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Kinetic energy of an electron gas

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We derive a simple expression for the correlation part of the kinetic energy of an inhomogeneous electron gas from density-functional theory. We show that in the local density approximation, this expression reduces to the virial theorem result $t_{xc}=3v_{xc}-4\epsilon_{xc}$. We also derive the correction for an inhomogeneous gas using Langreth and Mehl's expression for the exchange-correlation energy from a nonuniform density.

The correlation contribution to the kinetic energy plays a special role in assessing the quality of approximations used in applications of the density-functional theorem.[1] A general expression for the complete kinetic energy in the density-functional formalism has not previously been available.

Bauer[2] has recently shown that the ground-state expectation value of any operator $\hat{o}$, can be evaluated in the Hohenberg-Kohn-Sham density-functional scheme,[3,4] subject to a generalized V-representability condition. He showed that if the Hamiltonian is augmented by the operator $\hat{o}$ via a scalar field λ,

$$\mathscr{H}=\mathscr{H}(\lambda=0)+\lambda\hat{o} \;, \tag{1}$$

and the exchange-correlation energy is computed for small values of the field λ, then the correction to the expectation value calculated using the Kohn-Sham single-determinant wave function is the derivative of the exchange-correlation energy with respect to the field, λ:

$$\langle\hat{o}\rangle-\langle\hat{o}\rangle_s=\frac{\partial E_{xc}}{\partial\lambda}\Big|_{\lambda=0} \;. \tag{2}$$

One case where this result can be applied directly and needs no extra V-representability condition is to the calculation of the correlation part of the kinetic energy. In this case the augmented Hamiltonian becomes

$$\mathscr{H}(\lambda)=(1+\lambda)T+W_{\text{int}}=\frac{e^2}{2}\left[\sum_i(1+\lambda)a_0\nabla_i^2+\sum_{i\neq j}\frac{1}{r_{ij}}\right] , \tag{3}$$

where T is the kinetic-energy operator, W_{int} is the electron-electron interaction operator, and a_0 is the Bohr radius. As the Hamiltonian depends on λ and a_0 only through the combination $(1+\lambda)a_0$, it is immediately obvious that the exchange-correlation energy depends on these parameters only through the same combination. We then use the resulting identity

$$\frac{\partial E_{xc}}{\partial\lambda}\Big|_{\lambda=0}=a_0\frac{\partial E_{xc}}{\partial a_0} \tag{4}$$

to find the exchange-correlation contribution to the kinetic energy as

$$T_{xc}=a_0\frac{\partial E_{xc}}{\partial a_0} \;, \tag{5}$$

where we are now setting $\lambda=0$ in all formulae. This is the primary result in this paper.

In an homogenous electron gas, the exchange-correlation energy density can be written in terms of a_0 as

$$\epsilon_{xc}=\epsilon_x g(a_0^3 n) \;, \tag{6}$$

where $\epsilon_x=-0.75e^2(3n/\pi)^{1/3}$ does not depend explicitly on a_0. Since we can write

$$a_0\frac{\partial g(a_0^3n)}{\partial a_0}=3n\frac{\partial g(a_0^3n)}{\partial n}=3n\frac{\partial(\epsilon_{xc}/\epsilon_x)}{\partial n} \;, \tag{7}$$

and

$$\frac{\partial\epsilon_x}{\partial n}=-\frac{\epsilon_x}{3n} \;, \tag{8}$$

we see that the correlation kinetic-energy density can be written as

$$t_c=3v_{xc}-4\epsilon_{xc} \;, \tag{9}$$

where v_{xc} is the exchange-correlation potential,

$$v_{xc}=\frac{\partial n\,\epsilon_{xc}}{\partial n} \;,$$

in agreement with the virial theorem result.[5]

We can also apply Eq. (5) to an inhomogeneous electron gas by writing the exchange-correlation energy density in terms of $g(a_0^3n,\, a_0^4|\nabla n|,\, a_0^5\nabla^2 n,\,\ldots)$, so that Langreth and Mehl's expression[6] for the extra exchange-correlation energy due to inhomogeneity yields an extra exchange-correlation kinetic-energy contribution,

$$\Delta T_{xc}=\int d^3r\; n\,\Delta t_{xc} \;, \tag{10}$$

where, in atomic units,

$$\Delta t_{xc}=-(1.712\times10^{-2})\frac{|\nabla n|^2}{n^{7/3}}[\exp(-F)-\tfrac{7}{9}] +(3.36\times10^{-3})\frac{|\nabla n|^3}{n^{7/2}}\exp(-F) \;, \tag{11}$$

and

$$F=0.262\frac{|\nabla n|}{n^{7/3}} \;.$$

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[1] M. Levy and J. P. Perdew, Bull. Am. Phys. Soc. **30**, 225 (1985).
[2] G. E. W. Bauer, Phys. Rev. B **27**, 5912 (1983).
[3] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
[4] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
[5] See, for example, A. R. Williams and U. von Barth, in *Theory of the Inhomogeneous Electron Gas,* edited by S. Lundqvist and N. H March (Plenum, New York, 1983).
[6] D. C. Langreth and M. J. Mehl, Phys. Rev. Lett. **47**, 446 (1981); Phys. Rev. B **28**, 1809 (1983)

