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The role of the von Weizsäcker kinetic energy gradient term in independent harmonically confined fermions for arbitrary two-dimensional closed-shell occupancy

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Abstract
The search for the single-particle kinetic energy functional $T_S[n]$ continues to be of major interest for density functional theory. Since it is expected to be generally applicable, exactly solvable models are of obvious interest. Here we focus on one, which is also of interest experimentally in magnetic trapping of ultracold fermion vapours. This is the model of independent harmonically trapped fermions in two dimensions. Here, the role of the von Weizsäcker inhomogeneity kinetic energy is a focal point, prompted also by the work of Delle Site (2005 *J. Phys. A: Math. Gen.* **38** 7893).

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1. Introduction

Current usage of density functional theory (DFT) [1] relies on the solution of one-electron Schrödinger equations [2, 3] to bypass the lack of knowledge of the single-particle (s) kinetic energy functional $T_S[n]$, where n is the ground-state fermion density.

In our earlier work, we have been concerned with many fermions subject to harmonic confinement. Here we present results specifically for independent fermions in two dimensions (2D) for an arbitrary number of closed shells, denoted below by $M + 1$.

Some further motivation for the present study has been afforded in [4] by Delle Site, who has argued for a reduction in weight of the von Weizsäcker contribution $T_W[n]$ to $T_S[n]$, where $T_W[n]$ is given by [5]

$$T_W[n] = \frac{\hbar^2}{8m}\int \frac{(\nabla n)^2}{n}\,\mathrm{d}\mathbf{r} = \int t_W(\mathbf{r})\,\mathrm{d}\mathbf{r}. \tag{1.1}$$

The outline of the present paper is then as follows. In section 2, we first set out the exact form of $T_S[n]$ for harmonic trapping in 2D. Then in section 3, the positive definite kinetic energy density ($(\nabla\psi)^2$ form) $t_g(\mathbf{r})$ is calculated for various numbers of closed shells and is compared numerically with the contribution $t_W(\mathbf{r})$ for the von Weizsäcker form (1.1). Section 4 deals explicitly with the various contributions to the exact functional $T_S[n]$ for the present 2D harmonically confined fermions. Contact is made with a proposal of Delle Site [4] for the reduction of the weight of the von Weizsäcker term. Section 5 constitutes a summary together with some proposals for future studies which should prove fruitful.

2. Form of single-particle kinetic energy functional T_S[n] for an arbitrary number of closed shells of 2D harmonically confined independent fermions

Minguzzi *et al* [6] wrote the single-particle kinetic energy density $T_S[n]$ for this 2D example of harmonic trapping as

$$T_S[n] = \int t_g(r)\,\mathrm{d}\mathbf{r}, \tag{2.1}$$

where

$$t_g(r) = \frac{1}{2}t_W(r) + \left[C_2 + \frac{\hbar^2}{8m}\int_0^r \mathrm{d}s \frac{n'(s)^2}{n(s)^3}\left(\frac{2}{s} + \frac{3n'(s)}{n(s)}\right)\right]n^2(r), \tag{2.2}$$

with C_2 being a constant [6] and $t_W(r)$ as given in equation (1.1).

In spite of the factor 1/2 multiplying $t_W(r)$ in equation (2.2), our purpose immediately below is to demonstrate that $t_g(r) \to t_W(r)$ for a sufficiently large r for harmonic confinement in 2D.

3. Asymptotic large r form of $t_g(r)$ in equation (2.2) compared with $t_W(r)$ in equation (1.1)

We have used the known ground-state density for $M + 1$ closed shells, which in 2D satisfies the differential equation [6]

$$\frac{\hbar^2}{8m}\frac{\partial}{\partial r}\nabla^2 n(r) + \left[\left(M + \frac{3}{2}\right)\hbar\omega - V(r)\right]n'(r) + \frac{\partial V(r)}{\partial r}n(r) = 0, \tag{3.1}$$

where the confining potential $V(r) = \frac{1}{2}m\omega^2 r^2$. Figure 1 shows the results for $M = 5$, the exact $t_g(r)$ in equation (2.2) being compared with the von Weizsäcker form $t_W(r) = (\hbar^2/8m)(n'^2/n)$ in equation (1.1), using of course the same exact 2D fermion density. Figure 1(*a*) shows this comparison over the entire range of interest of r, while figure 1(*b*) shows a restricted range. Notwithstanding the factor of 1/2 multiplying $t_W(r)$ in equation (2.2), to which we return below, it can be seen from figure 1(*b*) especially that for $M = 5$, $t_g(r)$ approaches $t_W(r)$ asymptotically at sufficiently large r.

