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One-dimensional kinetic energy density functionals compatible with the differential virial theorem

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Abstract. For a system of one-dimensional fermions moving in a common effective potential $V(x)$, a method is described to find the most general kinetic energy functional ε_k which satisfies the requirements that ε_k (i) is a sufficiently differentiable function of the density ρ and of its first n derivatives $\rho, \rho', \ldots \rho^{(n)}$; (ii) is non-negative for arbitrary density distributions ≥ 0; (iii) obeys the differential virial theorem. The cases $n = 0, 1, 2$ have been worked out yielding the result that $\varepsilon_k = \tilde{\kappa}\rho^3 + \lambda_w \rho'^2/\rho$ is the only solution compatible with these conditions, where $\tilde{\kappa} \geq 0$ is an indetermined coefficient to the Thomas-Fermi term and $\lambda_w = \hbar^2/8m$ is the full Weizsäcker coefficient.

1. Introduction

The usual approximations to the kinetic energy density functional ε_k of a fermion gas with density ρ have the form

$$\varepsilon_k = \kappa\rho^{5/3} + \lambda(\nabla\rho)^2/\rho + \ldots \tag{1}$$

in three dimensions and

$$\varepsilon_k = \tilde{\kappa}\rho^3 + \tilde{\lambda}\rho'^2/\rho + \ldots \tag{2}$$

in one dimension where the two first terms only are given here. Here κ, $\tilde{\kappa}$, λ, $\tilde{\lambda}$ are certain coefficients and $\rho' \equiv d\rho/dx$. For $\lambda = 0$ ($\tilde{\lambda} = 0$) and $\kappa = \kappa_{TF}$ ($\tilde{\kappa} = \tilde{\kappa}_{TF}$) the well known Thomas-Fermi (TF) approximation in three (one) dimensions is obtained where we have put $\kappa_{TF} = 3(3\pi^2)^{2/3}\hbar^2/10m$ [1] and $\tilde{\kappa}_{TF} = \hbar^2\pi^2/6m$ [2].

The gradient correction term of (1) was first introduced by von Weizsäcker [3] with $\lambda = \lambda_w \equiv \hbar^2/8m$. A corresponding argument leads to the same value for $\tilde{\lambda}$. Later on several authors [4-6] set up a more systematic procedure of expanding ε_k into a gradient series under the supposition that ρ is sufficiently slowly variable so that gradient terms can be regarded as small corrections to the leading TF term. It is found that the original value of λ_w as given by von Weizsäcker should be diminished by a factor of 9.

When the first two terms of (1) are taken into account, insertion of Hartree-Fock densities leads to a total kinetic energy which differs from the true HF kinetic energy by less than 1% [7]; agreement becomes still better when the third term of (1) (not given here) is included, however, the fourth term yields an infinite result for atoms [8].

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When densities are calculated self-consistently from the Euler equation which arises from the minimisation of the total energy functional results for ρ, total energy and various other properties are far less favourable when the approximation (1) with $\lambda = \lambda_w/9$ is used [9-11]. This approximation has also been criticised on theoretical grounds and it has been proposed to modify the coefficient κ_{TF} rather than λ_w, see [10-16].

Thus, in summary, the answers to the question how to choose the coefficients of the Thomas-Fermi and of the Weizsäcker term are still controversial, although there is general agreement that approximations of the type (1) (or (2)) are not capable of reproducing quantum oscillations, irrespective of the value of λ [17, 18].

As has been shown by Szasz *et al* [19] the two requirements on ε_k

(i) to depend on ρ and $\nabla\rho$ only (ρ, ρ' in one dimension),

(ii) to satisfy the virial theorem,

are compatible to Thomas-Fermi-Weizsäcker functionals with still completely unspecified coefficients. Therefore, the virial theorem cannot help to fix the coefficients in expressions (1) and (2).

