}\right) \quad (3.3)$$

or

$$\gamma(\xi, \eta) = \frac{1}{\sqrt{\pi}} \exp(-(\xi^2 + \eta^2)). \quad (3.4)$$

Here units are used in which  $m = \hbar = \omega = 1$ , and then it is an elementary matter to show that  $\gamma(\xi, \eta)$  in equation (3.4) satisfies the partial differential equation (2.5).

For general  $N$ , we have in terms of the Hermite polynomials that

$$\psi_N(x) = \mathcal{N}_{N-1} \exp(-x^2/2)H_{N-1}(x) \quad (3.5)$$

and

$$\psi'_N(x) = \mathcal{N}_{N-1} \exp(-x^2/2)[-xH_{N-1}(x) + 2(N-1)H_{N-2}(x)] \quad (3.6)$$

where the normalization constant is given by

$$\mathcal{N}_{N-1} = \frac{1}{\pi^{1/4}} \sqrt{\frac{1}{2^{N-1}(N-1)!}}. \quad (3.7)$$

Then

$$\gamma(\xi, \eta) = \mathcal{N}_{N-1}^2 e^{-(\xi^2 + \eta^2)} \left[ H_{N-1}(\xi + \eta)H_{N-1}(\xi - \eta) + \frac{N-1}{2\eta} \{H_{N-1}(\xi + \eta)H_{N-2}(\xi - \eta) - H_{N-2}(\xi + \eta)H_{N-1}(\xi - \eta)\} \right]. \quad (3.8)$$

For two levels occupied, equation (3.8) reduces to

$$\gamma(\xi, \eta) = \frac{e^{-(\xi^2 + \eta^2)}}{\sqrt{\pi}} [1 + 2(\xi^2 - \eta^2)] \quad (3.9)$$

and for three and four levels only occupied the Dirac density matrices are, respectively,

$$\gamma(\xi, \eta) = \frac{e^{-(\xi^2 + \eta^2)}}{2\sqrt{\pi}} [3 - 8\eta^2 + 4\xi^4 + 4\eta^4 - 8\xi^2\eta^2] \quad (3.10)$$

and

$$\gamma(\xi, \eta) = \frac{e^{-(\xi^2+\eta^2)}}{6\sqrt{\pi}} [9 + 18\xi^2 - 42\eta^2 - 12\xi^4 + 36\eta^4 - 24\eta^2\xi^2 + 8(\xi^6 - \eta^6) + 24\xi^2\eta^4 - 24\xi^4\eta^2]. \tag{3.11}$$

It is straightforward, by substitution in the partial differential equations (2.5) or (2.8), to verify that these results (3.9)–(3.11) are exact solutions.

It is of some interest, in concluding this section for  $d = 1$ , to note from equations (3.9)–(3.11) that in terms of  $f(p, q)$  entering equations (2.6) and (2.8), with  $p$  and  $q$  related to  $\xi$  and  $\eta$  through equation (2.7), the highest powers of  $p$  and  $q$  and their corresponding cross-terms, have the form of a constant times  $(p - q)^{N-1}$ , where  $N = 2, 3$  and  $4$  for equations (3.9), (3.10) and (3.11), respectively. The coefficient of this highest-order contribution is known if the fermion density  $\varrho(r)$  has been obtained, since the function  $f(p, q = 0)$  determines this quantity  $\varrho$  through equation (2.6).

**4. Two-dimensional harmonic confinement: Dirac density matrix together with some numerical results for the diagonal fermion particle density**

In this section we turn to the case of two-dimensional harmonic confinement. We shall begin by stating a result, in the form of a multidimensional integral, for the Dirac density matrix. Some background to this is summarized in appendix A. It will then be shown that the diagonal element of this result, the Fermi particle density  $\varrho(r)$ , can be readily computed for a selected number of closed shells. This result then prompts an alternative solution for  $\varrho(r)$  from the third-order linear homogeneous differential equation established by Minguzzi *et al* [12]. The numerical results from the multiple integral form (4.1) immediately below, with  $\vec{r}_0 = \vec{r}$ , are thereby confirmed to be correct.

