

## ARTICLES

## Strictly correlated electrons in density-functional theory

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Electrons at a fixed density approach a strictly correlated limit as their Coulomb interaction is scaled to infinity. We find the exact energy for strictly correlated electrons in spherical two-electron densities, and a useful gradient expansion for general densities. We also propose a model for the coupling-constant dependence, which interpolates between the weak- and strong-interaction limits. This model defines a density functional which predicts accurate ground-state correlation energies for real atoms and the two-dimensional uniform electron gas. [S1050-2947(99)10001-5]

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Most physical properties of atoms, molecules, and solids arise from the quantum-mechanical behavior of the electrons. A simple but accurate theoretical description of these systems is very desirable. The most difficult contribution to the ground-state energy is due to electronic correlations, resulting from both Pauli exclusion and Coulomb repulsion. In density-functional theory (DFT [1]), this exchange-correlation energy  $E_{xc}[\rho]$  is exactly represented as an integral, involving a series of hypothetical systems which have the same ground-state electron density  $\rho(\mathbf{r})$  as the real system, but where the electronic repulsion is scaled by a factor  $\alpha$  ("coupling constant").

The present paper demonstrates that this "coupling-constant integration" can be performed very accurately if information on two extreme limits is considered. The familiar limit  $\alpha \rightarrow 0$  of weak interaction is dominated by the exchange energy and by the second-order correlation energy [2]. The limit  $\alpha \rightarrow \infty$  of strong interaction is also found to be mathematically simple, but in a different way. To describe this strong interaction, we introduce the concept "SCE" of *strictly correlated electrons*, and present an exact solution for spherical two-electron systems. An accurate approximation to SCE is provided by a simple gradient expansion which applies to any many-electron system. Using this information in a model for the coupling-constant dependence, we obtain a density functional for the correlation energy  $E_c[\rho]$  of real systems with  $\alpha = 1$ .

In DFT, the ground-state energy of a system of interacting electrons is presented as a functional

$$E[\rho] = T_s[\rho] + \int d^3r v_{\text{ext}}(\mathbf{r})\rho(\mathbf{r}) + U[\rho] + E_{xc}[\rho]$$

of the electron density  $\rho(\mathbf{r})$ .  $T_s[\rho]$  is the kinetic energy of a system of noninteracting electrons with a ground-state density  $\rho$ . The second term is the interaction with the external potential  $v_{\text{ext}}(\mathbf{r})$ . The two remaining terms describe the electron-electron interaction. The classical Coulomb or Hartree term

$$U[\rho] = \frac{1}{2} \int d^3r \int d^3r' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

treats the electrons as a continuous distribution of charge. All aspects of the many-body problem ignored in this continuum description are included in the explicitly unknown exchange-correlation functional  $E_{xc}[\rho]$ .

An exact expression for this functional is the coupling-constant integral [3]

$$E_{xc}[\rho] = \int_0^1 d\alpha W_\alpha[\rho],$$

$$W_\alpha[\rho] = \langle \Psi^\alpha[\rho] | \hat{V}_{ee} | \Psi^\alpha[\rho] \rangle - U[\rho]. \quad (1)$$

The integrand  $W_\alpha[\rho]$  has only potential-energy contributions.  $\hat{V}_{ee} \equiv \sum_{i < j} |\mathbf{r}_i - \mathbf{r}_j|^{-1}$  is the two-particle Coulomb interaction operator for electrons.  $\Psi^\alpha[\rho]$  is that wave function which minimizes the expectation value  $\langle \hat{T} + \alpha \hat{V}_{ee} \rangle$  for a fictive electron system with the kinetic-energy operator  $\hat{T}$  and the interaction  $\alpha \hat{V}_{ee}$ , subject to the constraint that it has the ground-state density  $\rho$  of the real system with interaction  $\hat{V}_{ee}$  ( $\alpha = 1$ ).

