

**Gradient term in the Kohn-Sham exchange-correlation potential\***

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We show that the gradient expansion of the Kohn-Sham potential does not exist for the case of pure exchange but that when correlation is taken into account by screening the exchange, the expansion does exist and has a different dependence on the charge density than that assumed by Herman *et al.* and by Sham. We obtain the gradient term to all powers in  $e^2$ . Our gradient term vanishes in regions where the charge density vanishes, unlike the gradient term calculated by Herman *et al.* and Sham which becomes infinite.

I. INTRODUCTION

Hohenberg and Kohn<sup>1</sup> and Kohn and Sham<sup>2</sup> (KS) have shown that the energy of an interacting electron gas may be written as a functional of the charge density

$$E_v[n] = T_s[n] + \int v(\vec{r})n(\vec{r}) d\vec{r} + \frac{1}{2} \int \frac{n(\vec{r})n(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r} d\vec{r}' + E_{xc}[n], \quad (1)$$

where  $T_s[n]$  is the kinetic-energy functional for non-interacting electrons and  $E_{xc}[n]$  is the exchange and correlation energy functional,<sup>3</sup>

$$T_s[n] = \frac{3}{10} \int (3\pi^2 n)^{2/3} n d\vec{r} + \frac{1}{2} \int t^{(2)}(n) |\nabla n|^2 d\vec{r} + \dots, \quad (2)$$

$$E_{xc}[n] = \int g_{xc}(n) n d\vec{r} + \frac{1}{2} \int g_{xc}^{(2)}(n) |\nabla n|^2 d\vec{r} + \dots, \quad (3)$$

$g_{xc}^{(2)}$  and  $t^{(2)}$  are unknown functions of  $n$ ,  $v(r)$  is the external potential (i.e., the nuclear potential in an atom or crystal), and  $g_{xc}$  is the exchange plus correlation energy per electron in a free-electron gas.

Dropping the  $|\nabla n|^2$  terms, KS obtained from the stationary property of Eq. (1), subject to the condition

$$\int \delta n(\vec{r}) d\vec{r} = 0, \quad (4)$$

the equation

$$\delta n(\vec{r}) \left( \varphi(\vec{r}) + \frac{\delta T_s[n]}{\delta n(\vec{r})} + \mu_{xc}(n(\vec{r})) \right) d\vec{r} = 0, \quad (5)$$

where  $\varphi(\vec{r}) = v(\vec{r}) + \int d\vec{r}' n(\vec{r}') / |\vec{r} - \vec{r}'|$  and  $\mu_{xc}(n) = d[n g_{xc}(n)] / dn$ . Noting that Eqs. (4) and (5) are identical to what is obtained for a system of non-interacting electrons moving in a potential  $\varphi(\vec{r}) + \mu_{xc}(n(\vec{r}))$ , KS pointed out that one obtains the  $n(\vec{r})$  which satisfies these equations by solving the one-electron Schrödinger equation

$$\left[ -\frac{1}{2} \nabla^2 + \varphi(\vec{r}) + \mu_{xc}(n(\vec{r})) \right] \Psi_i(\vec{r}) = \epsilon_i \Psi_i(\vec{r}), \quad (6)$$

and setting

$$n(\vec{r}) = \sum_{i=1}^N |\Psi_i(\vec{r})|^2, \quad (7)$$

where  $N$  is the number of electrons. It is to be emphasized that the one-electron eigenvalues  $\epsilon_i$  and eigenfunctions  $\Psi_i(\vec{r})$  are meaningless in themselves. Only the total charge density (7) and total energy obtained by substituting (7) in (1) are meaningful.

Herman *et al.*<sup>4</sup> (dropping correlation effects) tried to include the  $|\nabla n|^2$  exchange terms in (6) by replacing  $\mu_{xc}(n(\vec{r}))$  by the variation of  $E_x[n]$  with respect to  $n$ ,  $\nabla n$ , and  $\nabla^2 n$ . They chose to write

$$E_x[n] = \frac{1}{2} \int n V_{xs}(n) d\vec{r} + \frac{3}{2} \beta \int n G(n) V_{xs}(n) d\vec{r}, \quad (8)$$

where  $\beta$  is a constant to be determined,

$$G(n) = n^{-2/3} \left[ \frac{4}{3} \left( \frac{\nabla n}{n} \right)^2 - \frac{2 \nabla^2 n}{n} \right], \quad (9)$$