As stated above, we will now simply give, as a starting point for this section, the multidimensional integral form of  $\gamma(\vec{r}, \vec{r}_0)$  for the two-dimensional isotropic harmonic oscillator with  $M + 1$  as the number of closed shells, and with  $\hbar, m$  taken as unity:

$$\gamma(x, y, x_0, y_0) = \frac{\omega e^{-\omega(r^2+r_0^2)/2}}{\pi^3 M!} \int_{\mathbb{R}^4} e^{-(t_1^2+t_2^2+t_3^2+t_4^2)} e^z \Gamma(M + 1, z) dt_1 dt_2 dt_3 dt_4 \tag{4.1}$$

where  $\Gamma(M + 1, z)$  is the incomplete gamma function and

$$z = 2[(\sqrt{\omega}x + it_1)(\sqrt{\omega}x_0 + it_2) + (\sqrt{\omega}y + it_3)(\sqrt{\omega}y_0 + it_4)]. \tag{4.2}$$

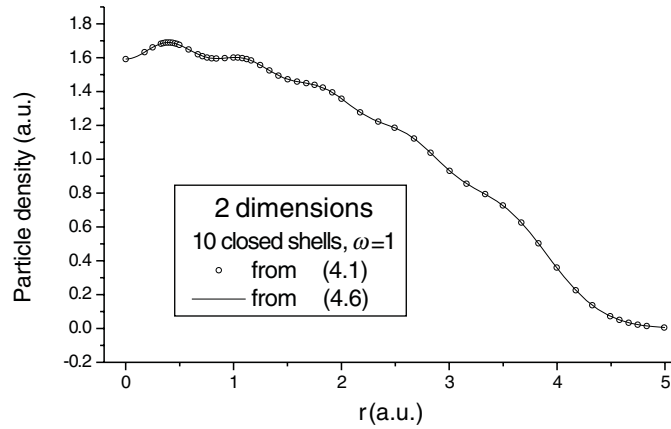
Since  $\Gamma(M + 1, z) = M! e^{-z} \sum_{n=0}^M z^n / n!$ , equation (4.1) is just

$$\gamma(x, y, x_0, y_0) = \frac{\omega e^{-\omega(r^2+r_0^2)/2}}{\pi^3} \sum_{n=0}^M \int_{\mathbb{R}^4} e^{-(t_1^2+t_2^2+t_3^2+t_4^2)} \frac{z^n}{n!} dt_1 dt_2 dt_3 dt_4. \tag{4.3}$$

The integrals can be readily evaluated.

We now turn to an approach which will allow a numerical check of the diagonal form of equation (4.3). The total density for the closed-shell isotropic two-dimensional oscillator has been discussed by Brack and van Zyl [21], and can be written in terms of the Laguerre polynomials as [12] (assuming single occupancy of levels)

$$\varrho(r) = \omega \sum_{\mu=0}^M (M + 1 - \mu)(-1)^\mu L_\mu(2\omega r^2) e^{-\omega r^2} \tag{4.4}$$



**Figure 1.** Fermi particle density for two-dimensional harmonic oscillator with ten closed shells. Agreement between the two cases shown, to the numerical accuracy employed, confirms the equivalence of the diagonal element of equation (4.1) for the Dirac density matrix and the well-established form (4.6) for the fermion density for this example.

with  $(M + 1)$  the number of filled shells. Starting from this expression, Minguzzi, March and Tosi derive the (third-order, linear) differential equation obeyed by the density [12]:

$$\frac{1}{8} \frac{\partial[\nabla^2 \varrho(r)]}{\partial r} + \left[ \left( M + \frac{3}{2} \right) \omega - \frac{\omega^2 r^2}{2} \right] \frac{\partial \varrho(r)}{\partial r} + \omega^2 r \varrho(r) = 0. \quad (4.5)$$

