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LETTER TO THE EDITOR

Density and near-diagonal Dirac density matrix for closed shells of isotropic harmonically confined fermions in three dimensions

I A Howard[1] **and N H March**[1,2]

[1] Department of Physics, University of Antwerp (RUCA), Groenenborgerlaan 171, B-2020 Antwerp, Belgium

[2] University of Oxford, Oxford, UK

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Abstract

In early work, Lawes and March obtained a differential equation for an arbitrary number of independent harmonically confined fermions in one dimension, and very recently this result has been generalized to apply to three-dimensional (3D) isotropic harmonic confinement. Here, an exact solution of this 3D equation for the fermion particle density $\rho(r)$ is constructed, and the near-diagonal form of the Dirac density matrix is also obtained.

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A long-term aim of density functional theory is to construct a differential equation for the particle density ρ of N fermions, for arbitrary N, without recourse to Schrödinger wavefunctions. For the admittedly very limited case of independent fermions, harmonically confined and restricted to one-dimensional motion, Lawes and March [1] in early work gave such a differential equation, namely

$$\frac{\rho'''(x)}{8} + \left(N - \frac{x^2}{2}\right)\rho'(x) + \frac{1}{2}\frac{\partial V}{\partial x}\rho(x) = 0 \qquad (1)$$

the lowest state corresponding to $N = 1$, with the potential energy given by $V(x) = (1/2)x^2$. Impetus for further theoretical study of harmonically confined fermions has come from the recent experimental work of Demarco and Jin [2]. This has motivated the study of Minguzzi *et al* [3], who have very recently generalized equation (1) to three dimensions, for isotropic harmonically confined fermions filling an arbitrary number $M + 1$ of closed shells. Their differential equation reads

$$\frac{1}{8}\frac{\partial}{\partial r}[\nabla^2\rho(r)] + [(M+2)\omega - V(r)]\rho'(r) + \frac{3}{2}\frac{\partial V}{\partial r}\rho(r) = 0 \qquad (2)$$

where the isotropic harmonic potential is now written as

$$V(r) = \tfrac{1}{2}\omega^2 r^2. \tag{3}$$

This equation is here shown to have a relatively simple solution for $\rho(r)$ of the form

$$\rho(r) = C\exp(-\omega r^2)\sum_{n=0}^{M} a(n)(\omega r^2)^n. \tag{4}$$

In equation (4), the normalization constant C is given by

$$C = \left[\frac{\sqrt{\pi}}{2}\left(\frac{\omega}{\pi}\right)^{3/2} N\right] \Big/ \sum_{n=0}^{M} a(n)\Gamma(n+3/2). \tag{5}$$

Here, N is the total fermion number for $(M+1)$ filled shells, which is readily obtained from the degeneracy of the three-dimensional (3D) oscillator levels as

$$N = (M+1)(M+2)(M+3)/6. \tag{6}$$

Finally, in equation (5) the coefficients $a(n)$, which depend on the number of closed shells considered, are related by the recursion relation

$$0 = a(n+2)\left[\frac{(n+2)(2n+5)}{2}\right] + a(n+1)[2(M+1) - 3(n+1)] + a(n)\left[\frac{2(n-M)}{(n+1)}\right] \tag{7}$$

with

$$a(M) = 2^M.$$

After noting at this point that these results have been confirmed by explicit calculation for the first few values of M, we sketch the derivation of equations (4)–(7). From the known form of the 3D harmonic-oscillator wavefunctions [4], it is obvious that the total density must have a factor $\exp(-\omega r^2)$. If it is assumed that the full solution for the density can be written in the form of the product of this factor and a finite series in powers of r, it is found by simple substitution in equation (2) that equation (4) is a valid solution provided the $(M+1)$ terms in the series have coefficients related by the recursion relation of equation (7).