There is, however, at least in one dimension, a 'differential' virial theorem derived independently and using different methods by Baltin [20] and March and Young [21] which connects exactly the kinetic energy density, the particle density and the potential pointwise, contrary to the usual virial theorem which is an integral relation. The 'differential' virial theorem, from which the ordinary virial theorem follows by integration over all x, states that, for one-dimensional fermions moving independently in an effective common potential $V(x)$,

$$\varepsilon_k'(x) = \frac{\hbar^2}{8m}\rho'''(x) - \tfrac{1}{2}V'(x)\rho(x) \tag{3}$$

where the positive definite definition

$$\varepsilon_k(x) \equiv 2\frac{\hbar^2}{2m}\sum_{i=1}^{N/2}[\psi_i'(x)]^2 \tag{4}$$

has been used (ψ_i real chosen wavefunctions, doubly occupied by a total of N fermions).

It is the purpose of this work to investigate to what extent the coefficients of the gradient expansion (2) can be fixed provided ε_k is required to be non-negative for all trial densities $\rho \geq 0$ and to satisfy equation (3).

After the next section where the general method is described, specific cases are worked out. In § 3 it is supposed that ε_k depends only on ρ or on ρ and ρ', § 4 deals with the fairly cumbersome case that the second derivative of ρ is included, too, besides ρ, ρ'. Results are summarised and discussed in the last section.

2. General method

Suppose we approximate the functional ε_k by a function of the first n derivatives

$$\varepsilon_k = f(\rho, \rho', \rho'', \ldots, \rho^{(n)}). \tag{5}$$

The first variation of the kinetic energy with respect to variations of the density is then

given by

$$\delta T = \delta \int_{-\infty}^{+\infty} f(\rho, \rho', \ldots, \rho^{(n)})\, \mathrm{d}x$$

$$= \int_{-\infty}^{+\infty} \sum_{\nu=0}^{n} \frac{\partial f}{\partial \rho^{(\nu)}} \delta\rho^{(\nu)}\, \mathrm{d}x \tag{6}$$

$$\delta T = \int_{-\infty}^{+\infty} \left[\sum_{\nu=0}^{n} (-1)^{\nu} \frac{\mathrm{d}^{\nu}}{\mathrm{d}x^{\nu}} \left(\frac{\partial f}{\partial \rho^{(\nu)}} \right) \right] \delta\rho\, \mathrm{d}x$$

where integration by parts has been used repeatedly.

When the total energy

$$E = T + U$$

$$= \int_{-\infty}^{+\infty} \varepsilon_k\, \mathrm{d}x + \int_{-\infty}^{+\infty} V\rho\, \mathrm{d}x \tag{7}$$

is minimised under the constraint

$$\int_{-\infty}^{+\infty} \rho\, \mathrm{d}x = N \tag{8}$$

the Euler equation is

$$\delta T / \delta\rho + V = \mu \tag{9}$$

where the Lagrange multiplier μ has the meaning of the chemical potential. Using (6) we obtain

$$\sum_{\nu=0}^{n} (-1)^{\nu} \frac{\mathrm{d}^{\nu}}{\mathrm{d}x^{\nu}} \left(\frac{\partial f}{\partial \rho^{(\nu)}} \right) + V(x) = \mu. \tag{9a}$$

When this equation is differentiated with respect to x, V' can be eliminated from (3) yielding

$$\sum_{\nu=0}^{n} \left[(-1)^{\nu} \rho \frac{\mathrm{d}^{\nu+1}}{\mathrm{d}x^{\nu+1}} \left(\frac{\partial f}{\partial \rho^{(\nu)}} \right) - 2\rho^{(\nu+1)} \frac{\partial f}{\partial \rho^{(\nu)}} \right] = -\frac{\hbar^2}{4m} \rho''' \tag{10}$$

where ε_k' in (3) has been rewritten as

$$\varepsilon_k' = \frac{\mathrm{d}\varepsilon_k}{\mathrm{d}x} = \sum_{\nu=0}^{n} \frac{\partial f}{\partial \rho^{(\nu)}} \frac{\mathrm{d}\rho^{(\nu)}}{\mathrm{d}x} = \sum_{\nu=0}^{n} \frac{\partial f}{\partial \rho^{(\nu)}} \rho^{(\nu+1)}. \tag{11}$$