#### 4.1. An alternative 'recursion' form of the total density $\varrho(r)$ for $M + 1$ closed shells

Direct solution of equation (4.5) as a Gaussian times a finite polynomial in  $(\omega r^2)$  allows one to write  $\varrho(r)$  in a simpler form as

$$\varrho(r) = C_2 \exp(-\omega r^2) \sum_{n=0}^M a(n) (\omega r^2)^n \quad (4.6)$$

where

$$C_2 = \frac{N\omega/\pi}{\sum_{n=0}^M a(n)n!} \quad (4.7)$$

$N$  is the total particle number and the  $a(n)$  are related by the recursion relation

$$n(n+1)^2 a(n+1) + n(2(M+1) - 3n)a(n) + 2(n - (M+1))a(n-1) = 0 \quad (4.8)$$

with  $a(M) = 2^M$ . Note that, in two dimensions, the total particle number is  $N = (M+2)(M+1)/2$ . This form of the solution is analogous to those previously derived for total particle density for the one- and three-dimensional isotropic oscillator [14, 22]. It is worth reiterating here that the 1D analogue of equation (4.6) reproduces the diagonal ( $\eta = 0$ ) forms in equations (3.4) and (3.9)–(3.11).

Turning briefly to some numerical results for  $d = 2$ , we have used both the diagonal form of equation (4.1) and the alternative form of  $\varrho(r)$  given in equation (4.6) for ten closed shells. A plot is shown in figure 1: the results being in accord with the numerical accuracy to which we have worked. This confirms the correctness of the integral form (4.1) on the diagonal.

4.2. The kinetic energy density  $t(r)$

As in the one- and three-dimensional cases, the form (4.6) for the total density means that we can evaluate analytically the kinetic energy density  $t(r)$ . It is more convenient to express this in terms of the average  $\bar{t}(r) \equiv [t(r) + t_G(r)]/2$  of the  $\psi \nabla^2 \psi$  and  $(\nabla \psi)^2$  wavefunction forms, respectively, of the kinetic energy density. We then make use of the two-dimensional form of the ‘differential virial theorem’ [12],

$$\frac{\partial \bar{t}}{\partial r} = -\varrho(r) \frac{\partial V(r)}{\partial r} \tag{4.9}$$

where  $\partial V(r)/\partial r = \omega^2 r$ , and the density of equation (4.6) to find

$$\bar{t}(r) = -\frac{\omega C_2}{2} \exp(-\omega r^2/2) \sum_{n=0}^M \frac{a(n)}{(n+1)} (\omega r^2)^{n/2} \mathcal{M}_W \left( \frac{n}{2}, \frac{n+1}{2}, \omega r^2 \right) + \lambda_2 \tag{4.10}$$

with  $\mathcal{M}_W(b, c, z)$  being the Whittaker function [23] and

$$\lambda_2 = \frac{\omega^2 N}{2\pi} \tag{4.11}$$

for  $\bar{t}(r) \rightarrow 0$  as  $r \rightarrow \infty$ . Again, this form is analogous to those found in the one-dimensional [22] and three-dimensional [14] cases.

4.3. Total density and kinetic energy density in momentum ( $p$ ) space for the isotropic 2D oscillator

It is well known that the 1D harmonic oscillator wavefunctions have the same functional form in  $r$ -space as in  $p$ -space. The same is true in 2D, since we can always write the wavefunction in  $r$ -space as  $\psi_{n,m}(x, y) = \phi_n(x)\phi_m(y)$ . The implication therefore is that the particle density  $n(p)$  in  $p$ -space for the isotropic 2D oscillator also has the same functional form as  $\varrho(r)$  in  $r$ -space. Thus, we can write at once

$$n(p) = \tilde{C}_2 \exp(-p^2/\omega) \sum_{n=0}^M a(n) (p^2/\omega)^n \tag{4.12}$$

with

$$\tilde{C}_2 = \frac{N/(\pi\omega)}{\sum_{n=0}^M a(n)n!} \tag{4.13}$$

and the same recursion relations as in equation (4.8) for the  $a(n)$ . It follows that the density in  $p$ -space is also a solution of a differential equation of the same form as that for  $r$ -space, i.e.

$$\frac{1}{8} \frac{\partial [\nabla_p^2 n(p)]}{\partial p} + \left[ \left( M + \frac{3}{2} \right) \omega - \frac{p^2}{2\omega^2} \right] \frac{\partial n(p)}{\partial p} + \frac{pn(p)}{\omega^2} = 0. \tag{4.14}$$

Note that the kinetic energy density in  $p$ -space,  $t(p) = p^2 n(p)/2$ , is consequently also determined.