$W_\alpha[\rho]$  is expected to be a smooth function of the coupling constant  $\alpha$  [4,5]. Some key properties are known exactly [5-7]:

$$W_\alpha[\rho] = \alpha W_1[\rho_{1/\alpha}], \quad \rho_\lambda(\mathbf{r}) \equiv \lambda^3 \rho(\lambda \mathbf{r}), \quad (2)$$

$$W'_\alpha[\rho] \equiv dW_\alpha[\rho]/d\alpha < 0 \quad (\alpha \geq 0), \quad (3)$$

$$W_0[\rho] = E_x[\rho], \quad (4)$$

$$W'_0[\rho] = 2E_c^{\text{GL2}}[\rho], \quad (5)$$

$$W_\infty[\rho] \equiv \lim_{\alpha \rightarrow \infty} W_\alpha[\rho] \quad (\text{finite}). \quad (6)$$

$E_x[\rho]$ , the exchange energy, is the Fock integral with the (occupied) Kohn-Sham (KS) orbitals.  $E_c^{\text{GL2}}[\rho]$ , the second-

TABLE I. The approximations  $E_c^{\text{mod}}$  [Eq. (8)] of the exact correlation energy  $E_c$  [11,4(b)] for  $N$ -electron systems, using exact exchange energies  $W_0$  [11], exact or accurate  $W'_0$  [2,12], and  $W_{\text{SCE}}$  from Eq. (10) (for two-electron systems) or  $W_{\text{PC}}$  from Eq. (11) (in parentheses) as models for  $W_\infty$ .  $E_c$  (exact) for the exponential two-electron density (Exp.) is taken from Ref. [4(b)]. No exact value is available for the Gaussian two-electron density (Gau.). Hartree-Fock densities [10] have been used to calculate  $W_{\text{SCE}}$  and  $W_{\text{PC}}$  for the real atoms and ions. The less accurate energies  $E_c^{\text{GL2}}$  result from ignoring the information in  $W_\infty$ . (All energies in hartree.)

	$N$	$W_0$	$\frac{1}{2}W'_0 = E_c^{\text{GL2}}$	$W_{\text{SCE}}$	$(W_{\text{PC}})$	$E_c^{\text{mod}}$	$E_c^{\text{mod}}(\text{PC})$	$E_c$ (exact)
He	2	-1.0246	-0.0503	-1.500	(-1.463)	-0.042	(-0.041)	-0.042
Exp.	2	-0.6250	-0.0467	-0.910	(-0.886)	-0.036	(-0.035)	-0.037
Gau.	2	-0.7978	-0.0497	-1.152	(-1.102)	-0.040	(-0.038)	-
Ne <sup>8+</sup>	2	-6.0275	-0.0467	-8.795	(-8.554)	-0.045	(-0.045)	-0.046
Be	4	-2.6740	-0.125		(-3.943)		(-0.105)	-0.096
Ne	10	-12.084	-0.469		(-20.02)		(-0.420)	-0.394

order coefficient in Görling-Levy perturbation theory [7], can also be expressed in terms of the (occupied and unoccupied) KS orbitals [Eq. (4) in Ref. [7(a)]]. In this sense, quantities (4) and (5) represent the weak-interaction limit ( $\alpha \rightarrow 0$ ). Extrapolating  $W_\alpha[\rho]$  linearly from  $\alpha=0$ , we obtain from Eq. (1) the estimate  $E_c^{\text{GL2}}[\rho]$  for the correlation energy  $E_c \equiv E_{\text{xc}} - E_x$ .

This approximation can be improved substantially if information on the opposite limit  $\alpha \rightarrow \infty$  of strong interaction,  $W_\infty[\rho]$ , is included. The simple model

$$W_\alpha^{\text{mod}}[\rho] = W_\infty + \frac{W_0 - W_\infty}{\sqrt{1 + 2X\alpha}}, \quad X \equiv \frac{W'_0}{W_\infty - W_0} \quad (7)$$

for the integrand  $W_\alpha[\rho]$  fulfills requirements (3)–(6). In particular, it also fulfills Eq. (2), because [6,7]  $W_{0,\infty}[\rho_\lambda] = \lambda W_{0,\infty}[\rho]$  and  $W'_0[\rho_\lambda] = W'_0[\rho]$ .  $W_\alpha^{\text{mod}}$  is chosen so that there is an asymptotic  $\alpha^{-1/2}$  term which is expected [8] to result from zero-point oscillations of the strongly correlated system at large  $\alpha$  around its strictly correlated state at  $\alpha = \infty$  [see also Eq. (14) below]. Model (7) for  $W_\alpha[\rho]$  yields, in Eq. (1), after elementary integration (and subtraction of the exchange energy  $E_x \equiv W_0$ ), a new density functional for the correlation energy of real systems,

$$E_c^{\text{mod}}[\rho] = (W_0 - W_\infty) \left[ \frac{1}{X} (\sqrt{1 + 2X} - 1) - 1 \right]. \quad (8)$$