The potential V (and, of course, the particle number N) determines the density ρ. Therefore, for f given, equation (10) cannot be regarded as a differential equation (of order $\leqslant l \equiv \max(2n+1, 3)$, $n = 0, 1, 2, \ldots$) for ρ since V has been eliminated. Rather this equation has to be looked upon as a relation to be satisfied identically with respect to the variables $\rho, \rho', \ldots \rho^{(l)}$ occurring in it. In other words, equation (10) is a condition to be imposed on the dependence of f upon the variables $\rho, \rho', \ldots, \rho^{(n)}$. Thus, for n chosen, we may expect information about the constants in equation (2).

Let us examine the cases $n = 0$, 1 and 2 in detail, i.e. $\varepsilon_k = f(\rho)$, $\varepsilon_k = f(\rho, \rho')$ and $\varepsilon_k = f(\rho, \rho', \rho'')$.

3. Approximation that ε_k be dependent on ρ and ρ' only

3.1. Case $\varepsilon_k = f(\rho)$

If $\varepsilon_k = f(\rho)$ equation (10) is

$$\rho \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}f}{\mathrm{d}\rho}\right) - 2\rho' \frac{\mathrm{d}f}{\mathrm{d}\rho} = -\frac{\hbar^2}{4m}\rho'''$$

or

$$\rho\rho' \frac{\mathrm{d}^2 f}{\mathrm{d}\rho^2} - 2\rho' \frac{\mathrm{d}f}{\mathrm{d}\rho} + \frac{\hbar^2}{4m}\rho''' = 0. \tag{12}$$

Evidently, this equation cannot be satisfied for arbitrary ρ, ρ', ρ'' and ρ''' since $\mathrm{d}^2 f/\mathrm{d}\rho^2$ and $\mathrm{d}f/\mathrm{d}\rho$ are not dependent on ρ'''. Thus the assumption that ε_k depends only on ρ leads to a contradiction.

If the term with ρ''' were absent, we would obtain

$$\rho \frac{\mathrm{d}^2 f}{\mathrm{d}\rho^2} - 2\frac{\mathrm{d}f}{\mathrm{d}\rho} = 0 \tag{13}$$

having the general solution

$$f = \tilde{\kappa}\rho^3 + c \tag{14}$$

with integration constants $\tilde{\kappa}$ and c. Since from physical grounds we have to demand $f(0) = 0$ it would follow that

$$f = \tilde{\kappa}\rho^3 \tag{14a}$$

which is just the TF term of (2) with unspecified coefficient.

3.2. Case $\varepsilon_k = f(\rho, \rho')$

When $\varepsilon_k = f(\rho, \rho')$ is inserted in (10), one obtains

$$\rho \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial \rho}\right) - \rho \frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\frac{\partial f}{\partial \rho'}\right) - 2\rho' \frac{\partial f}{\partial \rho} - 2\rho'' \frac{\partial f}{\partial \rho'} + \frac{\hbar^2}{4m}\rho''' = 0 \tag{15}$$

which leads to

$$\rho'\left(\rho \frac{\partial^2 f}{\partial \rho^2} - \rho\rho' \frac{\partial^3 f}{\partial \rho' \partial \rho^2} - 2\frac{\partial f}{\partial \rho}\right) - \rho''\left(2\rho\rho' \frac{\partial^3 f}{\partial \rho\, \partial \rho'^2} + \rho\rho'' \frac{\partial^3 f}{\partial \rho'^3} + 2\frac{\partial f}{\partial \rho'}\right)$$
$$+ \rho'''\left(\frac{\hbar^2}{4m} - \rho \frac{\partial^2 f}{\partial \rho'^2}\right) = 0 \tag{16}$$