and the Slater exchange potential

$$V_{xs} = 2 \mathcal{E}_x = -3 [(3/8\pi)n(\vec{r})]^{1/3}. \quad (10)$$

Integrating by parts on the  $\nabla^2 n$  term one sees that (8) is identical to (3), providing

$$g_{xc}^{(2)}(n) = -3\beta(3/\pi)^{1/3} n^{-4/3}. \quad (11)$$

Taking  $V_x = \delta_{n, \nabla n, \nabla^2 n} (\frac{1}{2} n V_{xs}(n) + \frac{3}{2} \beta n G(n) V_{xs}(n))$ , Herman *et al.* obtained

$$V_x = \frac{2}{3} V_{xs}(n) + \beta G(n) V_{xs}(n). \quad (12)$$

The choice of Herman *et al.* for  $G(n)$ , or equivalently  $g_{xc}^{(2)}(n)$ , was dictated by the requirement that the gradient terms in  $V_x$  be dimensionally equivalent to  $V_{xs}$ . Substituting  $V_x$  for  $\mu_x$  in Eq. (6) they adjusted  $\beta$  either to minimize the total energy or to make the total energy equal to the Hartree-Fock

energy. They found  $\beta = 5 \times 10^{-3}$  and  $3.14 \times 10^{-3}$ , respectively, for atomic krypton with little variation for other atoms. Sham<sup>5</sup> attempted a first-principles calculation of  $\beta$  (which we discuss in Sec. II) and found<sup>6</sup>  $\beta = 1.13 \times 10^{-3}$ . Thus,  $V_x$  presents two paradoxes; the "experimental" values differ from the theoretical value by a factor of 3 or 5, and in the limit of zero charge density  $V_x$  becomes infinite rather than zero (Herman *et al.* multiplied  $V_x$  by an exponential damping factor to remove this infinity).

The resolution of these paradoxes is simply that both Herman *et al.* and Sham were wrong when they assumed  $g_x^{(2)}(n)$  must be proportional to  $n^{-4/3}$  [Eq. (11)] in order that the gradient term of  $E_x[n]$  scale in the same way as the local term. The local term is a pure exchange energy, i. e., a Coulomb potential energy, whereas the gradient term contains both potential- and kinetic-energy contributions and therefore does not scale as a Coulomb energy. This is obvious from Eq. (1), where  $E_x$  is seen to be the total energy minus the Hartree potential energy minus the kinetic energy of a *noninteracting* charge distribution. Thus  $E_x$  represents the exchange energy, plus the actual kinetic energy, minus the kinetic energy of noninteracting electrons with the same charge density. These two kinetic-energy terms cancel only in the trivial case of a free-electron gas, and therefore the local term of  $E_x$  is a pure exchange term while the gradient term is not. Although we are unable to give an absolute proof of our assertion that the kinetic-energy functional in a system with exchange differs from the noninteracting kinetic-energy functional, the following argument seems quite convincing. Consider an electron gas in the Hartree approximation with a weak applied potential  $V_G^H e^{i\mathbf{G}\cdot\mathbf{r}}$ . This will induce a Fourier component of charge density  $\rho_G^H$ . Consider also the Hartree-Fock case with a  $V_G^{HF}$  and  $\rho_G^{HF}$ . Now choose  $V_G^{HF}$  to be such that  $\rho_G^{HF} = \rho_G^H$ . If the two kinetic-energy functionals are identical then the two systems will have the same kinetic energy. But the one-electron wave functions for the two systems are entirely different. This follows from the fact that the nonlocal exchange operator may be replaced by a *different* local potential for each electron; thus the total potential seen by each electron is different and therefore different from the Hartree potential. Since the two systems consist of different wave functions, it seems most unlikely that the expectation value of the kinetic-energy operator will be the same for both systems.

Assuming the Kohn-Sham theory to be correct, the virial theorem must hold. However it is not clear whether or not it should hold term by term in the gradient expansion. Many, including Sham,<sup>7</sup> have shown that it holds in the case of exchange without correlation for the first term of the expansion (i. e., local charge density approximation) and

Sham<sup>7</sup> has stated that it holds for the gradient terms as well. However, this assertion was based on the assumption that the gradient term in  $E_x$  scaled like pure exchange. In Sec. II we show that the gradient term in  $E_x$  is singular, so that the question becomes moot. We then derive the gradient term for the case of screened exchange (the screening is an effect of correlation). The expression is so complicated that the kinetic, exchange, and correlation parts cannot be separated. Even if they could, however, it is not likely that the virial theorem would hold because of the approximations inherent in screened exchange.

