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ADDENDUM

On possible gradient approximations to the one-dimensional kinetic energy density functional compatible with the differential virial theorem

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Abstract. When the kinetic energy density ε_k (defined positive definite) of a system of one-dimensional, non-interacting fermions is approximated by an ordinary function of the density ρ, and of the lowest n derivatives of ρ, $\varepsilon_k \geqslant 0$ can satisfy the differential virial theorem for arbitrary density distributions only if ε_k actually depends on ρ and ρ' only. Thus the case $n > 1$ is ruled out, and one is left with the result $\varepsilon_k = \kappa\rho^3 + \rho'^2/(8\rho)$ $(\kappa \geqslant 0)$ already obtained in previous work.

The construction of the kinetic energy density functional (KEDF) ε_k has been a challenge in density functional theory since its very beginning [1]-[3]. Since it seems impossible to obtain the exact KEDF, one has to resort to approximations.

In one of the most important approximations, $\varepsilon_k(x)$ at some point x is expressed by the fermion density ρ and by its lowest derivatives taken as the *same* point x. In one dimension, this means that

$$\varepsilon_k(x) = f(\rho(x), \rho'(x), \ldots, \rho^{(n)}(x)) \tag{1}$$

with f being an ordinary function of n variables.

For $n = 0$, 1 and 2, one of the authors [4] investigated the most general function f compatible with the differential virial theorem [5], [6]

$$\varepsilon_k'(x) = \tfrac{1}{8}\rho'''(x) - \tfrac{1}{2}V'(x)\rho(x) \tag{2}$$

where $V(x)$ is the one-body potential in which the particles are moving. Equation (2) is valid in this form if the positive definite expression

$$\varepsilon_k = \frac{1}{2}\sum_{i=1}^{N} |\psi_i'|^2 \geqslant 0 \tag{3}$$

is used for a system of N fermions occupying the bound states ψ_i singly up to ψ_N.

When equation (2) is combined with the Euler equation of density functional theory the potential can be eliminated yielding [4]

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

This equation governs the dependence of f upon the variables $\rho, \rho', \ldots, \rho^{(n)}$ which are allowed to take on independently arbitrary values each (except for ρ being $\geqslant 0$). For $n \leqslant 2$, it turned out that

$$\varepsilon_k = \kappa\rho^3 + \frac{\rho'^2}{8\rho} \tag{5}$$

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($\kappa \geqslant 0$ indeterminced constant) is the most general expression among the class (1) of functions. Especially, in the case of $n = 2$, one finds that ρ'' actually cannot occur in ε_k, on account of the constraint $\varepsilon_k \geqslant 0$.

In this addendum, this result is generalized to arbitrary n. Thus we shall prove the following theorem.

Theorem. If ε_k is approximated by an expression of the form (1) with $n \geqslant 2$ then the requirements both of

(i) compatibility with the differential virial theorem (2)

(ii) positive definiteness (3)

imply that ε_k actually is dependent upon ρ and ρ' only, i.e. that ε_k is given by (5).

Proof. Introducing the notation

$$f_\nu \equiv \frac{\partial f}{\partial \rho^{(\nu)}} \qquad f_{\nu\lambda} \equiv \frac{\partial^2 f}{\partial \rho^{(\nu)} \partial \rho^{(\lambda)}} \tag{6}$$

and

$$\Theta_{\lambda,\nu} \equiv \frac{\mathrm{d}^{\lambda+1} f_\nu}{\mathrm{d}x^{\lambda+1}} \tag{7}$$

etc, equation (4) reads

$$\sum_{\nu=0}^{n} [(-1)^\nu \rho \Theta_{\nu,\nu} - 2\rho^{(\nu+1)} f_\nu] = -\tfrac{1}{4}\rho'''. \tag{8}$$

Let us now look for the highest derivative occurring in $\Theta_{\lambda,\nu}$. For $\lambda = 1$ we have that

$$\begin{aligned}
\Theta_{1,\nu} &= \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}f_\nu}{\mathrm{d}x}\right) \\
&= \frac{\mathrm{d}}{\mathrm{d}x}\left(\sum_{\sigma=0}^{n} f_{\nu\sigma}\rho^{(\sigma+1)}\right) \\
&= \sum_{\tau=0}^{n}\sum_{\sigma=0}^{n} f_{\nu\sigma\tau}\rho^{(\tau+1)}\rho^{(\sigma+1)} + \sum_{\sigma=0}^{n} f_{\nu\sigma}\rho^{(\sigma+2)} \\
&\equiv R(\rho, \rho', \ldots, \rho^{(n+1)}) + f_{\nu n}(\rho, \rho', \ldots, \rho^{(n)})\rho^{(n+2)}
\end{aligned} \tag{9}$$

where R stands for an expression not further specified which, however, contains no terms with derivatives of order $n+2$. Differentiating further and focusing on the term associated with the highest derivative only we evidently can write

$$\Theta_{\lambda,\nu} = R(\rho, \rho', \ldots, \rho^{(n+\lambda)}) + f_{\nu n}(\rho, \rho', \ldots, \rho^{(n)})\rho^{(n+\lambda+1)}. \tag{10}$$

Therefore the only term involving the highest derivative $\rho^{(2n+1)}$ in equation (8) is given by

$$(-1)^n \rho \Theta_{n,n} = (-1)^n \rho [R(\rho, \rho', \ldots, \rho^{(2n)}) + f_{nn}\rho^{(2n+1)}] \tag{11}$$

(for $n \geqslant 2$). If equation (8) is to hold identically with respect to all variables $\rho, \rho', \ldots, \rho^{(2n+1)}$ it follows that the coefficient of $\rho^{(2n+1)}$ has to vanish, i.e.

$$f_{nn} = \frac{\partial^2 f}{\partial [\rho^{(n)}]^2} \equiv 0. \tag{12}$$

Thus f must be linear with respect to $\rho^{(n)}$,

$$\varepsilon_k = \alpha(\rho, \rho', \ldots, \rho^{(n-1)}) + \beta(\rho, \rho', \ldots, \rho^{(n-1)})\rho^{(n)} \tag{13}$$

where α and β are some functions not depending on $\rho^{(n)}$.

Condition (3), however, rules out linear dependence of ε_k upon $\rho^{(n)}$ (and, likewise, upon any $\rho^{(\nu)}$, $\nu > 0$). Otherwise ε_k could become negative for sufficiently negative $\rho^{(n)}$ at some point, in contrast to the requirement that $\varepsilon_k \geqslant 0$ for *all* density functions. Thus

$$\beta \equiv 0 \tag{14}$$

and hence ε_k can depend at most on $\rho, \ldots, \rho^{(n-1)}$. However, repeating the above arguments we finally end up with the result that ε_k is allowed to depend on ρ and ρ' only. This proves our theorem.

References

[1] Callaway J and March N H 1984 *Solid State Phys.* **38** 135
[2] March N H 1955 *Proc. Phys. Soc.* **70** 839
[3] Gombas P 1949 *Die statistische Theorie des Atoms und ihre Anwendungen* (Berlin: Springer)
[4] Baltin R 1987 *J. Phys. A: Math. Gen.* **20** 111
[5] March N H and Young W H 1959 *Nuclear Phys.* **12** 23
[6] Baltin R 1986 *Phys. Lett.* **113A** 121