ρ''' does not occur in f, thus the factor of ρ''' must vanish, i.e.

$$\frac{\partial^2 f}{\partial \rho'^2} = \frac{\hbar^2}{4m\rho} \tag{17}$$

which is integrated immediately yielding

$$f = \frac{\hbar^2}{8m}\frac{\rho'^2}{\rho} + \rho' g(\rho) + h(\rho) \tag{17a}$$

where $g(\rho)$ and $h(\rho)$ are functions of ρ only yet to be determined.

Furthermore, since f does not contain ρ'', the coefficient of $\rho\rho''^2$ must be zero, i.e.

$$\partial^3 f/\partial\rho'^3 = 0. \tag{18}$$

Expression (17a) satisfies this equation.

Equating now the term linear in ρ'' to zero we obtain from (16)

$$\frac{\partial f}{\partial \rho'} + \rho\rho' \frac{\partial^3 f}{\partial \rho\, \partial \rho'^2} = 0. \tag{19}$$

When expression (17a) is inserted in (19) it follows that

$$g(\rho) = 0 \tag{20}$$

so that

$$f = \frac{\hbar^2}{8m}\frac{\rho'^2}{\rho} + h(\rho). \tag{21}$$

We are left from equation (16) with

$$\rho'\left(\rho\frac{\partial^2 f}{\partial \rho^2} - \rho\rho'\frac{\partial^3 f}{\partial \rho'\, \partial \rho^2} - 2\frac{\partial f}{\partial \rho}\right) = 0. \tag{22}$$

From (21) we find that (22) leads to

$$\rho\frac{\mathrm{d}^2 h}{\mathrm{d}\rho^2} - 2\frac{\mathrm{d}h}{\mathrm{d}\rho} = 0 \tag{23}$$

having the solution

$$h(\rho) = \tilde{\kappa}\rho^3 \tag{24}$$

(cf (13), (14) and (14a)) with $h(0) = 0$.

Thus we finally end up with

$$\varepsilon_k = \tilde{\kappa}\rho^3 + \frac{\hbar^2}{8m}\frac{\rho'^2}{\rho} \tag{25}$$

i.e. a kinetic energy density with indetermined coefficient of the TF term and with the original Weizsäcker term.

4. Inclusion of the second derivative of density in the functional

In a further step let us assume $\varepsilon_k = f(\rho, \rho', \rho'')$ so that equation (10) becomes

$$\rho\left[\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial \rho}\right) - \frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\frac{\partial f}{\partial \rho'}\right) + \frac{\mathrm{d}^3}{\mathrm{d}x^3}\left(\frac{\partial f}{\partial \rho''}\right)\right] - 2\left(\rho'\frac{\partial f}{\partial \rho} + \rho''\frac{\partial f}{\partial \rho'} + \rho'''\frac{\partial f}{\partial \rho''}\right) + \frac{\hbar^2}{4m}\rho''' = 0. \tag{26}$$

When the derivatives of $\partial f/\partial\rho$, $\partial f/\partial\rho'$ and $\partial f/\partial\rho''$ with respect to x are performed, expressions of considerable length emerge, so we will not quote them.

The left-hand side of equation (26) contains derivatives of ρ up to the fifth. Among these ρ''', $\rho^{(4)}$ and $\rho^{(5)}$ do not occur implicitly in f and in its partial derivatives, by supposition. Therefore we have to equate the coefficients of these highest-order derivatives and of their powers (if any) to zero, according to the considerations of § 2.

The coefficient of $\rho^{(5)}$ is $\rho\,\partial^2 f/\partial\rho''^2$, so

$$\partial^2 f/\partial\rho''^2 = 0 \tag{27}$$

so that

$$f(\rho, \rho', \rho'') = a(\rho, \rho')\rho'' + b(\rho, \rho') \tag{28}$$

with a, b being functions yet unknown.