We want to add some comments here as to the near-diagonal generalization of equation (4) to treat the Dirac [5] density matrix $\gamma(\boldsymbol{r}, \boldsymbol{r}_0)$, which is such that

$$\gamma(\boldsymbol{r}, \boldsymbol{r}_0)|_{\boldsymbol{r}_0=\boldsymbol{r}} = \rho(\boldsymbol{r}). \tag{8}$$

The density matrix γ satisfies the equation of motion [6]

$$\nabla_r^2\gamma - \nabla_{r_0}^2\gamma = \frac{2m}{\hbar}\left[\frac{1}{2}\omega^2(r^2 - r_0^2)\right]\gamma(\boldsymbol{r}, \boldsymbol{r}_0). \tag{9}$$

However, it is important at this point to stress that the canonical density matrix for the 3D oscillator, $C(\boldsymbol{r}, \boldsymbol{r}_0, \beta)$, also satisfies equation (9). In terms of wavefunctions $\psi_i(\boldsymbol{r})$ and corresponding eigenvalues ϵ_i

$$C(\boldsymbol{r}, \boldsymbol{r}_0, \beta) = \sum_{\text{all}\, i} \exp(-\beta\epsilon_i)\psi_i^*(\boldsymbol{r})\psi_i(\boldsymbol{r}_0). \tag{10}$$

Sondheimer and Wilson [7] showed for the isotropic 3D harmonic oscillator that

$$C(\boldsymbol{r}, \boldsymbol{r}_0, \beta, \omega) = \left[\frac{\omega}{2\pi\sinh(\beta\omega)}\right]^{3/2} \exp\left[-\frac{\omega|\boldsymbol{r}+\boldsymbol{r}_0|^2}{4}\tanh\left(\frac{\beta\omega}{2}\right)\right] \times \exp\left[-\frac{\omega|\boldsymbol{r}-\boldsymbol{r}_0|^2}{4}\coth\left(\frac{\beta\omega}{2}\right)\right]. \tag{11}$$

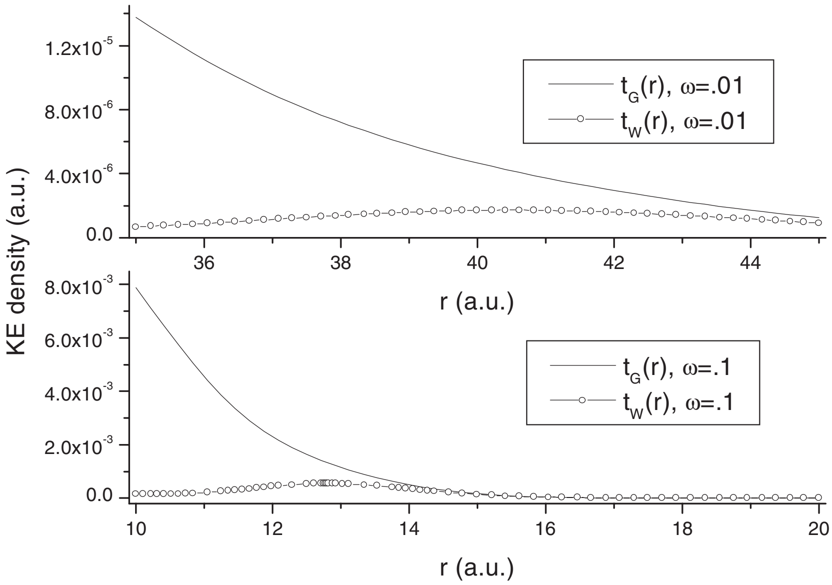

Figure 1. The (positive definite) kinetic energy density $t_G(r)$ compared with the von Weizsäcker $t_W(r)$ for $M = 9$, for $\omega = 0.01$ and 0.1 au.

