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Relativistic effects when many independent Fermions are confined in *d* dimensions

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Abstract

The study of the density of independent harmonically confined Fermions is of considerable current interest because of (a) quantum dots and (b) the experiments of DeMarco and Jin on some alkali metal vapours in magnetic traps. Our concern here is with relativistic effects, first in harmonically confined assemblies of electrons as in (a) above and secondly with a stronger type of Fermion confinement typified again by electrons but now in a quartic rather than quadratic potential. While our numerical illustrations are for dimensionalities $d = 1$ and 3, some analytical results are presented in d dimensions.

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1. Introduction

Harmonic confinement has been of considerable interest because of (a) quantum dots and following experiments on Bose–Einstein condensation [1–3]; (b) the study of DeMarco and Jin [4] (see also [5–7]) on magnetically trapped Fermion vapours. Since magnetic traps are well represented by harmonic confinement, and different geometries can span two and three dimensions, the experiments in [4–7] above motivated Minguzzi *et al* [8, 9] to construct differential equations for the Fermion density $\rho(r)$ for isotropic harmonic confinement in two and three dimensions. Their studies generalized the early work of Lawes and March [10] on one-dimensional harmonic confinement. These three studies in [8–10] can be subsumed into the d-dimensional differential equation [11]

$$\frac{\hbar^2}{8m_0}\frac{\partial[\nabla^2\rho(r)]}{\partial r} + \left[\left(M + \frac{d+1}{2}\right)\hbar\omega - \frac{m_0\omega^2 r^2}{2}\right]\frac{\partial\rho(r)}{\partial r} + dm_0\omega^2 r\rho(r)/2 = 0 \qquad (1)$$

with ω the characteristic frequency and $(M + 1)$ the number of closed shells. For $d = 3$, Howard and March [12] solved equation (1) in a finite series form, and we depict their result for $\rho(r)$ for 13 closed shells (or $N = 455$ one-particle levels with single occupancy) in figure 1.

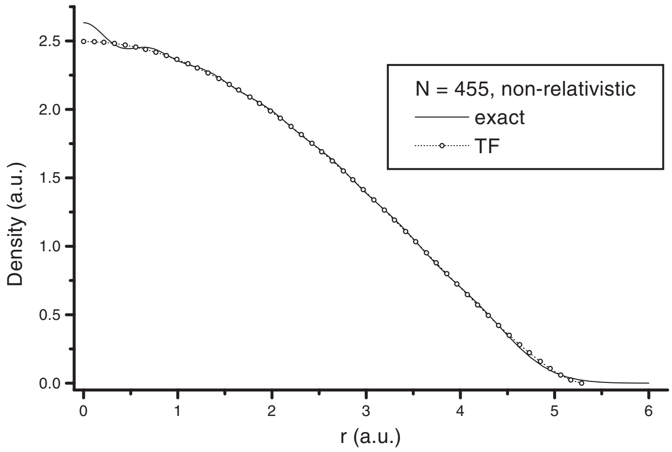

Figure 1. Fermion densities for three-dimensional harmonic confinement. Exact density shown from solution of equation (1) for 13 closed shells ($N = 455$ is number of particles with single occupancy of levels). Choice of variables is $m_0 = 1$ (electron rest mass in atomic units; i.e., for quantum dot example in three dimensions), $c = 137$ and $\hbar\omega = 1$. The non-relativistic Thomas–Fermi (TF) density is also plotted. For this value of N, the relativistic TF density of equations (5) and (6) is graphically indistinguishable from the non-relativistic TF results.

For comparison with this result, we show the Thomas–Fermi semiclassical approximation given by

$$\rho^{\mathrm{TF}}(r) = \frac{4\pi}{3h^3}(2m_0)^{3/2}[\mu - V(r)]^{3/2} \tag{2}$$

where m_0 denotes the Fermion (rest) mass, and $V(r) = kr^2/2$ with k the force constant characterizing the harmonic confinement. The chemical potential μ is evidently to be determined from the normalization requirement

$$N = \int_0^{r_c} \rho^{\mathrm{TF}}(r) 4\pi r^2 \, \mathrm{d}r = \frac{4\pi}{3h^3}(2m_0)^{3/2} \int_0^{r_c} [\mu - V(r)]^{3/2} 4\pi r^2 \, \mathrm{d}r \tag{3}$$

where the classical radius r_c is determined from $\mu = kr_c^2/2$. This yields

$$N = \frac{1}{6}\left(\frac{\mu}{\hbar\omega}\right)^3. \tag{4}$$

The focus of this paper is to study relativistic effects when many independent Fermions are confined in d dimensions.

