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Kinetic energy density and Pauli potential: dimensionality dependence, gradient expansions and non-locality

A Holas†, P M Kozlowski‡ and N H March§

† Institute of Physical Chemistry of the Polish Academy of Sciences, ul Kasprzaka 44/52, 01-224 Warsaw, Poland
‡ Department of Chemistry, University of Arizona, Tucson, AZ 85721, USA
§ Theoretical Chemistry Department, University of Oxford, 5 South Parks Road, Oxford OX1 3UB, UK

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Abstract. For arbitrary level filling, the fully non-local kinetic energy density and Pauli potential for the one-dimensional harmonic oscillator can be constructed explicitly. In the present work, these exact results are eventually compared with the low-order gradient expansions. This prompts a fuller study of the dimensionality dependence of low-order gradient expansions for systems with general one-body potentials, and its relevance to the theory of the Pauli potential. One consequence of the present work is to display the generalization to D-dimensions as $(D-2)/3D$ of the three-dimensional Kirzhnits coefficient $\frac{1}{9}$ of the von Weizsäcker term in the kinetic energy density.

1. Introduction

A major aim of density functional theory (e.g. Parr and Yang 1989) remains the direct calculation of the electron density $\rho(\boldsymbol{r})$ from a given one-body potential $v(\boldsymbol{r})$. Since we shall be concerned with D-dimensional systems in the present work, let us first note the explicit result of the Thomas–Fermi statistical method:

$$\rho = C_D\{\mu_D - v\}^{D/2} \tag{1.1}$$

where C_D is a known constant, while the constant μ_D is the chemical potential. Equation (1.1) is, of course, only quantitative when v varies by but a small fraction of itself over a characteristic electron wavelength. When more rapid spatial variation occurs, then density gradients must be introduced in order to correct equation (1.1). The simplest of these 'corrections' stems from the von Weizsäcker inhomogeneity kinetic energy T_{W} which is given by

$$T_{\mathrm{W}}[\rho] = \frac{\hbar^2}{8m}\int \frac{(\nabla\rho)^2}{\rho}\,\mathrm{d}\tau. \tag{1.2}$$

As Kirzhnits (1957) was the first to demonstrate, for weakly inhomogeneous systems equation (1.2) must be reduced by some factor, to yield the lowest-order correction T_2 to the Thomas–Fermi (TF) kinetic energy, say T_0, as

$$T_2 = \lambda_D \frac{\hbar^2}{m}\int \frac{(\nabla\rho)^2}{\rho}\,\mathrm{d}\tau = \frac{\lambda_D}{\lambda_{\mathrm{W}}} T_{\mathrm{W}} \qquad \lambda_{\mathrm{W}} = \tfrac{1}{8}. \tag{1.3}$$

In three dimensions, Kirzhnits showed that $\lambda_D/\lambda_{\mathrm{W}} = \frac{1}{9}$, an alternative proof being given subsequently by Jones and Young (1971); see also Hodges (1973).

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2. Exact results for one-dimensional harmonic oscillator

2.1. Kinetic energy density

With this as background, let us next confront the above approximate results with an *exact model problem: the one-dimensional harmonic oscillator potential with N levels* singly occupied by non-interacting electrons and N quite general. Following early work by Husimi (1940) on the density matrix, Lawes and March (1979) obtained for this case the following relation between the potential $v(x)$ and the density $\rho(x)$ ($\hbar = m = 1$):

$$(N-v)\rho' + \tfrac{1}{2}v'\rho + \tfrac{1}{8}\rho''' = 0 \tag{2.1}$$

where we denote $\mathrm{d}f(x)/\mathrm{d}x$ as f', etc. These functions, together with the kinetic energy density $t_s(x)$, are related by the differential form of the virial theorem derived by March and Young (1959; see also Baltin 1985), valid for an arbitrary one-dimensional system:

$$t_s' + \tfrac{1}{2}v'\rho + \tfrac{1}{8}\rho''' = 0. \tag{2.2}$$

Here the following microscopic definition of t_s is adopted:

$$t_s = -\frac{1}{2}\sum_{i=1}^{N} \psi_i^* \nabla^2 \psi_i. \tag{2.3}$$

One can verify immediately that the expression for the harmonic potential in the form

$$v = \tfrac{1}{2}x^2 = -\frac{3t_s}{\rho} - \frac{\rho''}{4\rho} + N \tag{2.4}$$

satisfies equations (2.1) and (2.2). Then, by substitution of equation (2.4) into (2.2) we eliminate v to find the result (see also Kozłowski and March 1989, 1990)

$$\left(\frac{t_s}{\rho^3}\right)' = \frac{1}{8}\frac{((\rho')^2)'}{\rho^4}. \tag{2.5}$$