Correspondingly, the fourth-order term yields

$$3\rho\left(\rho'\frac{\partial^3 f}{\partial\rho\,\partial\rho''^2} + \rho''\frac{\partial^3 f}{\partial\rho'\partial\rho''^2} + \rho'''\frac{\partial^3 f}{\partial\rho''^3}\right) = 0. \tag{29}$$

However, this equation is already satisfied because of equation (27).

The third-order terms lead to

$$\rho\left(2\frac{\partial^2 f}{\partial\rho\,\partial\rho''} + \rho'\frac{\partial^3 f}{\partial\rho\,\partial\rho'\partial\rho''} + \rho''\frac{\partial^3 f}{\partial\rho'^2\,\partial\rho''} - \frac{\partial^2 f}{\partial\rho'^2}\right) - 2\frac{\partial f}{\partial\rho''} + \frac{\hbar^2}{4m} = 0 \tag{30}$$

where (27) has already been taken into account. Inserting (28) in (30) we obtain

$$\rho\left(2\frac{\partial a}{\partial\rho} + \rho'\frac{\partial^2 a}{\partial\rho\,\partial\rho'} - \frac{\partial^2 b}{\partial\rho'^2}\right) - 2a + \frac{\hbar^2}{4m} = 0. \tag{31}$$

Consider now all terms of equation (26) which do not contain ρ''', $\rho^{(4)}$ and $\rho^{(5)}$. When equation (28) is used, it is possible to collect terms associated with ρ''^2, ρ'' and without ρ''. Equating the coefficients of these powers to zero each we obtain respectively

$$\rho\left(3\frac{\partial^2 a}{\partial\rho\,\partial\rho'} + \rho'\frac{\partial^3 a}{\partial\rho\,\partial\rho'^2} - \frac{\partial^3 b}{\partial\rho'^3}\right) - 2\frac{\partial a}{\partial\rho'} = 0 \tag{32}$$

$$\rho\left(2\rho'\frac{\partial^2 a}{\partial\rho^2} + \rho'^2\frac{\partial^3 a}{\partial\rho^2\partial\rho'} - \rho'\frac{\partial^3 b}{\partial\rho\,\partial\rho'^2}\right) - \rho'\frac{\partial a}{\partial\rho} - \frac{\partial b}{\partial\rho'} = 0 \tag{33}$$

and

$$\rho\left(\frac{\partial^2 b}{\partial\rho^2} - \rho'\frac{\partial^3 b}{\partial\rho'\partial\rho^2} + \rho'^2\frac{\partial^3 a}{\partial\rho^3}\right) - 2\frac{\partial b}{\partial\rho} = 0. \tag{34}$$

Equation (32) may be discarded because it follows from equation (31) by partial differentiation with respect to ρ'. When (31) is differentiated with respect to ρ we obtain an equation by use of which we are able to eliminate $\partial^3 b/\partial\rho\,\partial\rho'^2$ from (33). Thus we find

$$\rho\frac{\partial b}{\partial\rho'} = \rho'\left(\rho\frac{\partial a}{\partial\rho} - 2a + \frac{\hbar^2}{4m}\right) \tag{35}$$

and differentiating this equation with respect to ρ' we can eliminate $\partial^2 b/\partial\rho'^2$ from (31) whence we obtain

$$\rho\frac{\partial a}{\partial\rho} + 2\rho'\frac{\partial a}{\partial\rho'} = 0. \tag{36}$$

This simple homogeneous first-order partial differential equation for $a(\rho, \rho')$ can be solved immediately by the method of characteristics (see, e.g., [22]).