The inverse Laplace transform $\mathcal{L}^{-1}$ of C/β with respect to β yields $\mathcal{L}^{-1}[C/\beta] \to \gamma(\boldsymbol{r}, \boldsymbol{r}_0, E)$. This establishes, by using equation (11), that γ depends only on two space variables $|\boldsymbol{r} + \boldsymbol{r}_0|$ and $|\boldsymbol{r} - \boldsymbol{r}_0|$. This is a huge simplification over the general central field case for closed shells, when γ depends on $|\boldsymbol{r}|$, $|\boldsymbol{r}_0|$ and the angle between the two vectors. One is led then to write, by expansion around the diagonal,

$$\gamma(\boldsymbol{r}, \boldsymbol{r}_0) = \rho\left(\frac{|\boldsymbol{r} + \boldsymbol{r}_0|}{2}, \omega\right) + f\left(\frac{|\boldsymbol{r} + \boldsymbol{r}_0|}{2}\right)|\boldsymbol{r} - \boldsymbol{r}_0|^2 + \mathcal{O}(|\boldsymbol{r} - \boldsymbol{r}_0|^4). \qquad (12)$$

The first term is known from equation (4), while

$$f(r) = -\frac{t_G(r)}{3} + \frac{\nabla^2\rho}{24} \qquad (13)$$

where $t_G(r)$ is defined from the wavefunction form $\frac{1}{2}\sum_i(\nabla\psi)^2$ (see [8]). However, we already know that [3]

$$\frac{t'(r)}{\rho'(r)} = (M+2)\hbar\omega - \frac{1}{2}\omega^2 r^2 \qquad (14)$$

and

$$t_G(r) = t(r) + \tfrac{1}{4}\nabla^2\rho(r). \qquad (15)$$

Thus we have also determined the near-diagonal behaviour of the Dirac density matrix from a knowledge of $\rho(r)$ plus the potential $V(r)$.

The averaged kinetic energy density $\bar{t}(r) = [t_G(r) + t(r)]/2$ can be determined explicitly from equations (4)–(7) as

$$\bar{t}(r) = \sum_{n=0}^{M} \tau_n(r) + \lambda \qquad (16)$$

with

$$\tau_n(r) = -\frac{3}{8}\frac{N\omega^{5/2}}{\pi(n+1)}\frac{(\omega r^2)^{n/2}}{\sum_{n=0}^{M} a(n)\Gamma(n+3/2)}\exp(-\omega r^2/2)a(n)\mathcal{M}\left(\frac{n}{2}, \frac{(n+1)}{2}, \omega r^2\right) \quad (17)$$

and $\mathcal{M}(\kappa, \mu, z)$ the Whittaker $\mathcal{M}$-function with parameters (κ, μ) [9]. Here the constant λ on the right-hand side of equation (16) can be evaluated as

$$\lambda = \frac{3}{8}\frac{N\omega^{5/2}}{\pi}\frac{\sum_{n=0}^{M} a(n)\Gamma(n+1)}{\sum_{n=0}^{M} a(n)\Gamma(n+3/2)}. \quad (18)$$

The final point we wish to make is the expectation that the (positive definite) kinetic energy $t_G(r)$ will eventually, outside the classical radius, tend to the von Weizsäcker kinetic energy density $t_W(r)$ defined by

$$t_W(r) = \frac{1}{8}\frac{\rho'^2(r)}{\rho(r)} \quad (19)$$

at sufficiently large r. In figure 1 we show $t_G(r)$ and $t_W(r)$ for $M = 9$ (i.e. for ten filled shells) and for the cases $\omega = 0.1$ and 0.01 au. Especially in the lower part of the figure it is plain that $t_G(r)$ approaches $t_W(r)$ as one exceeds the classical radius.

In summary, equation (4) constitutes an exact solution, for $(M + 1)$ closed shells, of the differential equation (2) of [3]. This has then been employed, together with equations (13) and (14), to determine the near-diagonal behaviour of the Dirac density matrix $\gamma(\boldsymbol{r}, \boldsymbol{r}_0)$ through equation (12). Finally, the positive definite kinetic energy density $t_G(r)$ has been shown to approach the von Weizsäcker form (16) in the tunnelling region outside the classical radius of the oscillator potential.

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