The integral of equation (2.5) is evidently

$$t_s(x) = \frac{1}{8}\frac{(\rho'(x))^2}{\rho(x)} + \tfrac{1}{2}\rho^3(x)\left(\int_0^x \mathrm{d}y\,\frac{(\rho'(y))^3}{\rho^5(y)} + C_t\right) \tag{2.6}$$

where, because of symmetry, it proves convenient to choose 0 for the lower limit of integration. The constant C_t is determined from equation (2.4) at $x = 0$ to be

$$C_t[\rho] = \tfrac{2}{3}\rho^{-2}(0)N[\rho] - \tfrac{1}{6}\rho^{-3}(0)\rho''(0) \tag{2.7}$$

where, evidently,

$$N = N[\rho] = \int \mathrm{d}y\,\rho(y). \tag{2.8}$$

Therefore, equation (2.6) with equation (2.7) represents the explicit functional dependence of the kinetic energy density on particle density, for the harmonic oscillator example considered above. It must be emphasized that this dependence on ρ has for $N > 1$ inherently non-local character (see also section 5).

It is worthy of note that with the above $t_s = t_s[\rho; x]$, equation (2.4) represents the one-body potential written as an explicit functional of the particle density.

2.2. *Pauli potential*

The Pauli potential $v_P(x)$ (March 1985, Herring and Chopra 1988) can be defined in general as the functional derivative of the Pauli energy E_P,

$$E_P[\rho] = T_s[\rho] - T_W[\rho] \tag{2.9}$$

that is,

$$v_P(x) = \frac{\delta E_P[\rho]}{\delta\rho(x)} = \frac{\delta T_s[\rho]}{\delta\rho(x)} - \frac{\delta T_W[\rho]}{\delta\rho(x)} \tag{2.10}$$

where T_s is the total kinetic energy of the non-interacting electron system, to be obtained from the density (2.3) as

$$T_s = \int \mathrm{d}x\, t_s(x) \tag{2.11}$$

and T_W is given by equation (1.2).

The first term of the expression (2.10) for v_P can be obtained from the exact Euler equation of density functional theory

$$\frac{\delta T_s[\rho]}{\delta\rho(x)} + v(x) = \lambda \tag{2.12}$$

where λ is the Lagrange multiplier connected with the condition (2.8). The second term is obtained by direct functional differentiation of equation (1.2):

$$\frac{\delta T_W[\rho]}{\delta\rho(x)} = \frac{1}{8}\left(\frac{\rho'(x)}{\rho(x)}\right)^2 - \frac{1}{4}\frac{\rho''(x)}{\rho(x)}. \tag{2.13}$$

So, from equation (2.10) we have

$$v_P = -v + \frac{1}{4}\frac{\rho''}{\rho} - \frac{1}{8}\left(\frac{\rho'}{\rho}\right)^2 + \text{constant} \tag{2.14}$$

a result valid for arbitrary one-dimensional systems.

Inserting v from equation (2.4), we obtain finally for the harmonic oscillator case

$$v_P = \frac{3t_s}{\rho} + \frac{1}{2}\frac{\rho''}{\rho} - \frac{1}{8}\left(\frac{\rho'}{\rho}\right)^2 + \text{constant}. \tag{2.15}$$

With $t_s = t_s[\rho; x]$, equations (2.6) and (2.7), the expression (2.15) achieves the aim of constructing the Pauli potential (see also Nalewajski and Kozlowski 1988) as an explicit functional of ρ for the one-dimensional harmonic oscillator.

2.3. *Pauli energy density*

We define the Pauli energy density in correspondence with the definition (2.9) of the total Pauli energy, namely

$$e_P(x) = e_s(x) - e_W(x) \tag{2.16}$$

where the density e_W of the von Weizsäcker energy according to equation (1.2) is

$$e_W = \tfrac{1}{8}\rho^{-1}|\nabla\rho|^2. \tag{2.17}$$

For the kinetic energy density e_s it proves convenient to adopt here the alternative to equation (2.3), namely

$$e_s = \tfrac{1}{2} \sum_{i=1}^{N} |\nabla \psi_i|^2 \tag{2.18}$$

which integrates to the same total kinetic energy

$$T_s = \int \mathrm{d}x\, e_s(x) \tag{2.19}$$

since the two densities are related by

$$e_s = t_s + \tfrac{1}{4}\nabla^2 \rho. \tag{2.20}$$

The total Pauli energy E_P is likewise given by

$$E_P = \int \mathrm{d}x\, e_P(x). \tag{2.21}$$

The above definitions have the useful properties that $e_s \geqslant 0$ (which is obvious from equation (2.18)) and also $e_P \geqslant 0$ (shown by Holas and March 1991).