## II. GRADIENT TERM IN THE EXCHANGE-CORRELATION ENERGY

Following Sham,<sup>5</sup> we write the integral equation for the irreducible vertex function

$$\bar{\Lambda}(\vec{k} + \vec{q}, \vec{k}) = 1 - \int \frac{d^3k'}{(2\pi)^3} \bar{\chi}(\vec{k}' + \vec{q}, \vec{k}') u(\vec{k} - \vec{k}') \bar{\Lambda}(\vec{k}' + \vec{q}, \vec{k}'), \quad (13)$$

where for the case of pure exchange

$$u(q) = 4\pi e^2 / q^2, \quad (14)$$

and

$$\theta(\vec{k}' + \vec{q}, \vec{k}') = (f_{\vec{k}'+\vec{q}} - f_{\vec{k}'}) / [E(\vec{k}' + \vec{q}) - E(\vec{k}')]. \quad (15)$$

$f_{\vec{k}}$  is the occupation number of the state  $\vec{k}$  and  $E(\vec{k})$  is the electron energy in a homogeneous system,

$$E(k) = \frac{1}{2} k^2 + E_{xc}(k). \quad (16)$$

When correlation is included, Eq. (13) is an approximation which assumes that the spin symmetric part of the effective particle-hole interaction is energy independent. The major effect of correlation is to screen the exchange interaction and so we will replace (14) by

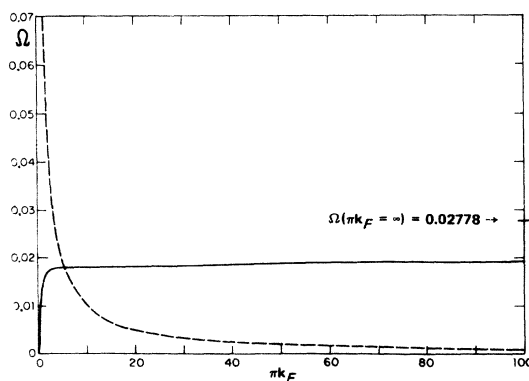


FIG. 1. Graph of  $\Omega$  as a function of  $\pi k_F$  in Hartree atomic units;  $\Omega$  is defined in Eq. (34) in the text. The dashed curve is Sham's  $\Omega$ .

$$u(q) = 4\pi e^2 / (q^2 + \lambda^2). \quad (17)$$

For computational ease Sham also worked with (17) but took the limit  $\lambda \rightarrow 0$  at the end. Because he worked only to first order in  $e^2$ , he obtained a finite result for  $g^{(2)}(n)$ , but, as we shall see, due to the infinite density of states at the Fermi surface in the Hartree-Fock approximation,  $g^{(2)}(n)$  is actually infinite in the  $\lambda \rightarrow 0$  limit and one cannot separate the exchange and correlation terms in the gradient expansion.

Expanding the density response function

$$\chi(q) = 2 \int \frac{d^3k}{(2\pi)^3} \theta(\vec{k} + \vec{q}, \vec{k}) \bar{\Lambda}(\vec{k} + \vec{q}, \vec{k}) \quad (18)$$

in a Taylor series

$$\chi(q) = \chi^{(0)} + \chi^{(2)} q^2 + \dots, \quad (19)$$

Sham obtained

$$g_{xc}^{(2)}(n) = \chi^{(2)} / (\chi^{(0)})^2 - \chi_0^{(2)} / (\chi_0^{(0)})^2. \quad (20)$$

Because he assumed the density dependence of  $g_x^{(2)}$  is  $n^{-4/3}$ , Sham inserted (13) into (18) iterating  $\bar{\Lambda}$  and retaining only terms to first order in  $e^2$ , higher powers of  $e^2$  entering as  $e^2/\pi k_F$  which yield extra factors of  $n^{-1/3}$ . The screened exchange energy is given by

$$E_{xc}(k) = - \int \frac{d^3k'}{(2\pi)^3} f_{k'} u(k - k') = - \frac{e^2 k_F}{\pi} \left[ 1 - \frac{\lambda}{k_F} \left( \tan^{-1} \frac{k + k_F}{\lambda} - \tan^{-1} \frac{k - k_F}{\lambda} \right) + \frac{k_F^2 + \lambda^2 - k^2}{4k k_F} \ln \frac{(k + k_F)^2 + \lambda^2}{(k - k_F)^2 + \lambda^2} \right], \quad (21)$$

