Brief Reports

Exact single-particle kinetic energy functional for general two-level and model n-level one-dimensional systems: Dependence only on electron density and its gradient

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From the explicit solution of a two-level problem previously obtained, it is proved that the single-particle kinetic energy density functional $t_s[\rho]$ is the density ρ times a function solely of the ratio ρ'/ρ, with ρ' the first derivative of ρ. For an n-level system with a harmonic-oscillator potential, the form of $t_s[\rho]$ is explicitly obtained. Again $t_s[\rho]$ involves only ρ and ρ'; no higher derivatives appear.

I. INTRODUCTION

Recently we have been treating n-level one-dimensional systems of electrons moving in a one-body potential $V(x)$. These lead to an explicit expression for the kinetic energy density though this is given only implicitly in terms of the density $\rho(x)$. Our purpose here is to consider more explicitly the single-particle kinetic energy functional $T_s[\rho]$. We shall show below that the corresponding kinetic energy density $t_s[\rho]$ is, in fact, for a two-level system in one dimension, a product of ρ and a function only of ρ'/ρ. Then, for n-levels, we shall work out completely $t_s[\rho]$ for the example of a harmonic-oscillator potential. As illustrative of the philosophy of this work, we recall first the approximation due to von Weizsäcker,[1] as refined by Kirzhnits[2] (WK). These workers wrote the low-order expression

$$T_s^{WK}[\rho]=c_k \int \rho^3 dx + \frac{\lambda \hbar^2}{8m} \int \frac{(\rho')^2}{\rho} dx , \qquad (1.1)$$

with c_k the appropriate kinetic constant in the Thomas-Fermi limit which is valid asymptotically for large numbers of electrons N. The constant λ in Eq. (1.1) was set equal to unity by von Weizsäcker. The latter work of Kirzhnits proved that, in the limit of a slowly varying electron density, required to validate the Thomas-Fermi term, the correct value of λ is $\frac{1}{9}$.

The argument below will demonstrate that, while Eq. (1.1) is a relatively crude approximation to the single-particle kinetic energy functional, the philosophy of expressing $T_s[\rho]$ as a function of ρ and ρ' is, in fact, well justified. We note here, for reference later, that the inhomogeneity term involving λ in Eq. (1.1), is simply written in terms of $\ln\rho \equiv s$: namely

$$\frac{\lambda \hbar^2}{8m} \int \frac{(\rho')^2}{\rho} dx = \frac{\lambda \hbar^2}{8m} \int (s')^2 \exp(s) dx . \qquad (1.2)$$

In Sec. II, the two-level system will be exploited using the earlier work of Dawson and March[3] and March and Nalewajski.[4] Since this argument is somewhat formal and abstract for a general potential, Sec. III treats, quite explicitly, the single-particle kinetic density $t_s[\rho]$ for a harmonic-oscillator potential, but for a general n-level case.

II. GENERAL FORM OF $t_s[\rho]$ FOR TWO-LEVEL SYSTEM

The work in Refs. 3 and 4 allows the two-level system to be characterized, for a given potential $V(x)$, by wave functions

$$\sqrt{2}\psi_1(x)=\sqrt{\rho(x)}\cos\theta(x) \qquad (2.1)$$

and

$$\sqrt{2}\psi_2(x)=\sqrt{\rho(x)}\sin\theta(x) . \qquad (2.2)$$

From these references one can eliminate $V(x)$ to obtain a differential equation for the phase θ solely in terms of ρ'/ρ, namely[5]

$$\theta'' + \frac{\rho'}{\rho}\theta' = 2\xi \sin(2\theta) , \qquad (2.3)$$

where $\xi=(\varepsilon_1-\varepsilon_2)/2$, the eigenvalues ε_1 and ε_2 corresponding to the functions ψ_1 and ψ_2. The single-particle kinetic energy density $t_s[\rho]$ is readily found[3,4] as

$$t_s[\rho]=\frac{1}{8}\frac{(\rho')}{\rho}+\frac{1}{2}\rho(\theta')^2-\frac{1}{4}\rho'' . \qquad (2.4)$$