By inserting equations (2.20) and (2.17) into equation (2.16) we obtain the general result

$$e_P = t_s + \tfrac{1}{4}\rho'' - \frac{1}{8}\frac{(\rho')^2}{\rho}. \tag{2.22}$$

Evidently, with known $t_s = t_s[\rho; x]$ for the harmonic oscillator, the Pauli energy is known for that example as an explicit functional of ρ. In fact the expression (2.22) with equation (2.6) can be usefully rearranged as

$$e_P[\rho; x] = \frac{\rho^3(x)}{4}\left[\int_0^x \mathrm{d}y \left(\frac{\rho'(y)}{\rho(y)}\right)'' \rho^{-2}(y) + C_P[\rho]\right] \tag{2.23}$$

with

$$C_P[\rho] = \tfrac{2}{3}\rho^{-3}(0)\rho''(0) + \tfrac{1}{3}\rho^{-2}(0)N[\rho]. \tag{2.24}$$

This may serve also as an alternative to the form (2.6) for the kinetic energy functional t_s (in terms of e_P using equation (2.22)).

Finally, we obtain from equation (2.15) a relation between v_P, e_P and ρ (of a local character) after inserting there t_s from equation (2.22):

$$v_P = \frac{3e_P}{\rho} - \frac{1}{4}\left(\frac{\rho'}{\rho}\right)' + \text{constant}. \tag{2.25}$$

Of course, it must not be assumed that equations (2.4), (2.6), (2.15), (2.23) and (2.25), derived for a harmonic oscillator potential, will be valid for a general one-dimensional potential energy. To make progress for this latter case, we shall press first, in section 3 immediately below, the consequences of the differential form (2.2) of the virial theorem in one dimension, and then, to allow some discussion of higher-dimensional problems, we turn in section 4 to the extension of the result (1.1) by inclusion of gradient corrections in D-dimensions.

3. General non-local theory in one dimension

To emphasize the role of non-locality for general one-dimensional potentials $v(x)$, let us make use of equation (2.2) again. Taking t_s from equation (2.20), eliminating e_s from equation (2.16) and v using equation (2.14), readily yields

$$e'_P = \tfrac{1}{2}\rho v'_P \tag{3.1}$$

all terms involving derivatives of ρ explicitly cancelling from the equation. Equation (3.1) may now be integrated to relate the Pauli potential and energy via $\rho(x)$:

$$v_P[\rho; x] = \frac{2e_P[\rho; x]}{\rho(x)} + 2\int_{x_0}^{x} dy\, \frac{e_P[\rho; y]\rho'(y)}{\rho^2(y)} + \text{constant.} \tag{3.2}$$

This equation generalizes the local relation (2.25) for the harmonic oscillator to arbitrary one-dimensional potentials. Thus, in all such one-dimensional problems it follows from equation (3.2) that knowledge of $e_P[\rho; x]$ allows not only $v_P[\rho; x]$ to be obtained, but the other density functionals: $e_s[\rho; x]$ from equations (2.16) and (2.17) and hence $t_s[\rho; x]$ using equation (2.20) and also $v[\rho; x]$ from equation (2.14).

Unfortunately, it has not proved possible to date to extend the above argument beyond one dimension. Therefore, to treat higher dimensions, and in particular to generalize equation (1.1), we must resort to a fuller study of the gradient corrections introduced in section 1.

4. Gradient expansion of kinetic energy density in *D*-dimensional space

4.1. General form and leading term

The gradient expansion of the kinetic energy density may be viewed as a generalization of the TF approximation:

$$\tilde{e}_s[\rho; \boldsymbol{r}] = e_0(\rho(\boldsymbol{r})) + e_2(\rho(\boldsymbol{r}))(\nabla\rho(\boldsymbol{r}))^2 + \text{higher-gradient terms.} \tag{4.1}$$

The leading TF term e_0 is the same as the kinetic energy density of a uniform electron gas having the local density $\rho(\boldsymbol{r})$. For the D-dimensional case the result is known (e.g. see Iwamoto 1984):

$$e_0(\rho) = \frac{D}{D+2}\rho\tfrac{1}{2}k_F^2 = \kappa_D\rho^{(D+2)/D} \tag{4.2}$$

where

$$k_F = k_F(\rho) = 2\pi^{1/2}\left[\tfrac{1}{2}\Gamma\left(\frac{D}{2}+1\right)\rho\right]^{1/D} \tag{4.3}$$

and therefore

$$\kappa_D^P = \frac{2\pi D}{D+2}\left[\tfrac{1}{2}\Gamma\left(\frac{D}{2}+1\right)\right]^{2/D} \tag{4.4}$$

for double occupancy (paramagnetic P case) or

$$\kappa_D^F = 2^{2/D}\kappa_D^P \tag{4.5}$$

for the single occupancy (ferromagnetic F case); see also table 1. In connection with this table, Baltin (1987) quotes the paramagnetic κ_D for $D = 3$, while his quoted result for $D = 1$ is the ferromagnetic value.