4.4. Fourier transform of  $n(p)$  and  $t(p)$  related to total kinetic energy

The relation

$$t'(r) = \left( (M + 3/2)\omega - \frac{\omega^2 r^2}{2} \right) \varrho'(r) \tag{4.15}$$



derived in [12], can be used to evaluate the total kinetic energy of the 2D system; multiplying both sides by  $r$  and integrating by parts over all space, we find for  $N$  particles

$$T/N = (M + 3/2)\omega/3 \quad (4.16)$$

where use has been made of the equality of potential and kinetic energies and the integral form of the virial theorem.

In [24] the Fourier transforms of the  $p$ -space particle density  $n(p)$  and of the kinetic energy density  $t(p)$  into  $r$ -space are shown to give information on the density matrix and on the total kinetic energy of a system. Specifically, the Fourier transform  $\tilde{n}(\vec{r})$  of  $n(p)$  is such that

$$\tilde{n}(\vec{r}) = \int \gamma(\vec{r}' - \vec{r}, \vec{r}') d\vec{r}' \quad (4.17)$$

where  $\gamma(\vec{r}, \vec{r}')$  is the first-order density matrix, while the transform  $\tilde{t}(\vec{r})$  of  $t(p)$  is such that  $\tilde{t}(0) = T$ , the total kinetic energy of the system. In the present case of the 2D oscillator,  $\tilde{n}(\vec{r})$  can be evaluated explicitly as

$$\tilde{n}(r) = \frac{\tilde{C}_2 \omega \pi}{2} \sum_{n=0}^M a(n) n! M(n+1, 1, -\omega r^2/4) \quad (4.18)$$

where  $M(a, b, z)$  is Kummer's  $M$ -function [23]. This form for  $\tilde{n}(r)$  is analogous to that constructed for the three-dimensional case in [24]. We note that at  $r = 0$ ,  $\tilde{n}(0) = N$  as it must be. Likewise  $\tilde{t}(\vec{r})$  can be evaluated as

$$\tilde{t}(r) = \frac{\tilde{C}_2 \omega^2 \pi}{2} \sum_{n=0}^M a(n) (n+1)! M(n+2, 1, -\omega r^2/4). \quad (4.19)$$

As  $r \rightarrow 0$ , it can be verified that

$$\tilde{t}(0) = \frac{\tilde{C}_2 \omega^2 \pi}{2} \sum_{n=0}^M a(n) (n+1)! \quad (4.20)$$

gives back the kinetic energy  $T$  of equation (4.16).

## 5. Cases $d = 3$ and $4$

Let us, very briefly, summarize some rather simple results for the final examples to be tackled here, namely  $d = 3$  and  $4$ . For the case of two closed shells and  $d = 3$ , Minguzzi *et al* [13] give  $\gamma(\vec{r}, \vec{r}_0)$  solely in terms of  $r^2 + r_0^2$  and  $\vec{r} \cdot \vec{r}_0$ . But we have the elementary identities

$$r^2 + r_0^2 = \frac{1}{2} [|\vec{r} + \vec{r}_0|^2 + |\vec{r} - \vec{r}_0|^2] \quad (5.1)$$

and

$$\vec{r} \cdot \vec{r}_0 = \frac{1}{4} [|\vec{r} + \vec{r}_0|^2 - |\vec{r} - \vec{r}_0|^2]. \quad (5.2)$$

Then, a straightforward calculation gives the Dirac matrix  $\gamma$  for the lowest two filled shells as

$$\begin{aligned} \gamma(|\vec{r} + \vec{r}_0|, |\vec{r} - \vec{r}_0|) &= \left(\frac{\omega}{\pi}\right)^{3/2} \exp\left(-\frac{\omega|\vec{r} + \vec{r}_0|^2}{4}\right) \exp\left(-\frac{\omega|\vec{r} - \vec{r}_0|^2}{4}\right) \\ &\times [1 + 2\omega (|\vec{r} + \vec{r}_0|^2 - |\vec{r} - \vec{r}_0|^2)]. \end{aligned} \quad (5.3)$$

It is a straightforward matter, by explicit substitution of form (5.3) in the partial differential equation (2.11) written specifically for three dimensions, to show that it satisfies this equation.

