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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

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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 $\rho$ 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

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

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

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

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

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

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 $\gamma$ 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 $\epsilon_i$

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

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

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

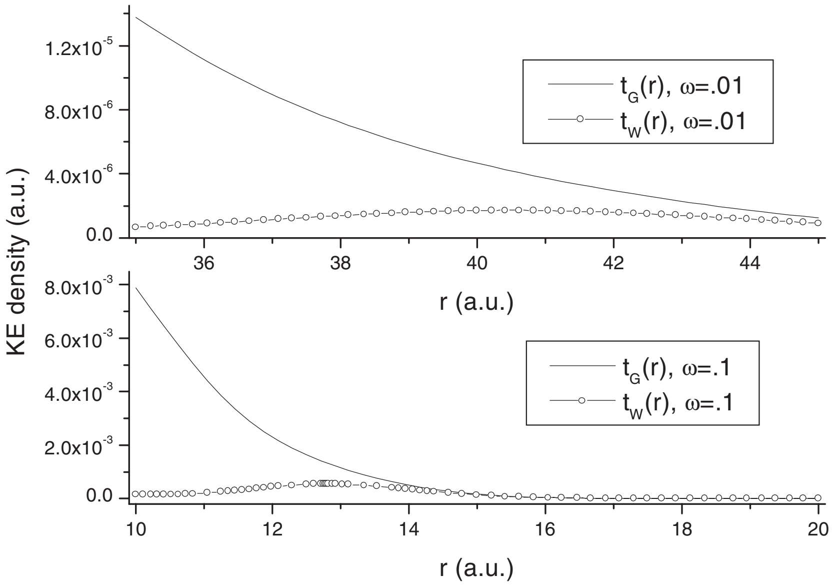


**Figure 1.** The (positive definite) kinetic energy density $t_G(r)$ compared with the von Weizsäcker $t_W(r)$ for $M = 9$, for $\omega = 0.01$ and 0.1 au.

The inverse Laplace transform $\mathcal{L}^{-1}$ of $C/\beta$ with respect to $\beta$ yields $\mathcal{L}^{-1}[C/\beta] \to \gamma(\boldsymbol{r}, \boldsymbol{r}_0, E)$. This establishes, by using equation (11), that $\gamma$ 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 $\gamma$ 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,

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

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

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

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]

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

and

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

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

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

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 $(\kappa, \mu)$ [9]. Here the constant $\lambda$ 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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