For a practical use of this functional, we need a quantitative interpretation of the unknown limit  $W_\infty[\rho]$ .

As  $\alpha$  grows, the electrons repel each other with an increasingly strong force. At the same time, however, according to the definition of  $W_\alpha[\rho]$  in Eq. (1), they must form a fixed smooth density distribution  $\rho(\mathbf{r})$ . Therefore, these electrons become strongly correlated [6]. In the very limit  $\alpha \rightarrow \infty$ , we expect the SCE state of strictly correlated electrons [8]. This means that the position of any one electron is completely determined by the positions of all the others. Therefore, if in a spherical two-electron system electron 1 is at a certain distance  $r_1$  from the center, electron 2 is on the opposite side of the center at the distance  $r_2 = f(r_1)$ . (This strictly correlated behavior is displayed in the exact ground state for two electrons bound by a very weak external

harmonic-oscillator potential [9].) The ‘‘correlation function’’  $f(r)$  can be obtained unambiguously from the given spherical density distribution  $\rho(r)$ . It is that particular solution to the nonlinear first-order differential equation

$$f'(r) = -\frac{r^2 \rho(r)}{f(r)^2 \rho(f(r))}, \quad (9)$$

which fulfills  $f(r_0) = r_0$ , where  $r_0$  is defined by  $\int_0^{r_0} dr (4\pi r^2) \rho(r) = 1$ . Equation (9) arises because the probability for electron 1 to be *inside* a sphere of radius  $r_1$  is the same as for electron 2 to be *outside* a sphere of radius  $f(r_1)$ . Since the distance  $|\mathbf{r}_1 - \mathbf{r}_2|$  between the two electrons is always  $r + f(r) > r_0$ , we can evaluate the expectation value  $\langle \hat{V}_{ee} \rangle_{\text{SCE}}$  to define the density functional

$$W_{\text{SCE}}[\rho] = 2\pi \int_0^\infty dr \frac{r^2 \rho(r)}{r + f(r)} - U[\rho] \quad (10)$$

as a candidate for an exact expression for the unknown limit  $W_\infty[\rho] = \langle \hat{V}_{ee} \rangle_\infty - U[\rho]$  in two-electron systems.  $W_{\text{SCE}}[\rho]$  has the correct scaling behavior  $W_{\text{SCE}}[\rho_\lambda] = \lambda W_{\text{SCE}}[\rho]$ , and other exact properties [8] of  $W_\infty[\rho]$ .

Solving the differential equation (9) with an accurate density profile  $\rho_{\text{He}}(r)$  for the ground state of the helium atom [10], we can, with the resulting  $f_{\text{He}}(r)$ , evaluate Eq. (10). With the exact exchange energy  $W_0$  of the helium ground state [11], an accurate value for the coefficient  $W'_0$  [2], and our result from Eq. (10) for  $W_\infty$ , Eq. (8) yields the accurate value  $E_c^{\text{mod}} = -0.0418$  for the exact correlation energy  $E_c[\rho_{\text{He}}] = -0.0421$  of the He ground state [11]. Ignoring the information provided by the quantity  $W_{\text{SCE}}[\rho_{\text{He}}]$  yields the poor result  $E_c^{\text{GL2}} = -0.0503$ , as shown in the first line in Table I.