2. Relativistic Thomas–Fermi theory

It seems natural enough then to begin with relativistic Thomas–Fermi theory, going back to Vallarta and Rosen [13]. Their treatment gives the relativistic (R) chemical potential as

$$\mu_R = \sqrt{c^2 p_F^2(\mathbf{r}) + m_0 c^4} - m_0 c^2 + V(\mathbf{r}) \tag{5}$$

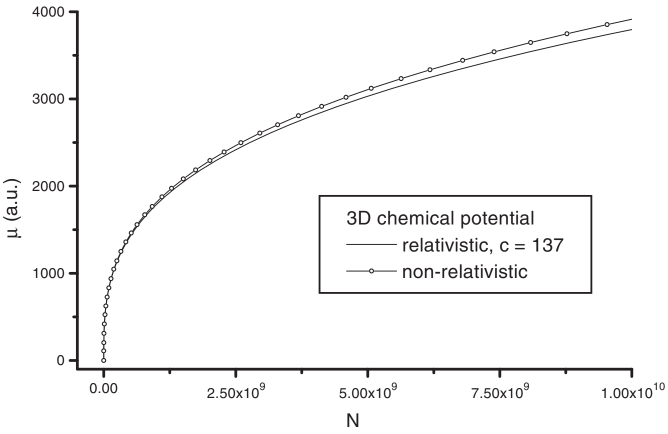

Figure 2. Chemical potentials for harmonic confinement in three dimensions as a function of Fermion number N ($m_0 = 1, c = 137$ and $\hbar\omega = 1$ as in figure 1). The upper curve is non-relativistic TF result. The lower curve is from relativistic TF theory. The asymptotic behaviour for N large is given explicitly for both non-relativistic and relativistic cases in equations (4) and (10).

where again the Fermi momentum $p_F(\mathbf{r})$ satisfies the phase-space relation, for singly occupied levels,

$$\rho_R^{\mathrm{TF}}(\mathbf{r}) = \frac{4\pi}{3h^3} p_F^3(\mathbf{r}) \tag{6}$$

or in d dimensions [14]

$$\rho_R^{\mathrm{TF}} = C_d p_F^d : \qquad C_d = \pi^{d/2} \bigg/ \left[h^d \Gamma\left(\frac{d}{2}+1\right)\right]. \tag{7}$$

Again, with $V(r) = kr^2/2$ inserted in equation (5) one finds with $d = 3$ the relativistic chemical potential μ_R, in units of $\hbar\omega$ and for $m_0 = 1$, as

$$N = -\frac{32}{945}\frac{(-4\mu_R^2c^6 - 41\mu_R^3c^4 - 24\mu_R^4c^2 - 4\mu_R^5 + 60\mu_Rc^8 + 64c^{10})}{\pi c^3\sqrt{4c^2+2\mu}} E\left(\frac{\sqrt{\mu_R}}{\sqrt{2c^2+\mu_R}}\right) - \frac{32}{945}\frac{(17\mu_R^3c^4 + 4\mu_R^4c^2 - 44\mu_Rc^8 + 12\mu_R^2c^6 - 64c^{10})}{\pi c^3\sqrt{4c^2+2\mu_R}} K\left(\frac{\sqrt{\mu_R}}{\sqrt{2c^2+\mu_R}}\right) \tag{8}$$

where K and E are the complete elliptic integrals of the first and second kinds, respectively. If we now plot $\rho_R(r)$ for $N = 455$, with $\hbar = m_0 = k = 1$ plus $c = 137$ in atomic units, we can hardly distinguish $\rho_R^{\mathrm{TF}}(\mathbf{r})$ from the non-relativistic TF curve.