so that making an expansion in powers of  $e^2$  is equivalent to assuming that  $[E_{xc}(\vec{k} + \vec{q}) - E_{xc}(k)] / [\frac{1}{2}(\vec{k} + \vec{q})^2 - \frac{1}{2}k^2] \ll 1$ . Because of the  $\delta$ -function nature of  $df_k/dE$ ,  $k$  ends up being evaluated on the Fermi surface, where in the  $\lambda \rightarrow 0$  limit the ratio is not much less than one but is actually infinite. Therefore, not only was Sham's physical reason for expanding in powers of  $e^2$  invalid, but it is also mathematically invalid as well.

We have solved for  $g^{(2)}(n)$  without any expansion in powers of  $e^2$ . We first expand  $\theta$  to order  $q^2$ ,

$$\theta(\vec{k} + \vec{q}, \vec{k}) = f'_k + \frac{1}{4} \frac{\nu}{k} (q^2 + 2qk\mu) f''_k + \left[ \frac{1}{4} \left( \frac{d\nu}{dk} - \frac{\nu}{k} \right) f''_k + \frac{1}{6} \nu^2 f'''_k \right] q^2 \mu^2, \quad (22)$$

where  $\mu$  is the cosine of the angle between  $\vec{k}$  and  $\vec{q}$ ,  $\nu = dE/dk$  with  $E$  given by (16) and (21) and the primes on  $f_k$  indicate differentiation with respect to  $E$ . We also expand  $\bar{\Lambda}$  to order  $q^2$ ,

$$\bar{\Lambda}(\vec{k} + \vec{q}, \vec{k}) = a + bq^2/k_F^2 + cq\mu/k_F + dq^2\mu^2/k_F^2, \quad (23)$$

where  $a$ ,  $b$ ,  $c$ , and  $d$  are functions of  $k$  to be determined. Substituting (22) and (23) in (18), we obtain

$$\chi = - \frac{k_F^2}{\pi^2 \nu_F} \left( a_F + \left\{ b_F + \frac{1}{3} d_F - \frac{1}{3} c_F - \frac{1}{6} k_F \left( \frac{dc}{dk} \right)_F - \frac{1}{18} a_F \left[ 1 + \frac{k_F}{\nu_F} \left( \frac{d\nu}{dk} \right)_F + \frac{1}{2} \frac{k_F^2}{\nu_F} \left( \frac{d^2\nu}{dk^2} \right)_F \right. \right. \right. \\ \left. \left. \left. - \frac{1}{2} \frac{k_F^2}{\nu_F^2} \left( \frac{d\nu}{dk} \right)_F^2 \right] - \frac{1}{18} k_F \left( \frac{da}{dk} \right)_F \left[ \frac{1}{2} \frac{k_F}{\nu_F} \left( \frac{d\nu}{dk} \right)_F - 1 \right] + \frac{1}{18} k_F^2 \left( \frac{d^2a}{dk^2} \right)_F \left( \frac{q^2}{k_F^2} \right) \right), \quad (24)$$

where the subscript  $F$  indicates that a quantity is to be evaluated on the Fermi surface. We next insert (22) and (23) in (13), use the spherical-harmonic addition formula inside the integral, and equate  $q$ -independent terms to solve for  $a$ , terms containing  $q\mu$  to solve for  $c$ , and terms containing  $q^2$  or  $q^2\mu^2$  to solve for  $b + \frac{1}{3}d$ . We get

$$a_F = \nu_F / k_F D_F, \quad (25)$$

$$k_F \left( \frac{da}{dk} \right)_F = 2c_F = \frac{e^2}{2\pi k_F D_F} \left( \frac{4k_F^2}{4k_F^2 + \lambda^2} - \ln \frac{4k_F^2 + \lambda^2}{\lambda^2} \right), \quad (26)$$

$$k_F^2 \left( \frac{d^2a}{dk^2} \right)_F = 2k_F \left( \frac{dc}{dk} \right)_F = \frac{e^2}{2\pi k_F D_F} \left( 2 \ln \frac{4k_F^2 + \lambda^2}{\lambda^2} - \frac{6k_F^2}{4k_F^2 + \lambda^2} - \frac{16k_F^4}{(4k_F^2 + \lambda^2)^2} - \frac{2k_F^2}{\lambda^2} \right), \quad (27)$$