When the parameter of a characteristic is denoted by s and $\dot{\rho} \equiv \mathrm{d}\rho/\mathrm{d}s$ the characteristic equations are

$$\dot{\rho} = \rho \tag{37a}$$

$$\dot{\rho}' = 2\rho' \tag{37b}$$

and

$$\dot{a} = 0 \tag{37c}$$

whence we find the characteristic curves

$$\rho = \rho_0 \, \mathrm{e}^{s} \tag{38a}$$

$$\rho' = \rho_0' \, \mathrm{e}^{2s} \tag{38b}$$

$$a = a_0. \tag{38c}$$

When the most general solution of (36) is required, the integration constants ρ_0, ρ_0' and a_0 have to be regarded as arbitrary functions (being, however, different from a characteristic) of a parameter t so that equations (38a)-(38c) constitute the parameter representation $\rho(t, s)$, $\rho'(t, s)$, $a(t, s)$ of an integral surface in three-dimensional (ρ, ρ', a) space. Elimination of s from (38a, b) yields

$$\frac{\rho'}{\rho^2} = \frac{\rho_0'(t)}{\rho_0^2(t)}. \tag{39}$$

Thus t has to be looked upon as an arbitrary function of ρ'/ρ^2, $t = q(\rho'/\rho^2)$, so that we finally find

$$a = a_0(t) = a_0(q(\rho'/\rho^2))$$

or

$$a(\rho, \rho') = r(\rho'/\rho^2) \tag{40}$$

where r is again an arbitrary function. Equation (40) is the most general solution of (36).

Using solution (40) we are now able to determine $b(\rho, \rho')$ from (35). Let

$$u \equiv \rho'/\rho^2. \tag{41}$$

It follows that

$$\rho \frac{\partial b}{\partial \rho'} = \rho' \left(\frac{\hbar^2}{4m} - 2 \frac{\mathrm{d}}{\mathrm{d}u}(ur(u)) \right)$$

or

$$\frac{\partial b}{\partial \rho'} = 2\rho u \left(\frac{\hbar^2}{8m} - \frac{\mathrm{d}}{\mathrm{d}u}(ur(u)) \right). \tag{42}$$

From this equation we obtain by integration with respect to ρ'

$$b(\rho, \rho') = \int_0^{\rho'} \frac{\partial b(\rho, v)}{\partial v} \, \mathrm{d}v + p(\rho) \tag{43}$$

where $p(\rho)$ has not yet been determined. With the new integration variable $w = v/\rho^2$ we find from (42) and (43)

$$b(\rho, \rho') = 2\rho^3 \int_0^u w\left(\frac{\hbar^2}{8m} - \frac{\mathrm{d}}{\mathrm{d}w}(wr(w))\right) \mathrm{d}w + p(\rho)$$

$$= \frac{\hbar^2}{8m}\rho^3 u^2 - 2\rho^3\left(u^2 r(u) - \int_0^u wr(w)\,\mathrm{d}w\right) + p(\rho)$$

$$b(\rho, \rho') = \left(\frac{\hbar^2}{8m} - 2r\left(\frac{\rho'}{\rho^2}\right)\right)\frac{\rho'^2}{\rho} + 2\rho^3 R\left(\frac{\rho'}{\rho^2}\right) + p(\rho) \tag{44}$$

where we have put

$$R(u) = \int_0^u wr(w)\,\mathrm{d}w. \tag{45}$$

Let us now evaluate equation (34). When the derivatives of expressions (40) and (44) are inserted in (34), we are left, after some algebra, with

$$\rho\frac{\mathrm{d}^2 p}{\mathrm{d}\rho^2} - 2\frac{\mathrm{d}p}{\mathrm{d}\rho} = 0 \tag{46}$$

which has the general solution

$$p(\rho) = \tilde{\kappa}\rho^3 + c \tag{47}$$

(cf equations (13) and (14)) with integration constants $\tilde{\kappa}$ and c.