Table 1. Characteristics of a D-dimensional electron gas.

D	$(k_F)^D/\rho$	κ_D^{P}	κ_D^{F}	λ_D/λ_W
1	$\pi/2$	$\pi^2/24$	$\pi^2/6$	$-\frac{1}{3}$
2	2π	$\pi/2$	π	0
3	$3\pi^2$	$\frac{3}{10}(3\pi^2)^{2/3}$	$\frac{3}{10}(6\pi^2)^{2/3}$	$\frac{1}{9}$

P, paramagnetic occupancy; F, ferromagnetic occupancy.

Expansion (4.1) does not include the $\nabla^2\rho$ term (compare equation (2.20)) since it does not contribute to the total kinetic energy $T_s[\rho]$. This is why the notation $\tilde{e}_s$ is adopted above in order to distinguish this energy density from e_s (equation (2.18)), and from t_s (equation (2.3)).

Terms higher than the leading one in the expansion (4.1) are presently known for $D=3$ only; e.g. e_2 was determined originally by Kirzhnits (1957), while Hodges (1973) and Murphy (1981) have calculated higher-gradient terms. As was pointed out by Hohenberg and Kohn (1964; see also Jones and Young 1971), the result of Kirzhnits can be found in an alternative way, from the response function of the electron assembly. This approach will be adopted below, in the form given by Hodges for $D=3$, because this is readily generalized to arbitrary dimensionality.

4.2. Response function approach for second-order term

For an almost uniform electron gas having density

$$\rho(\boldsymbol{r})=\rho_0+\tilde{\rho}(\boldsymbol{r}) \tag{4.6}$$

where $\tilde{\rho}$ is a small non-uniform component, the kinetic energy, with accuracy to second-order in $\tilde{\rho}$, is given by

$$T_s[\rho]=T_{\mathrm{U}}+T_{\mathrm{NU}}=T_{\mathrm{U}}+\tfrac{1}{2}\int K(\boldsymbol{q})|\tilde{\rho}(\boldsymbol{q})|^2\,\mathrm{d}^D\boldsymbol{q} \tag{4.7}$$

where the Fourier components of $\tilde{\rho}(\boldsymbol{r})$ are denoted by $\tilde{\rho}(\boldsymbol{q})$, while the kernel $K(\boldsymbol{q})$ is a function of both $\boldsymbol{q}$ and ρ_0. Vectors $\boldsymbol{r}$ and $\boldsymbol{q}$ are now evidently defined in D-dimensional spaces. The non-uniformity $\tilde{\rho}(\boldsymbol{r})$ arises from the application of a small non-uniform (NU) external potential having Fourier components $v_{\mathrm{ext}}(\boldsymbol{q})$ and it can be determined by minimizing the following energy:

$$\tfrac{1}{2}\int \mathrm{d}^D(\boldsymbol{q})[K(\boldsymbol{q})|\tilde{\rho}(\boldsymbol{q})|^2+(v_{\mathrm{ext}}(\boldsymbol{q})\tilde{\rho}^*(\boldsymbol{q})+\mathrm{cc})]. \tag{4.8}$$

This leads to the result

$$K(\boldsymbol{q})\tilde{\rho}(\boldsymbol{q})+v_{\mathrm{ext}}(\boldsymbol{q})=0. \tag{4.9}$$

But from linear response theory, $\tilde{\rho}(\boldsymbol{q})$ and $v_{\mathrm{ext}}(\boldsymbol{q})$ are related via $\chi_D^{\mathrm{L}}(\boldsymbol{q},0)$—the static susceptibility (or density–density response) function of a non-interacting electron gas (i.e. the Lindhard function for $D=3$)

$$\tilde{\rho}(\boldsymbol{q})=\chi_D^{\mathrm{L}}(\boldsymbol{q},0)\,v_{\mathrm{ext}}(\boldsymbol{q}) \tag{4.10}$$

which yields immediately

$$K(\boldsymbol{q})=-1/\chi_D^{\mathrm{L}}(\boldsymbol{q},0). \tag{4.11}$$

By Fourier transforming the quantities occurring in equation (4.7) we find

$$
\begin{aligned}
T_{\mathrm{NU}} &= \tfrac{1}{2}\int \mathrm{d}^D\boldsymbol{r}_1\,\mathrm{d}^D\boldsymbol{r}_2\,K(\boldsymbol{r}_1-\boldsymbol{r}_2)\tilde{\rho}(\boldsymbol{r}_1)\tilde{\rho}(\boldsymbol{r}_2)\\
&= \tfrac{1}{2}\int \mathrm{d}^D\boldsymbol{r}\,K(\boldsymbol{r})\int \mathrm{d}^D\boldsymbol{r}'\,\tilde{\rho}(\boldsymbol{r}'+\tfrac{1}{2}\boldsymbol{r})\tilde{\rho}(\boldsymbol{r}'-\tfrac{1}{2}\boldsymbol{r}).
\end{aligned}
\tag{4.12}
$$