and

$$b_F + \frac{1}{3} d_F = \frac{e^2}{\pi k_F D_F} \left\{ - \frac{1}{16} \left[ \frac{4}{3} + \frac{2}{3} \frac{k_F}{\nu_F} \left( \frac{d\nu}{dk} \right)_F \right] \left[ k_F \left( \frac{da}{dk} \right)_F \ln \frac{4k_F + \lambda^2}{\lambda^2} + \frac{4a_F k_F^2}{4k_F^2 + \lambda^2} \right] \right.$$

$$\begin{aligned}
& -\frac{1}{72} \left[ \frac{k_F}{\nu_F} \left( \frac{d\nu}{dk} \right)_F - \frac{k_F^2}{\nu_F^2} \left( \frac{d\nu}{dk} \right)_F^2 + \frac{k_F^2}{\nu_F} \left( \frac{d^2\nu}{dk^2} \right)_F \right] \ln \frac{4k_F^2 + \lambda^2}{\lambda^2} + \frac{1}{36} \left[ k_F^2 \left( \frac{d^2a}{dk^2} \right)_F \right. \\
& + \frac{k_F^2}{\nu_F} \left( \frac{d\nu}{dk} \right)_F \left( \frac{da}{dk} \right)_F + 2k_F \left( \frac{da}{dk} \right)_F \left. \right] \ln \frac{4k_F^2 + \lambda^2}{\lambda^2} + \frac{1}{36} \left[ \frac{k_F a_F}{\nu_F} \left( \frac{d\nu}{dk} \right)_F + 2a_F + 2k_F \left( \frac{da}{dk} \right)_F \right] \frac{4k_F^2}{4k_F^2 + \lambda^2} \\
& + \frac{1}{36} a_F \left( \frac{k_F^2 (-8k_F^2 + 2\lambda^2)}{(4k_F^2 + \lambda^2)^2} - \frac{2k_F^2}{\lambda^2} \right) - \frac{1}{12} c_F \left( \frac{4k_F^2}{4k_F^2 + \lambda^2} + 2 \ln \frac{4k_F^2 + \lambda^2}{\lambda^2} \right) - \frac{1}{12} k_F \left( \frac{dc}{dk} \right)_F \ln \frac{4k_F^2 + \lambda^2}{\lambda^2} \Big\} , \quad (28)
\end{aligned}$$

where

$$D_F = 1 - (e^2/\pi k_F) [1 - (\lambda^2/4k_F^2) \ln(4k_F^2 + \lambda^2)/\lambda^2] . \quad (29)$$

In addition, differentiating (16) we obtain

$$\frac{\nu_F}{k_F} = 1 - \frac{e^2}{\pi k_F} \left[ 1 - \left( \frac{1}{2} + \frac{\lambda^2}{4k_F^2} \right) \ln \frac{4k_F^2 + \lambda^2}{\lambda^2} \right] , \quad (30)$$

$$\left( \frac{d\nu}{dk} \right)_F = 1 - \frac{e^2}{\pi k_F} \left( -2 + \frac{2k_F^2}{4k_F^2 + \lambda^2} + \frac{k_F^2 + \lambda^2}{2k_F^2} \ln \frac{4k_F^2 + \lambda^2}{\lambda^2} \right) , \quad (31)$$

$$k_F \left( \frac{d^2\nu}{dk^2} \right)_F = -\frac{e^2}{\pi k_F} \left( \frac{k_F^2}{\lambda^2} + \frac{2\lambda^2 k_F^2}{(4k_F^2 + \lambda^2)^2} + \frac{15k_F^2 + 6\lambda^2}{4k_F^2 + \lambda^2} - \frac{3}{2} \frac{k_F^2 + \lambda^2}{k_F^2} \ln \frac{4k_F^2 + \lambda^2}{\lambda^2} \right) . \quad (32)$$