Therefore to understand how relativity becomes important as N increases, we have plotted in figure 2 μ_R from equation (8) as a function of N. For sufficiently large N, figure 2 shows how non-relativistic (μ) and relativistic (μ_R) chemical potentials begin to diverge. The range of Fermion number N in the plots is very large, involving $N \sim 10^9$. However, for K^{40} in magnetic traps a million atoms are involved in the experiments (see for example [15]). But our plot of μ_R is for electrons, i.e., $m_0 = 1$ in atomic units; it is for electrons that relativistic effects may eventually prove significant in harmonic confinement in three dimensions. Figure 2 shows clearly that relativity becomes significant for large N. Taking the asymptotic limit of equation (8) for large $\mu_R \equiv \mu_3$, we find for $d = 3$ that

$$N = \frac{64}{945}\frac{\sqrt{2}}{\pi c^3}\mu_3^{9/2} + \frac{32}{105}\frac{\sqrt{2}}{\pi c}\mu_3^{7/2} + \frac{4c}{15}\frac{\sqrt{2}}{\pi}\mu_3^{5/2} + \mathcal{O}\big(\mu_3^{3/2}\big). \tag{9}$$

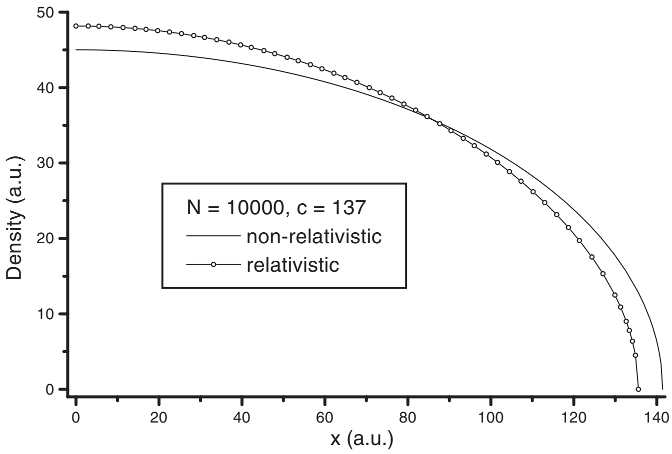

Figure 3. Electron densities for harmonic confinement in one dimension for 10 000 Fermions with single occupancy ($m_0 = 1, c = 137, \hbar\omega = 1$). Now there is a quite clearcut change in the electron density caused by relativistic effects. One can expect, in this example, that relativistic effects will be considerably larger than any changes in the non-relativistic TF density resulting from the exact solution of the analogue of equation (1) in one dimension, for $N = 10\,000$.

To lowest order, we then have for $d = 3$

$$\mu_3 = \frac{(945\pi)^{2/9}}{4} 2^{5/9} c^{2/3} N^{2/9} \tag{10}$$

and performing an equivalent expansion for $d = 1$ yields

$$\mu_1 = \frac{(3\pi)^{2/3}}{4} 2^{1/3} c^{2/3} N^{2/3} \qquad N \to \infty. \tag{11}$$

In general d dimensions, we find $\mu_d \propto c^{2/3} N^{2/3d}$ from the phase space equation (7).

The above considerations as to when relativistic effects become significant for $m_0 = 1$ have prompted us to consider next 10 000 singly occupied levels in one dimension. Then, from the TF approximation, both relativistic and non-relativistic densities are plotted in figure 3 for $\hbar\omega = 1$ and $c = 137$. Relativistic effects are clearly in evidence, the main qualitative features being that the Fermion density at the origin is increased noticeably, while the classically forbidden region, characteristic of semiclassical TF theories, is somewhat extended by inclusion of relativity. Plainly, for the parameters used in constructing figure 3 (especially $m_0 = 1$) there is little point in transcending the non-relativistic TF density using equation (1) for $d = 1$ and $N = 10\,000$, since relativistic effects will mask such non-relativistic corrections (except, of course, in the classically forbidden regions).