Of course, idempotency of  $\gamma$  is a further necessary requirement and that is ensured by the construction of the starting  $\gamma$  in [13] from orthonormal single-particle wavefunctions.

For the case  $d = 4$ , we shall consider two closed shells ( $M = 1$ ). The lowest shell is singly degenerate, while the second is four-fold degenerate; the density matrix has the form

$$\gamma(\vec{r}, \vec{r}_0) = \mathcal{N} \exp\left(-\frac{\omega|\vec{r} + \vec{r}_0|^2}{4}\right) \exp\left(-\frac{\omega|\vec{r} - \vec{r}_0|^2}{4}\right) [1 + b\omega(\vec{r} \cdot \vec{r}_0)] \tag{5.4}$$

where  $\vec{r}$  and  $\vec{r}_0$  are now four-component vectors and  $\mathcal{N}, b$  are constants. Applying equation (2.10) gives

$$\gamma(\vec{\xi}, \vec{\eta}) = \mathcal{N} \exp(-\omega(\xi^2 + \eta^2)) [1 + b\omega(\xi^2 - \eta^2)]. \tag{5.5}$$

The constants  $\mathcal{N}$  and  $b$  can be determined if  $\gamma(\vec{r}, \vec{r}_0)$  is known on the diagonal, i.e. if the density  $\varrho(r)$  is known.

In  $d$  dimensions the density  $\varrho(r)$  is determined by

$$\frac{1}{8} \frac{\partial[\nabla^2 \varrho(r)]}{\partial r} + \left[ \left( M + \frac{d+1}{2} \right) \omega - \frac{\omega^2 r^2}{2} \right] \frac{\partial \varrho(r)}{\partial r} + d\omega^2 r \varrho(r)/2 = 0 \tag{5.6}$$

where

$$\nabla^2 \varrho = \frac{\partial^2 \varrho}{\partial r^2} + \frac{d-1}{r} \frac{\partial \varrho}{\partial r}. \tag{5.7}$$

Evidently, equations (5.6) and (5.7) contain equation (4.5) for the special case when  $d = 2$ . For general  $d$ , the solution to (5.6) can be written in the ‘recursion’ form as

$$\varrho(r) = C_d \exp(-\omega r^2) \sum_{n=0}^M a(n) (\omega r^2)^n \tag{5.8}$$

for  $(M + 1)$  closed shells, with

$$C_d = \frac{2N\Gamma(1 + d/2)\omega^{d/2}}{d\pi^{d/2} \sum_{n=0}^M a(n)\Gamma(n + d/2)} \tag{5.9}$$

the number of particles  $N$  given by  $N = \prod_{i=1}^d (M + i)/d!$ , and the  $a(n)$  determined by the relation

$$n(n+1)(n+d/2)a(n+1) + 2n[(M+1) - 3n/2]a(n) + 2[n - (M+1)]a(n-1) = 0. \tag{5.10}$$

For  $M = 1$  and  $d = 4$ , we then find  $a(0) = 1$ ,  $a(1) = b = 2$  and  $\mathcal{N} = C_4 = \omega^2/\pi^2$ , so that  $\gamma(\vec{r}, \vec{r}_0)$  is completely determined. In figure 2 we plot, for comparison with the two-dimensional case in figure 1, the density for the case of ten closed shells in four dimensions.

A referee has asked us to comment on why the  $d = 4$  oscillator is relevant to ‘reality’. This is explained in the study of [25] on the Wigner function for a system of degenerate fermions moving in an oscillator potential. These authors emphasize the interest in retaining dimensionality since various properties corresponding to, say,  $d = 4$ , may be related to those of similar systems (for example, a Coulombic potential) in one dimension higher or lower.