Inserting Eqs. (25)–(32) into (24) we obtain  $\chi$ , whence from Eqs. (19) and (20)  $g_{xc}^{(2)}(n)$  is obtained. In the  $\lambda \rightarrow 0$  limit we find  $\chi^{(2)}$  and therefore  $g_{xc}^{(2)}$  proportional to  $\ln \lambda$ . This infinity<sup>8</sup> in the Taylor-series expansion is in all likelihood due not to the unscreened exchange  $\chi$  being infinite but merely non-analytic (probably with a  $q^2 \ln q$  dependence). This implies (for the case of unscreened exchange) that although the exchange-energy functional exists, its gradient expansion [Eq. (3)] does not. If the effect of correlation is taken into account by making  $\lambda$  finite then  $\chi$  is obviously analytic.<sup>9</sup> We have taken the Thomas-Fermi value

$$\lambda^2 = k_{FT}^2 = 4e^2 k_F / \pi \quad (33)$$

and evaluated  $g_{xc}^{(2)}$  as a function of  $k_F$ . We write

$$g_{xc}^{(2)}(k_F) = (\pi^2/k_F^3) \Omega(k_F) \quad (34)$$

and plot  $\Omega(k_F)$  in Fig. 1 where we compare it with Sham's<sup>5</sup> result (for unscreened exchange)

$$\Omega_{\text{Sham}} = 7/72 \pi k_F . \quad (35)$$

Note if for small  $k_F$  we write  $\Omega \sim k_F^{-3\alpha}$  and substitute (34) into

$$V_{xc} = d[n \mathcal{E}_{xc}(n)]/dn + \delta_{n, \nabla n} \left( \frac{1}{2} g_{xc}^{(2)}(n) |\nabla n|^2 \right) , \quad (36)$$

we obtain terms in  $V_{xc}$  of the form  $|\nabla n|^2/n^{2+\alpha}$  and  $\nabla^2 n/n^{1+\alpha}$ . Because for any reasonable charge distribution,  $|\nabla n|^2/n^2$  and  $\nabla^2 n/n$  will be finite even where  $n \rightarrow 0$ , we see that  $V_{xc}$  will approach zero or infinity when  $n \rightarrow 0$  according to whether  $\alpha$  is negative or positive. From Fig. 1 we see that  $V_{xc}$  does approach zero as the charge density approaches zero, which indeed it must for either screened or unscreened exchange. The infinite  $V_{xc}(n=0)$  of Sham and Herman *et al.* is a consequence of their neglecting the kinetic contributions to  $g_{xc}^{(2)}$ . Whether our  $V_{xc}$  gives better results than Sham's for atomic calculations can only be determined by performing the calculations, but we do note that his  $V_{xc}$  was a factor-of-3 smaller than the empirical value of Herman *et al.*, and that our  $g_{xc}^{(2)}$  gets rapidly larger than his as  $\pi k_F$  gets larger than 5.4. In krypton at the nucleus  $\pi k_F \sim 300$ , and it does not fall off to 5.4 until a point somewhat past the maximum of the outermost valence electron wave function.

Finally, it is worth noting that Ma and Brueckner<sup>10</sup> have calculated the gradient term in  $e^2$ . However, to all orders in  $e^2$  this must also be infinite in order that the gradient term of the exchange plus correlation energy be finite.

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<sup>1</sup>P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).

<sup>2</sup>W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).

<sup>3</sup>We work in the Hartree atomic units of Refs. 1, 2, and 5 rather than the Rydberg atomic units of Ref. 4.

<sup>4</sup>F. Herman, J. P. Van Dyke, and I. B. Ortenburger, Phys. Rev. Lett. 22, 807 (1969) and Intern. J. Quan. Chem. 35, 827 (1969).

<sup>5</sup>L. J. Sham, in *Computational Methods in Band Theory*, edited by P. J. Marcus, J. F. Janak, and A. R. Williams (Plenum, New York and London, 1971), p. 458.

<sup>6</sup>The same value of  $\beta$  was found by Ma and Ortenburger

(unpublished).

<sup>7</sup>L. J. Sham, Phys. Rev. A 1, 969 (1970).

<sup>8</sup>If we keep only terms to first order in  $e^2$ , we obtain the finite result of Ref. 4.

<sup>9</sup>A. M. Beattie, J. C. Stoddart, and N. H. March, Proc. R. Soc. A 326, 97 (1971) find the exchange potential is singular even though they use a screened exchange dielectric function. The reason for this singularity can be traced back to their approximating the Hartree-Fock energy in an energy denominator by the kinetic energy.

<sup>10</sup>S. K. Ma and K. A. Brueckner, Phys. Rev. 165, 18 (1968).