3. Difference equation approach

However, it will surely be important, for the future, to improve the relativistic TF theory for harmonic confinement by accounting for tunnelling tails in the region referred to above where the semiclassical density is identically zero. Therefore to obtain an estimate of the relativistic density which we believe should transcend the Vallarta–Rosen TF approximation we shall proceed heuristically by replacing the differential equation (1) by a difference equation which reads

$$\frac{(\rho(r+2\varepsilon)-\rho(r-2\varepsilon)-2\rho(r+\varepsilon)+2\rho(r-\varepsilon))}{16\varepsilon^3} + \left[M+\frac{(d+1)}{2}-\frac{r^2}{2}-\frac{(d-1)}{8r^2}\right]\frac{(\rho(r+\varepsilon)-\rho(r-\varepsilon))}{2\varepsilon} + \mathrm{d}r\frac{\rho(r)}{2}+\frac{(d-1)}{r}\frac{(\rho(r+\varepsilon)+\rho(r-\varepsilon)-2\rho(r))}{8\varepsilon^2}=0. \tag{12}$$

To our knowledge, such an approach for density functional theory is novel, though for individual wavefunctions Wall [16] already wrote a difference equation. Following his proposal, we note that the length scale of the interval ε in equation (12) is the Compton wavelength h/m_0c. Obviously, as $\varepsilon \to 0$ or $c \to \infty$, i.e. the non-relativistic limit, the heuristic proposal made here, which is embodied in the difference equation (12), reduces precisely to equation (1), as any correct density functional theory for an arbitrary number of closed shells must do.

We shall discuss the analytic solution of equation (12) in more detail elsewhere. Suffice it to say that we can write a solution for the relativistic Fermion density $\rho_R(r)$ in the form

$$\rho_R(r+n\varepsilon) = b^n(r,\varepsilon)\rho(r) \tag{13}$$

with $\rho(r)$ the corresponding non-relativistic density, n being an integer. Then b satisfies a quartic equation which we have solved exactly for three-dimensional harmonic confinement. Taking $c = 137$, the density is graphically indistinguishable from the exact non-relativistic density for $N = 455$ in figure 1 for any reasonable choice of ε.

Therefore, it seemed natural to return to the one-dimensional example in figure 3, with $N = 10\,000$, where, with $m_0 = 1, \hbar\omega = 1, c = 137$ we know that relativistic effects are significant. Though the choice of ε, proportional to the Compton wavelength h/m_0c, is somewhat arbitrary, and will need beyond the present heuristic arguments a first-principles theory for, say, harmonic confinement, to $\varepsilon = \varepsilon(N)$ apart from its scale h/m_0c, equation (11) for the relativistic chemical potential for large N compared to the non-relativistic counterpart $\mu_1 \propto N$ suggests that c is linked 'in scaling' with $N^{1/2}$, to convert equation (11) to $\mu \propto N$. Thus, with admittedly some arbitrariness, we have solved the quartic equation for the one-dimensional analogue of b in equation (13) exactly for $\varepsilon = 44$ a.u., and the result is shown in figure 4(*a*); $b(x)$ obtained approximately for $n = 1$ and this value of ε from equation (13) by inserting TF and Vallarta–Rosen densities is shown for comparison. We stress that we have made no attempt to find the 'best' ε, as its determination is outside the scope of our heuristic approach based on a difference equation exemplified by equation (12). However, to show what relativistic Fermion density the choice $\varepsilon = 44$ implies, we have used the exact $b(x)$ in figure 3 for $N = 10\,000$, together with the non-relativistic TF density of figure 3 to construct figure 4(*b*). The result seems sufficiently encouraging to justify a fuller first-principles study of the role of difference equations in relativistic density functional theory.

Before concluding, we wish to mention a further example we have studied, in which many Fermions are more strongly confined than by the harmonic potential discussed at length above. Briefly, we shall now summarize our findings for such a stronger confining potential