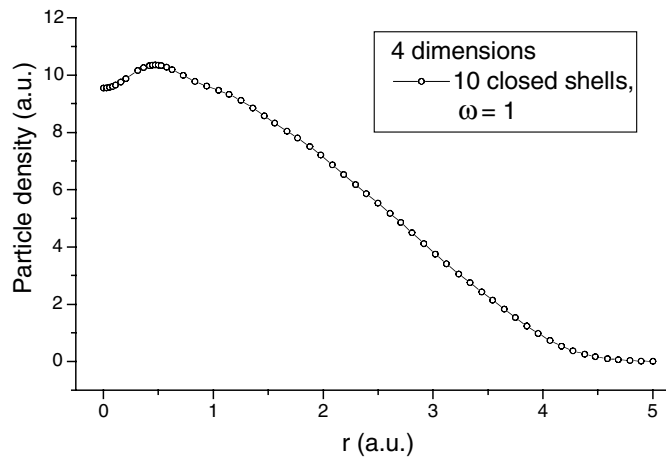


Figure 2. Fermi particle density for four-dimensional harmonic oscillator with ten closed shells.

## 6. Kinetic energy density in $d$ dimensions

While the kinetic energy density has been discussed earlier, with the most emphasis given to the case of  $d = 2$ , we want to summarize some results with general  $d$ -dimensional application for the harmonic oscillator in this penultimate section. Here, we focus entirely on the positive definite form of the kinetic energy density,  $t_G(\vec{r})$  say, corresponding to the  $(\nabla\psi)^2$  form in terms of wavefunctions. This can immediately be translated, in terms of the Dirac density matrix  $\gamma(\vec{r}_1, \vec{r}_2)$ , to

$$t_G(\vec{r}) = \frac{\hbar^2}{2m} (\nabla_{\vec{r}} \cdot \nabla_{\vec{r}_0}) \gamma(\vec{r}, \vec{r}_0) \Big|_{\vec{r}_0=\vec{r}}. \quad (6.1)$$

Again, as emphasized throughout the paper, we exploit the fact that  $\gamma$  in equation(6.1) depends only on the two scalar variables  $|\vec{\xi}|$  and  $|\vec{\eta}|$ , where the two vectors  $\vec{\xi}$  and  $\vec{\eta}$  are defined explicitly in equation (2.10).

By straightforward use of the chain rule, employing these new variables, one has the following identity for this specific case when  $\gamma = \gamma(|\vec{\xi}|, |\vec{\eta}|)$ :

$$(\nabla_{\vec{r}} \cdot \nabla_{\vec{r}_0}) \gamma(\vec{r}, \vec{r}_0) \Big|_{\vec{r}_0=\vec{r}} = \frac{1}{4} \left( \nabla_{\vec{\xi}}^2 - \nabla_{\vec{\eta}}^2 \right) \gamma \Big|_{|\vec{\eta} \rightarrow 0}. \quad (6.2)$$

In  $d$  dimensions, we have the further result

$$\nabla_{\vec{\xi}}^2 \gamma = \frac{\partial^2 \gamma}{\partial \xi^2} + \frac{d-1}{r} \frac{\partial \gamma}{\partial \xi} \quad (6.3)$$

with a corresponding formula for  $\nabla_{\vec{\eta}}^2 \gamma$ .

As a very specific example, let us utilize the 3D example in equation (5.3), applicable to the lowest two filled shells. Then, choosing  $\omega = 1$  for notational simplicity, we obtain

$$t_G(\vec{r}) = \frac{1}{8\pi^{3/2}} \exp(-\xi^2) [24 - 12\xi^2 + 8\xi^4] \quad (6.4)$$

which, on integration to find  $T = \int_0^\infty t(r) 4\pi r^2 dr$ , gives  $E/2$  where  $E$  is the total energy (sum of eigenvalues) for two closed shells.

In general, in  $d$  dimensions, the basic results of this section are embodied in equations (6.1)–(6.3), and, of course, to find the  $d$ -dimensional total kinetic energy the correct ‘volume’ element in  $d$  dimensions must be employed, to replace  $4\pi r^2 dr$  used above for the 3D example.