Figure 2 shows similar results for $M = 14$, (*a*) showing the whole relevant range of r, and (*b*) focussing again on the large-r regime. The same conclusion is apparent, with the difference between $t_g(r)$ and $t_W(r)$ being of short range compared to the range of the total positive-definite kinetic energy $t_g(r)$.

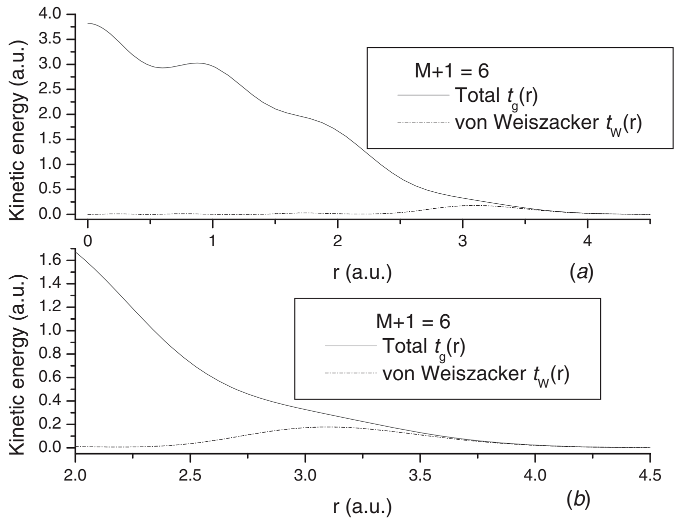

Figure 1. Kinetic energy densities $t_g(r)$ (solid line) and von Weizsäcker contribution $t_W(r)$ (dashed line) for $M + 1 = 6$ closed shells. (*a*) shows the whole *r*-range, while (*b*) is expanded to show agreement between $t_g(r)$ and $t_W(r)$ at large *r*.

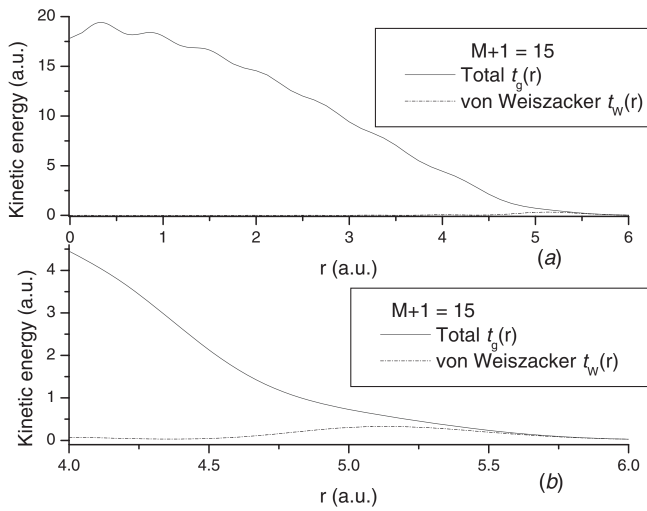

Figure 2. Kinetic energy densities $t_g(r)$ (solid line) and von Weizsäcker contribution $t_W(r)$ (dashed line) for $M + 1 = 15$ closed shells. (*a*) shows the whole *r*-range, while (*b*) is expanded to show agreement between $t_g(r)$ and $t_W(r)$ at large *r*.