Using the long-wave expansion of $K(\boldsymbol{q})$:

$$
K(\boldsymbol{q}) = k_0 + k_2\boldsymbol{q}^2 + \mathrm{O}(\boldsymbol{q}^4)
\tag{4.13}
$$

where the coefficients k_0, k_2 etc are functions of the uniform density ρ_0, we obtain for its Fourier transform

$$
K(\boldsymbol{r}) = [k_0 - k_2\nabla_{\boldsymbol{r}}^2 + \mathrm{O}(\nabla_{\boldsymbol{r}}^4)]\delta(\boldsymbol{r}).
\tag{4.14}
$$

After substituting this into equation (4.12), and with some manipulation, we find

$$
T_{\mathrm{NU}} = \tfrac{1}{2}k_0\int \mathrm{d}^D\boldsymbol{r}\,\tilde{\rho}^2(\boldsymbol{r}) + \tfrac{1}{2}k_2\int \mathrm{d}^D\boldsymbol{r}(\nabla\tilde{\rho}(\boldsymbol{r}))^2 + \ldots .
\tag{4.15}
$$

The first term is to be identified with the second-order correction term of the expansion of the TF energy density, occurring in equation (4.1),

$$
e_0(\rho) = e_0(\rho_0+\tilde{\rho}) = e_0(\rho_0) + \frac{\mathrm{d}e_0}{\mathrm{d}\rho}\tilde{\rho} + \frac{1}{2}\frac{\mathrm{d}^2e_0}{\mathrm{d}\rho^2}\tilde{\rho}^2 + \ldots
\tag{4.16}
$$

that is,

$$
\frac{\mathrm{d}^2e_0(\rho)}{\mathrm{d}\rho^2} = k_0(\rho)
\tag{4.17}
$$

while the second term in equation (4.15) should correspond to the second term in equation (4.1), that is,

$$
e_2(\rho) = \tfrac{1}{2}k_2(\rho).
\tag{4.18}
$$

The static susceptibility for D-dimensional space is known to be (e.g. see Holas 1990)

$$
\begin{aligned}
\chi_D^{\mathrm{L}}(\boldsymbol{q},0) &= \chi_D^{\mathrm{L}}(0)F\left[1, 1-\frac{D}{2}; \frac{3}{2}; \left(\frac{q}{2k_{\mathrm{F}}}\right)^2\right]\\
&= \chi_D^{\mathrm{L}}(0)\left[1 + \frac{2-D}{12}\left(\frac{q}{2k_{\mathrm{F}}}\right)^2 + \mathrm{O}(q^4)\right]
\end{aligned}
\tag{4.19}
$$

for $q < 2k_{\mathrm{F}}$, where $F\ (\alpha, \beta; \gamma; z)$ is the hypergeometric function,

$$
\chi_D^{\mathrm{L}}(0) = -D\rho k_{\mathrm{F}}^{-2}
\tag{4.20}
$$

while k_{F} as a function of ρ is given in equation (4.3). Using equation (4.11) we find for the coefficients of the expansion (4.13):

$$
k_0 = k_{\mathrm{F}}^2/D\rho \qquad k_2 = (D-2)/12D\rho.
\tag{4.21}
$$

By differentiation of equation (4.2), it can readily be verified that k_0 given in equation (4.21) satisfies equation (4.17). The k_2 in equation (4.21) leads, according to equation (4.18) to the following form of the squared gradient term

$$
e_2(\rho)(\nabla\rho)^2 = \lambda_D\rho^{-1}(\nabla\rho)^2
\tag{4.22}
$$

with

$$\lambda_D = (D-2)\lambda_W/3D \qquad \lambda_W = \tfrac{1}{8}. \tag{4.23}$$

It is clear from equation (4.23) that, as in the three-dimensional case, equation (1.3), this term differs from the von Weizsäcker energy density by a constant factor. However, this factor is strongly dependent on dimensionality as $(D-2)/3D$. It is immediately clear that this contribution is zero for the two-dimensional case, and has the negative value $-\frac{1}{3}$ for one dimension. In contrast to the TF term, the modified von Weizsäcker gradient correction has the same form for both single and double occupancy (P and F cases).