## 7. Summary and possible future directions

The main achievements of the present theoretical study are:

- (i) The partial differential equation (2.13) in terms of sum and difference of variables  $|\vec{r} + \vec{r}_0|$  and  $|\vec{r} - \vec{r}_0|$ . This equation holds in  $d$  dimensions and is readily shown to embrace equation (2.5) derived in the early investigation of March and Young [17]. With the change of dependent variable made in equation (2.6), one is led to equation (2.8), which is a simple partial differential equation also valid for the  $d$ -dimensional harmonic oscillator.
- (ii) The explicit multiple-integral form (4.1) for the 2D isotropic harmonic oscillator. This diagonal form  $\varrho(x, y) = \varrho(r)$  has been shown numerically (for ten closed shells) to be identical to that derived directly from the ‘recursion’ form (4.6), which in turn solves the (ordinary) differential equation (4.5).
- (iii) The demonstration for the 2D fermion density  $\varrho(r)$  that the properties of the highest occupied shell alone determine  $\varrho(r)$  completely (compare, in 1D, equation (3.8) with difference variable  $\eta$  set equal to zero).
- (iv) Directly from the Dirac matrix, the positive definite kinetic energy density  $t_G(r)$  is derived in section 6.

As to future directions, precise mathematics by which one could pass from exact results such as the 2D  $\gamma(\vec{r}, \vec{r}_0)$  in equation (4.1) to the asymptotic form as one approaches the limit  $N \rightarrow \infty$  would be of interest. Such a limiting form of  $\gamma$  must evidently have the Thomas–Fermi 2D density  $\varrho(r)$  as its limiting diagonal result.

## Acknowledgments

It is a pleasure for NHM to thank Professor J A Alonso for most generous hospitality during a visit to the University of Valladolid, which made this collaborative study possible. NHM also acknowledges many valuable discussions on the area embraced by this paper with Professor A Holas, Dr A Minguzzi and Professor M P Tosi. IAH wishes to acknowledge support from the Flemish Science Foundation (FWO) under grant no G.0347.97. We also thank the University of Antwerp (RUCA) for its support in the framework of the Visiting Professors Programme. This work is also supported by the Concerted Action Programme of the University of Antwerp, and by the Spanish DGES (PB98-0370) and Junta de Castilla y León (CO2/199).

## Appendix A. Multidimensional integral for the Dirac density matrix in two dimensions

In Cartesian coordinates, the normalized wavefunction  $\psi_{n,m}(x, y)$  for the state of the 2D oscillator specified by state numbers  $n, m$  is ( $\hbar = m = 1$ )

$$\psi_{n,m}(x, y) = \frac{\sqrt{\omega} e^{-\omega(x^2+y^2)/2}}{(2^{n+m}\pi n!m!)^{1/2}} H_n(\sqrt{\omega}x) H_m(\sqrt{\omega}y) \quad (\text{A.1})$$

with  $H_j$  the Hermite polynomials. If we now use the integral representation of the Hermite polynomials [26],

$$H_j(x) = \frac{2^j}{\sqrt{\pi}} \int_{-\infty}^{\infty} (x + it)^j \exp(-t^2) dt \quad (\text{A.2})$$

we can write

$$\psi_{n,m}(x, y) = \frac{\sqrt{\omega} 2^{(n+m)/2} \exp(-\omega(x^2 + y^2)/2)}{\pi^{3/2} \sqrt{n!m!}} \int_{\mathbb{R}^2} (\sqrt{\omega}y + it_3)^m (\sqrt{\omega}x + it_1)^n e^{-t_1^2 - t_3^2} dt_1 dt_3. \quad (\text{A.3})$$

Then the 1DM becomes

$$\begin{aligned} \gamma(x, y, x_0, y_0) &= \sum_{n,m} \psi_{n,m}^*(x, y) \psi_{n,m}(x_0, y_0) \\ &= \frac{\omega e^{-\omega(r^2+r_0^2)/2}}{\pi^3} \int_{\mathbb{R}^4} e^{-t_1^2-t_2^2-t_3^2-t_4^2} dt_1 dt_2 dt_3 dt_4 \sum_{n,m} \frac{2^{n+m}}{n!m!} \\ &\quad \times [(\sqrt{\omega}x + it_1)(\sqrt{\omega}x_0 + it_2)]^n [(\sqrt{\omega}y + it_3)(\sqrt{\omega}y_0 + it_4)]^m. \end{aligned} \quad (\text{A.4})$$

For the isotropic oscillator with  $(M + 1)$  closed shells, the sum over  $n, m$  becomes a sum over  $n$ , with  $m = N - n$ , as  $n$  goes from 0 to  $N$ , and a subsequent sum over  $N$  from 0 to  $M$ . With these restrictions, the summations in equation (A.4) result in equation (4.1). This form of  $\gamma$  can be straightforwardly generalized to arbitrary dimensionality.