4. Study of the individual contributions to the kinetic energy functional $T_S[n]$ for 2D harmonically trapped fermions in equation (2.2)

As a brief background to this section, we wish to stress here that many fermions subjected to harmonic confinement are currently of major interest because of experimental work on ultracold vapours of ^{40}K and ^{6}Li isotopes populating hyperfine states inside magnetic traps

Table 1. Individual contributions to the single-particle kinetic energy $T_S[n]$ for 2D harmonic confinement for $M+1$ closed shells containing N particles. Here, T_W refers to the second term in equation (4.1); T_1, T_3 and T_4 refer to the first, third and fourth terms, respectively.

M	N	T_{TF}	T_W	T_1	T_3	T_4
0	1	0.25	0.25	0.50	0.125	−0.375
1	3	1.25	0.5193	2.50	0.1923	−0.712
2	6	3.5	0.8132	7.00	0.3170	−1.1303
5	21	22.75	1.8028	45.50	0.5454	−2.3482
9	55	96.25	3.2840	192.50	0.8875	−4.1715
14	120	310.0	5.3029	620.00	1.3458	−6.6487

Table 2. Individual contributions to the single-particle kinetic energy $T_S[n]$ for 2D harmonic confinement for $M+1$ closed shells. Here, $T_{\text{non-univ}}$ denotes the 'non-universal' contribution, and T_S is the total single-particle kinetic energy.

M	$T_{\text{non-univ}} = T_1 + T_3 + T_4 - T_{TF}$	$T_S = T_1 + T_W + T_3 + T_4$
0	0	0.50
1	0.7307	2.50
2	2.6868	7.00
5	20.9472	45.50
9	92.9660	192.5
14	304.6972	620.0

[7–10]. For these experiments, it turns out to be possible to range from a fully spherical three-dimensional (3D) trap to a quasi-two-dimensional system. Here, we focus exclusively on the 2D case for the single-particle kinetic energy functional $T_S[n]$. The basic result given in [11] and in equations (2.1) and (2.2) above may be rewritten as

$$T_S[n] = c_2 \int n(s)^2 \,\mathrm{d}^2 s + \frac{\hbar^2}{16m} \int \frac{n'^2(s)}{n(s)} \,\mathrm{d}^2 s + \frac{\hbar^2}{m} \int n(s)^2 \left[\frac{1}{8} \int_0^s \frac{n'^2(u)}{n(u)^3} \,\mathrm{d}u + \frac{3}{16} \int_0^s \frac{n'^3(u)}{n(u)^4} \,\mathrm{d}u \right] \mathrm{d}^2 s. \tag{4.1}$$

The above result (4.1) of [11] is exact for 2D harmonic confinement for an arbitrary number $(M+1)$ of closed shells, the constant c_2 multiplying the TF-like kinetic energy density proportional to n^2 in the first term on the right-hand side of equation (4.1) being explicitly given by

$$c_2 = \frac{1}{2}\left(M + \frac{3}{2}\right)\frac{\hbar\omega}{n(0)} - \frac{\hbar^2}{16m}\left[\frac{\nabla^2 n}{n^2}\right]_0. \tag{4.2}$$

The tables above analyse the contributions to (4.1) for small numbers $M+1$ of closed shells between 1 and 15.

5. Summary and future directions

Focusing on 2D harmonic confinement, we have first demonstrated clearly the fact that the kinetic energy density $t_g(r)$ defined equivalently in equations (2.1) and (4.1) tends to the full von Weizsäcker contribution $t_W(r) = (\hbar^2/8m)(n'^2/n)$ at sufficiently large r. This is notwithstanding the 'dimensionality' reduction of $t_W(r)$ by 1/2 in equation (2.2). We display this equivalence for 6 and 15 closed shells respectively in figures 1 and 2.

Referring to the suggestion of Delle Site [4] as to the reduction of the von Weizsäcker contribution in $T_S[n]$ by a factor the author denotes by q, we see that such a reduction applies by a 'dimensionality' factor 1/2 in our 2D example of harmonically trapped fermions. The detailed analysis of the individual contributions to the single-particle kinetic energy $T_S[n]$ listed in table 4 will, we hope, stimulate further work in this area, for forms of confinement other than harmonic trapping, though we have stressed the relevance to ultracold fermion vapour experiments in this case.

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