5. Examples of non-local functional dependence

To make quite clear the role of non-locality, which is in some sense lost by gradient expansions employed in section 4, we return now to the harmonic oscillator example. To gain insight, let us write the non-local part of the kinetic energy density t_s, equation (2.6) as

$$t_s^{\mathrm{nl}}[\rho; x] = \tfrac{1}{2}\rho(x)\mathrm{F}_t[\rho; x] + \tfrac{1}{2}\rho^3(x)C_t[\rho] \tag{5.1}$$

where

$$\mathrm{F}_t[\rho; x] = \int_0^x \mathrm{d}y \left(\frac{\rho(x)}{\rho(y)}\right)^2 \left(\frac{\rho'(y)}{\rho(y)}\right)^3. \tag{5.2}$$

We now investigate the case $N = 1$. The particle density and its derivatives are

$$\rho(x) = \pi^{-1/2}\exp(-x^2) \tag{5.3}$$

$$\rho'(x)/\rho(x) = -2x \tag{5.4}$$

$$\rho''(x)/\rho(x) = -2(1-2x^2). \tag{5.5}$$

Thus, according to equation (2.7),

$$C_t = (4\pi^{-1/2} + 2\pi^{-1/2})/6\pi^{-3/2} = \pi. \tag{5.6}$$

Then evaluating equation (5.2) we have

$$F_t(x) = \int_0^x \mathrm{d}y \exp(2y^2 - 2x^2)(-2y)^3. \tag{5.7}$$

In terms of the new variable $t = 2y^2 - 2x^2$ we find

$$F_t(x) = -\int_{-2x^2}^{0} \mathrm{d}t(t+2x^2)\exp t = 1 - 2x^2 - \exp(-2x^2) = \frac{-\rho''(x)}{2\rho(x)} - \pi\rho^2(x) \tag{5.8}$$

the last step in equation (5.8) having used equations (5.3) and (5.5). Hence from equations (5.1), (5.6) and (5.8)

$$t_s^{\mathrm{nl}}(x) = -\tfrac{1}{4}\rho''(x) \tag{5.9}$$

and using equations (2.6), (5.1) and (5.9) yields

$$t_s(x) = \tfrac{1}{8}(\rho'(x))^2/\rho(x) - \tfrac{1}{4}\rho''(x) = -\tfrac{1}{2}\rho^{1/2}(x)(\rho^{1/2}(x))''. \tag{5.10}$$

Since for $N=1$ one can choose $\psi_1(x)=\rho^{1/2}(x)$, the result (5.10) gives t_s in the form valid for an arbitrary system: equation (2.3). This is the reason why the apparently non-local form (5.2) becomes local after integration.

For the $N=2$ case, the particle density is

$$\rho(x)=\pi^{-1/2}\exp(-x^2)(1+2x^2) \tag{5.11}$$

the calculation of C_t and F_t can again be carried out, with the results

$$C_t=\pi \tag{5.12}$$

and

$$F_t(x)=-\pi\rho^2(x)+2(1+2x^2)^{-2}-6(1+2x^2)^{-1}+6-(1+2x^2). \tag{5.13}$$

The corresponding non-local contribution to the kinetic energy takes the form

$$t_s^{\mathrm{nl}}(x)=\tfrac{1}{2}\rho(x)[2(1+2x^2)^{-2}-6(1+2x^2)^{-1}+5-2x^2]. \tag{5.14}$$

While the terms within the square brackets in equation (5.14) can be viewed as a third-order polynomial in x^2, divided by $(1+2x^2)^2$, and a similar form holds for $(\rho'/\rho)^2$ and ρ''/ρ, it is not possible to express this polynomial in terms of the above local functionals of ρ (one needs two more functions, but higher derivatives of ρ involve higher powers of x^2). In this way we have shown that $t_s[\rho;x]$ for the harmonic oscillator case behaves as for any other system; for $N=1$ it is a general local functional of ρ given in equation (5.10); for $N=2$, t_s is inherently non-local and this cannot be removed by performing the integration in equation (5.2). Thus, early expectations (e.g. in Lawes and March (1979) and some other later papers) that the local density assumption for t_s holds in the harmonic oscillator case for $N\geqslant 2$ turn out to be unfounded.

6. Total energies: higher-order gradient terms for the harmonic oscillator

One can test the validity of the gradient approximation to local quantities such as $e_s(x)/\rho(x)$ or $v_B(x)$; below we check it with respect to the total energies; namely, kinetic energy†

$$T_s=\int \mathrm{d}x\,\rho(x)(e_s(x)/\rho(x))=\tfrac{1}{4}N^2 \tag{6.1}$$

to be compared with its gradient expansion

$$\begin{aligned} T_s&=\int \mathrm{d}x\,e_0-\frac{1}{3}\int \mathrm{d}x\,e_W+\int \mathrm{d}x\,e_s^{\mathrm{hgt}}\\ &=T_0-\tfrac{1}{3}T_W+T_s^{\mathrm{hgt}}=T_s^{\mathrm{g}}+T_s^{\mathrm{hgt}} \end{aligned} \tag{6.2}$$

(the superscript hgt indicates higher-gradient terms) and the Pauli potential energy

$$V_P=\int \mathrm{d}x\,\rho(x)\,v_P(x) \tag{6.3}$$

---

† The explicit result $\frac{1}{4}N^2$ is for the harmonic oscillator example.