$$V(x) = ax^4. \tag{14}$$

Then we can generalize the large-N scaling results above in one dimension to

$$\mu_1 = \text{const} \times N^{4/3} : N \to \infty \tag{15}$$

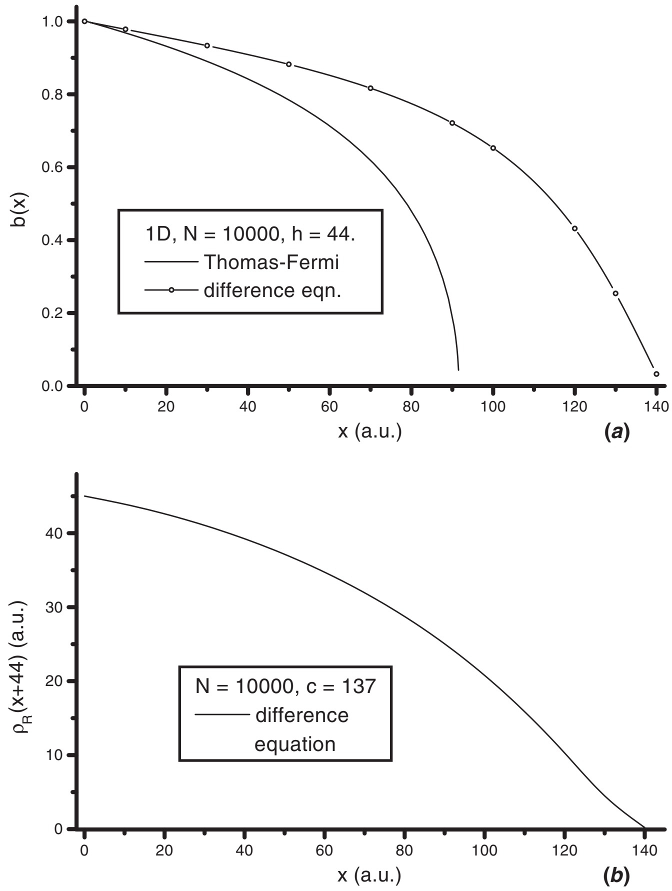

Figure 4. Illustrative use of the relativistic difference equation analogous to equation (12) in three dimensions for $N = 10\,000$ Fermions as in figure 3. The quantity $b(x)$ is shown for two cases in panel (*a*): (i) from the TF densities, as $b(x) = \rho_R(x+\varepsilon)/\rho(x)$, i.e. the ratio of the 'shifted' relativistic TF density to its non-relativistic counterpart and (ii) from the difference equation method proposed here. The choice of $\varepsilon = 44$ may eventually need refinement as we expect the relation of ε to the Compton wavelength to involve the number of Fermions N. Our TF estimates given in the body of the text lead us to conjecture that, for large N, $\varepsilon \sim N^{1/2}\lambda_{\mathrm{Compton}}$, but to refine that is a matter for first-principles theory, rather than for the heuristic method proposed here. Panel (*b*) shows the 'shifted' relativistic density $\rho_R(x+\varepsilon)$ with $\varepsilon = 44$, constructed, but now approximately as $\rho_R(x+\varepsilon) = b(x,\varepsilon)\rho_{\mathrm{TF}}(x)$, where $b(x,\varepsilon)$ is the exact solution of the difference equation (12) for $d = 1$, but the non-relativistic density is now approximated by its TF counterpart. This is an excellent approximation for $N = 10\,000$ considered here. We stress that we have not attempted to vary ε systematically, for reasons discussed in the caption to (*a*).

and the relativistic Thomas–Fermi counterpart to

$$\mu_{R1} = \mathrm{const} \times c^{4/5} N^{4/5} : N \to \infty. \tag{16}$$

The corresponding results in three dimensions are

$$\mu_3 = \mathrm{const} \times N^{8/21} : N \to \infty \tag{17}$$

and

$$\mu_{R3} = \mathrm{const} \times c^{4/5} N^{4/15} : N \to \infty. \tag{18}$$

To date, the differential equation for the non-relativistic density corresponding to equation (1), in the case of the potential $V = ax^4$ has not been obtained.

4. Summary and future directions

In summary, we have set out how one might make estimates of relativistic effects when many independent Fermions are subjected to confinement in *d* dimensions. As numerical examples, we have considered, for $d = 1$ and 3, two types of confinement: (a) harmonic as for quantum dots and very briefly (b) quartic confinement by the potential of equation (14). Finally, we have made a heuristic proposal whereby such a non-relativistic differential equation is to be replaced by a difference equation (see equation (12) for three-dimensional harmonic confinement). This aspect, we believe, makes a start on a relativistic density functional theory in terms of difference equations, but much further work is needed on the first-principles foundations of such a theory. Already, however, for wavefunction methods, but not to our knowledge density functional theory, in the studies of Wall [16], Ruijsenaars [17] and Ord [18], difference equations are in evidence, which encourages us as to the merit of the present heuristic approach to relativistic density functional theory. The heuristic treatment, while in its early stages of development of course as a density functional theory, has the considerable merit of avoiding a classically forbidden region, which is a consequence of semiclassical TF theories.

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