### Appendix B. Total 2D density in terms of one-dimensional densities, and of wavefunctions for highest occupied level

For the case of non-interacting particles, since the two-dimensional eigenfunctions  $\psi_{nm}(x, y)$  can be constructed as products of the known one-dimensional (1D) eigenfunctions  $\phi_n(x)$  and  $\phi_m(y)$ , the total density in 2D is given by an expression of the form

$$\varrho^{2D}(x, y) = \sum_{n,m} \psi_{nm}^2(x, y) = \sum_{n,m} \phi_n^2(x) \phi_m^2(y) \quad (\text{B.1})$$

where indices  $n, m$  sum over all allowed states. Since we can always write  $\phi_n^2 = \varrho_n^{1D} - \varrho_{n-1}^{1D}$ , where  $\varrho_n^{1D}$  is the total density associated with a 1D oscillator having  $(n + 1)$  filled shells, we can rewrite the isotropic 2D density in terms of 1D densities as

$$\varrho_M^{2D}(x, y) = \sum_{N=0}^M \sum_{n=0}^N [\varrho_n^{1D}(x) - \varrho_{n-1}^{1D}(x)] [\varrho_{N-n}^{1D}(y) - \varrho_{N-n-1}^{1D}(y)] \quad (\text{B.2})$$

where we take  $\varrho_{i-j}^{1D} = 0$  for  $j > i$ .

It is possible to confirm, starting from the above relation (as an extension of the case for the 1D harmonic oscillator [19]), that in the isotropic 2D case the total density  $\varrho_M^{2D}(x, y) = \varrho_M^{2D}(r)$  for the system with  $(M + 1)$  filled shells is completely characterized by the properties of the wavefunctions for the highest occupied shell alone. As noted by Lawes and March [19], for the 1D oscillator the work of Husimi [20] shows that the density  $\varrho_n^{1D}(x)$  for a system with  $n$  filled states can be related to the wavefunction  $\phi_n(x)$  for the  $n$ th state alone through

$$[\varrho_n^{1D}(x)]' = -x\phi_n^2(x) + \frac{1}{2} \frac{d}{dx} \phi_n^2(x) \quad (\text{B.3})$$

(we take units in this section such that  $\omega = 1$ ). If we define a quantity analogous to  $\phi_n^2$ ,  $\Psi_M^2(x, y) = \sum_{n=0}^M \phi_n^2(x) \phi_{M-n}^2(y) = \varrho_M^{2D}(x, y) - \varrho_{M-1}^{2D}(x, y)$ , for the  $(M + 1)$ st shell of the 2D oscillator, where  $\varrho_M^{2D}(x, y)$  is the total density of the oscillator with  $(M + 1)$  filled shells, then using equation (B.2) we can also write

$$\Psi_M^2(x, y) = \sum_{n=0}^M [\varrho_n^{1D}(x) - \varrho_{n-1}^{1D}(x)] [\varrho_{M-n}^{1D}(y) - \varrho_{M-n-1}^{1D}(y)]. \quad (\text{B.4})$$

We also know, using equation (23) of [12], that (using our present notation for indices)

$$\Psi_M^2(x, y) = \varrho_M^{2D}(r) - \varrho_{M-1}^{2D}(r) = \mathcal{Q}_0^{(M+1)}(y) \frac{e^{-y/2}}{\pi} \quad (\text{B.5})$$

where the  $Q_i^{(M+1)}(y)$  are defined in terms of the Laguerre polynomials. But  $Q_M^{2D}(r)$  can be completely expressed in terms of  $Q_0^{(M+1)}(y)$  and its derivatives (equations (4) and (7) of [12]). Therefore  $Q_M^{2D}(r)$  is completely determined by  $\Psi_M^2(r)$  and its derivatives.

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