Table 2. The gradient expansion of the kinetic energy and the Pauli potential energy of the N-particle system in the harmonic oscillator potential.

N	5	10	15	20
T_0	6.3616	25.1462	56.4199	100.1886
$-\frac{1}{3}T_W$	−0.1694	−0.2234	−0.2613	−0.2915
$T_s^g = T_0 - \frac{1}{3}T_W$	6.1922	24.9228	56.1586	99.8971
$T_s = \frac{1}{4}N^2$	6.2500	25.0000	56.2500	100.0000
$(T_s - T_s^g)/T_s$	0.0092	0.0031	0.0016	0.0010
$3T_0$	19.0848	75.4385	169.2597	300.5658
$-\frac{4}{3}T_W$	−0.6775	−0.8936	−1.0453	−1.1662
$V_P^g = 3T_0 - \frac{4}{3}T_W$	18.4073	74.5450	168.2144	299.3997
V_P	18.2419	74.3298	167.9660	299.1254
$(V_P - V_P^g)/V_P$	−0.0091	−0.0029	−0.0015	−0.0009

with corresponding gradient expansion for v_P in the form (A4) below

$$\begin{aligned} V_P &= 3\int \mathrm{d}x\, e_0 - \frac{4}{3}\int \mathrm{d}x\, \rho v_W + \int \mathrm{d}x\, \rho v_P^{\mathrm{hgt}} \\ &= 3T_0 - \tfrac{4}{3}T_W + V_P^{\mathrm{hgt}} = V_P^g + V_P^{\mathrm{hgt}}. \end{aligned} \tag{6.4}$$

Table 2 shows the values of all these energy terms defined above, for the harmonic oscillator. It can be seen that the relative error of gradient approximations to T_s and V_P is very small: it reduces from 0.9% for $N = 5$ to 0.1% for $N = 20$. Such high accuracy (an order of magnitude improvement on corresponding local quantities) is a consequence of the following properties. In the region of high density, both exact and approximate local quantities oscillate around the same mean value, so their integral values must be close. In the tail region where exact and approximate local quantities differ significantly, the density reduces rather abruptly to become exponentially small. Therefore, any quantity weighted with this density during integration gives only a small contribution.

In addition to the above examples, we have thought it useful to include as an appendix a discussion in terms of gradient expansions of the differential equation for the density amplitude $\rho^{1/2}$ (see equation (A7)), where the role of the higher-order gradient terms in the Pauli potential v_P is displayed explicitly. March and Murray (1960; see also Holas and March 1991) introduced such a potential v_P to replace the Euler equation (2.12) by this so-called boson equation (see (A5) and (A7)).

7. Summary

Though this paper is most explicit for one dimension, we have investigated the D-dimensional gradient expansion for the kinetic energy density. The Kirzhnits factor multiplying the von Weizsäcker term is shown to be dependent on dimensionality as $(D-2)/3D$.

For one dimension, explicit functional results have been obtained for N levels occupied in a harmonic oscillator potential†. The most useful result for general one-dimensional one-body potential problems is equation (3.2). This represents the solution

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† Table 2 demonstrates the overall high accuracy of gradient expansions. The dominant role of their zeroth-order terms was established.

to the problem of the evaluation of the functional derivative of E_{P}, in the case for which the Pauli energy E_{P} is known in the form of the integral of its density e_{P} as in equation (2.21). This also solves the same problem for the kinetic energy functional T_{s}, because T_{s} and E_{P}, through the definition (2.9), differ only by the von Weizsäcker term (1.2), the functional derivative of which is known (equation (2.13)).

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Appendix. Differential equation from gradient expansion applied to boson equation

The gradient expansion for the kinetic energy density obtained in section 4 leads to the following expansion for the Pauli energy in D-dimensions:

$$E_{\mathrm{P}}=T_{\mathrm{s}}-T_{\mathrm{W}}=T_0+\left(\frac{\lambda_D}{\lambda_{\mathrm{W}}}-1\right)T_{\mathrm{W}}+T_{\mathrm{s}}^{\mathrm{hgt}} \tag{A1}$$

where

$$T_0=\kappa_D\int \mathrm{d}^D\boldsymbol{r}[\rho(\boldsymbol{r})]^{(D+2)/D} \tag{A2}$$

$$T_{\mathrm{W}}=\lambda_{\mathrm{W}}\int \mathrm{d}^D\boldsymbol{r}|\nabla\rho(\boldsymbol{r})|^2/\rho(\boldsymbol{r}) \qquad \lambda_{\mathrm{W}}=\tfrac{1}{8}. \tag{A3}$$