Combining equations (28), (40), (44), and (47), we eventually obtain the most general solution of (26), namely

$$\varepsilon_k = r\left(\frac{\rho'}{\rho^2}\right)\rho'' + \left[\frac{\hbar^2}{8m} - 2r\left(\frac{\rho'}{\rho^2}\right)\right]\frac{\rho'^2}{\rho} + \left[2R\left(\frac{\rho'}{\rho^2}\right) + \tilde{\kappa}\right]\rho^3 + c. \tag{48}$$

From the condition that $\varepsilon_k \geq 0$ for arbitrary density distributions $\rho(x) \geq 0$ we conclude that

$$r(\rho'/\rho^2) = 0. \tag{49}$$

Otherwise ε_k could become negative for sufficiently negative ρ''. (49) implies, however, that $R(u) \equiv 0$ (see (45)) so we are left with

$$\varepsilon_k = \tilde{\kappa}\rho^3 + \frac{\hbar^2}{8m}\frac{\rho'^2}{\rho} \tag{50}$$

which is just the same expression as equation (25). The constant c, equation (48), vanishes because of the physical requirement that $\varepsilon_k \equiv 0$ for $\rho \equiv 0$.

5. Conclusion

In the preceding sections we have calculated the most general kinetic energy density functionals ε_k subject to the following constraints:

(i) ε_k is a function f of ρ and $\rho', \rho'', \ldots \rho^{(n)}$ ($n \geq 0$, integer),

(ii) ε_k is non-negative for arbitrary trial densities $\rho \geq 0$,

(iii) ε_k satisfies the differential virial theorem, equation (3).

The second and third conditions have to be obeyed exactly by the exact (unknown) kinetic energy density functional, whereas the first is a condition which seems to be a reasonable approximation.

On combining (i), (iii) and the Euler equation (9*a*) of the energy minimisation problem, we eliminate the potential and obtain for various n differential equations (10) not for $\rho(x)$, but for the unknown functions $f(\rho, \rho', \ldots \rho^{(n)})$ of the independent variables $\rho, \rho', \ldots \rho^{(n)}$.

These differential equations have been solved exactly for the cases $n = 0$, 1 and 2, the results being as follows.

(*a*) $n = 0$. When only local dependence $\varepsilon_k = f(\rho)$ is admitted equation (12) can be solved only if the term $\sim\rho'''$ is discarded. In this case, the solution is a TF term $\varepsilon_k \sim \rho^3$ with indetermined coefficient.

(*b*) $n = 1$. The partial differential equation (16) which arises from (10) for the case $\varepsilon_k = f(\rho, \rho')$ yields the solution

$$\varepsilon_k = \tilde{\kappa}\rho^3 + \frac{\hbar^2}{8m}\frac{\rho'^2}{\rho} \tag{25}$$

with arbitrary TF term, but with the original full Weizsäcker coefficient.

(*c*) $n = 2$. When still greater flexibility is admitted by letting $\varepsilon_k = f(\rho, \rho', \rho'')$ the corresponding partial differential equation (26) leads, by rather lengthy calculations, to the general solution (48) where, besides constants of integration, an arbitrary function r occurs. However, because of condition (ii), r has to be put to zero so that again we are left with the functional (25), thus ruling out any dependence of ε_k on ρ''.

In summary, when constraints (i)-(iii) are taken into account strictly, ε_k is necessarily given by (25), at least for $0 \leqslant n \leqslant 2$.

Of course, expression (25) cannot yet serve as functional for practical calculations since $\tilde{\kappa}$ cannot be fixed by the above conditions. However, results of this work clearly indicate, from a new point of view, that consistent corrections to functionals of the type of equations (2) have to be applied to the coefficient of the TF term, not to the coefficient of the Weizsäcker term. This result is in agreement with conclusions drawn by other authors [10-16]. Using different arguments these workers leave λ_w unchanged, but let the TF coefficient $\kappa(N)$ depend on the particle number N such that $\lim_{N\to\infty} \kappa(N) = \kappa_{TF}$.

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