Since the term in ρ'' integrates to zero when one calcu-

lates the total kinetic energy

$$T_s[\rho] = \int t_s dx , \qquad (2.5)$$

one need only note that the part of t_s contributing to $T_s[\rho]$ is $\rho[\frac{1}{8}(\frac{\rho'}{\rho})^2 + \frac{1}{2}(\theta')^2]$. But from Eq. (2.3), θ' is determined solely by ρ'/ρ, and hence one concludes that

$$T_s[\rho] = \int \rho(x) F\left[x, \frac{\rho'}{\rho}\right] dx. \qquad (2.6)$$

This clearly is consistent with the philosophy of von Weizsäcker and Kirzhnits, no derivative higher than ρ' entering the functional $T_s[\rho]$.

In the following section, we shall make the result (2.6) quite explicit for the simple model of a harmonic-oscillator potential. Indeed, this model, as will be demonstrated, can be solved for n levels, with n arbitrary. The same conclusion, namely that in this example for arbitrary n the kinetic energy involves only ρ and ρ' but no higher derivatives, again follows.

III. n-LEVEL SYSTEM FOR A HARMONIC-OSCILLATOR POTENTIAL

The object of this section is to make use of the admittedly simple example of a harmonic-oscillator potential with n-levels occupied to calculate $t_s[\rho]$ and $T_s[\rho]$ explicitly.

To do so one used the result[6] for this model,

$$\frac{\delta t}{\delta \rho} = 3\frac{t}{\rho} + \frac{1}{4}\frac{\rho''}{\rho} . \qquad (3.1)$$

Combining this with the customary Euler equation

$$\mu - V(x) = \frac{\delta t}{\delta \rho} \qquad (3.2)$$

of the density-functional theory, μ being the chemical potential, leads to

$$\rho(\mu - V) = 3t + \frac{1}{4}\rho'' . \qquad (3.3)$$

From the work of Lawes and March,[7] again specifically for the harmonic-oscillator model,

$$\frac{\delta t}{\delta \rho} = \frac{1}{\rho'}\frac{dt}{dx} . \qquad (3.4)$$

Hence, from Eqs. (3.1) and (3.4) one obtains

$$\frac{dt}{dx} = 3\frac{\rho' t}{\rho} + \frac{1}{4}\frac{\rho'\rho''}{\rho} . \qquad (3.5)$$

This first-order differential equation for the kinetic density t can be solved using the integrating factor ρ^{-3}, to yield

$$t = \frac{1}{8}\frac{(\rho')^2}{\rho} + \frac{1}{2}\rho^3 \int^x \frac{(\rho')^3}{\rho^5} dy . \qquad (3.6)$$

This demonstrates quite explicitly that for this model, with n levels occupied, and n arbitrary, t is determined solely by ρ and ρ', with no higher derivatives entering the functional. With regard to the lower limit of the integral appearing in Eq. (3.6), this has been calculated explicitly for the case of one level only and has the value $-(2)^{1/2}$.

The final step to be taken is to show that one can recover the correct Euler equation from the energy variation principle, built from the kinetic energy density t in Eq. (3.6) and the independent-particle potential energy $\int \rho(x)V(x)dx$ with $V(x) = \frac{1}{2}x^2$. The standard procedure of the calculus of variations leads straightforwardly to the result[7]

$$-\frac{1}{2}\rho V' - \frac{1}{8}\rho''' = (\mu - V)\rho' . \qquad (3.7)$$

IV. SUMMARY AND CONCLUSION

The main results of this work are embodied in Eqs. (2.6) and (3.6). The former Eq. is for a general potential $V(x)$ but for a two-level case only. As to Eq. (3.6), this is valid for the general n-level case, but only for the harmonic-oscillator model. The principal point to be stressed, based on these two equations, is that in both cases the single-particle kinetic energy functional involves ρ and ρ', but no higher derivatives of ρ. This seems encouraging in the context of the continuing search[8,9] for the general single-particle kinetic energy functional.

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