Therefore the Pauli potential is

$$v_{\mathrm{P}}=\delta E_{\mathrm{P}}/\delta\rho=\frac{(D+2)}{D}\kappa_D\rho^{2/D}+\left(\frac{\lambda_D}{\lambda_{\mathrm{W}}}-1\right)\frac{\delta T_{\mathrm{W}}}{\delta\rho}+v_{\mathrm{P}}^{\mathrm{hgt}}. \tag{A4}$$

After substituting this expression into the boson equation (i.e. equation (2.12) with $\delta T_{\mathrm{s}}/\delta\rho$ from (2.10))

$$\delta T_{\mathrm{W}}/\delta\rho(\boldsymbol{r})+v(\boldsymbol{r})+v_{\mathrm{P}}(\boldsymbol{r})=\lambda_{\mathrm{B}} \tag{A5}$$

using the fact that

$$\delta T_{\mathrm{W}}/\delta\rho=-\tfrac{1}{2}\nabla^2\chi/\chi \tag{A6}$$

the following differential equation for the density amplitude $\chi(\boldsymbol{r})=\rho^{1/2}(\boldsymbol{r})$ is obtained:

$$-\frac{1}{2}\frac{\lambda_D}{\lambda_{\mathrm{W}}}\frac{\nabla^2\chi}{\chi}+v+\frac{(D+2)}{D}\kappa_D\chi^{4/D}+v_{\mathrm{P}}^{\mathrm{hgt}}=\lambda_{\mathrm{B}}. \tag{A7}$$

Two cases must now be distinguished:

(i) $\lambda_D=0$, which holds for $D=2$ (see equation (4.23)).

Then equation (A7) yields

$$\rho(\boldsymbol{r})=\frac{1}{2\kappa_2}(\lambda_{\mathrm{B}}-v(\boldsymbol{r})+v_{\mathrm{P}}^{\mathrm{hgt}}(\boldsymbol{r}))\Theta(\lambda_{\mathrm{B}}-v(\boldsymbol{r})-v_{\mathrm{P}}^{\mathrm{hgt}}(\boldsymbol{r})) \tag{A8}$$

where the step function $\Theta(x)$ guarantees that $\rho \geqslant 0$ and that $\rho(\boldsymbol{r})$ is a nodeless function. The eigenvalue λ_{B} is determined from the normalization condition

$$\int \mathrm{d}\boldsymbol{r}\,\rho(\boldsymbol{r}) = N. \tag{A9}$$

If we neglect the higher-gradient term $v_{\mathrm{P}}^{\mathrm{hgt}}$, then equation (A8) reduces to the TF equation in the two-dimensional case.

(ii) $\lambda_D \neq 0$; $D=1$ or $D=3$. In this case equation (A7) may be rewritten in the standard form of the one-particle Schrödinger equation for $\chi(\boldsymbol{r})$:

$$-\tfrac{1}{2}\nabla^2\chi + v_{\mathrm{B}}^{\mathrm{eff}}\chi = \tilde{\lambda}_{\mathrm{B}}\chi \tag{A10}$$

where the effective boson potential is defined as

$$v_{\mathrm{B}}^{\mathrm{eff}} = \frac{\lambda_{\mathrm{W}}}{\lambda_D}\left(v + \frac{(D+2)}{D}\kappa_D\chi^{4/D} + v_{\mathrm{P}}^{\mathrm{hgt}}\right). \tag{A11}$$

If the unknown term $v_{\mathrm{P}}^{\mathrm{hgt}}$ is neglected, then equation (A10) can be solved iteratively in a standard way to achieve self-consistency, seeking the lowest eigenvalue $\tilde{\lambda}_{\mathrm{B}}$ corresponding to the nodeless solution for $\chi(\boldsymbol{r})$.

For $D=3$ the coefficient $\lambda_{\mathrm{W}}/\lambda_D$ is positive and equal to 9. Therefore the effective boson potential consists of 9 times the original external potential plus some positive term which falls to zero as $|\boldsymbol{r}|$ tends to infinity (to have finite integral (A9)). For that reason it is to be expected that in most cases such a potential will lead to a bound state.

However, the situation for $D=1$ seems much less favourable when $v_{\mathrm{P}}^{\mathrm{hgt}}$ is again dropped from equation (A11). In this case $\lambda_{\mathrm{W}}/\lambda_D$ is negative, having the value -3. It will usually be true that inclusion of some useful approximation to $v_{\mathrm{P}}^{\mathrm{hgt}}$ will be necessary to produce a bound state, as can readily be argued for the harmonic oscillator potential $v=\frac{1}{2}x^2$.

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