For hypothetical two-electron atoms with the ground-state densities  $\rho_\lambda^{\text{Exp.}}(\mathbf{r}) = 2\lambda^3 e^{-2\lambda r}/\pi$  and  $\rho_\lambda^{\text{Gau.}}(\mathbf{r}) = 2\lambda^3 e^{-(\lambda r)^2}/\pi^{3/2}$ , respectively, the quantities  $W_0[\rho] = -\frac{1}{2}U[\rho]$  [ $-\frac{5}{16}\lambda$  and  $-2\lambda/(2\pi)^{1/2}$ , respectively] and  $W'_0$  [12] are known exactly. Therefore, we can predict the unknown correlation energies. Table I gives the results for  $\lambda = 1$ . (For  $\lambda \neq 1$ , note that  $W_{0,\text{SCE,PC}}[\rho_\lambda] = \lambda W_{0,\text{SCE,PC}}[\rho_1]$  and  $W'_0[\rho_\lambda] = W'_0[\rho_1]$ .) For Ne<sup>8+</sup>, which has almost an expo-

nential density, we use in Table I as an approximation the value  $W'_0$  of Exp. For the two-electron densities in Table I, the ratio  $W_{\text{SCE}}[\rho]/\int d^3r \rho^{4/3}$  is about  $-1.25$ , consistent with and close to rigorous bounds [13] on  $W_\infty[\rho]/\int d^3r \rho^{4/3}$ .

The generalization of the SCE concept to systems with more than two electrons and/or without spherical symmetry is not straightforward. Strict correlation minimizes the electron-number fluctuation in any volume of space. A simple but accurate picture is the *point-charge-plus-continuum* (PC) model [14], originally established for the low-density limit. In this model, one point electron in a continuous rigid positive background is surrounded by a sharp-edged hole in a continuous fluid of negative charge which represents all the other electrons. Inside this hole, the negative fluid is completely removed. Outside, the fluid neutralizes the positive background perfectly. We note that the PC hole is not a model for the exchange-correlation hole as it is usually defined [1,3], but a different way of dividing up the charge around an electron. The PC division of the charge into neutral cells is a textbook way to estimate the energy of the Wigner crystal.

In a uniform system, the PC hole is a concentric sphere with radius  $r_s = (3/4\pi\rho)^{1/3}$ . In a system with a slowly varying positive background, it is assumed to be still of spherical shape but, to maintain minimum electrostatic energy and zero electric dipole moment, shifted into the direction of  $-\nabla\rho$  by the small displacement  $(\gamma/5)r_s$ , where  $\gamma = |r_s \nabla\rho|/\rho \ll 1$  [15]. This leads to the gradient expansion approximation (GEA)

$$W_{\text{PC}}[\rho] = \int d^3r [A\rho(\mathbf{r})^{4/3} + B\rho(\mathbf{r})^{-4/3}|\nabla\rho(\mathbf{r})|^2], \quad (11)$$

for the strongly interacting limit  $W_\infty[\rho]$  or for the functional  $W_{\text{SCE}}[\rho]$ . Both these functionals have the scaling property [6]  $W[\rho_\lambda] = \lambda W[\rho]$ , which is satisfied by Eq. (11). The coefficients in (11) are  $A = -\frac{9}{10}(4\pi/3)^{1/3} = -1.451$  and  $B = \frac{3}{350}(3/4\pi)^{1/3} = 5.317 \times 10^{-3}$  [15]. No dependence upon spin polarization is needed in Eq. (11).

A severe test for the functional (11) is provided by one-electron densities, where  $W_\alpha[\rho] = -U[\rho]$  for all  $\alpha$ . Therefore, for the scaled density  $\rho_\lambda(\mathbf{r}) = \lambda^3 e^{-2\lambda r}/\pi$  of the hydrogen atom,  $W_\alpha[\rho_\lambda] = -0.3125\lambda$  which is very close to  $W_{\text{PC}}[\rho_\lambda] = (-0.4179 + 0.1051)\lambda = -0.3128\lambda$ . Note the importance of the gradient (second) term. For the Gaussian one-particle density  $\rho_\lambda(\mathbf{r}) = \lambda^3 e^{-(\lambda r)^2}/\pi^{3/2}$ , we find  $W_\alpha[\rho_\lambda] = -0.399\lambda$ , while  $W_{\text{PC}}[\rho_\lambda] = (-0.532 + 0.156)\lambda = -0.376\lambda$ . These results clearly support the PC GEA [Eq. (11)].

Simple (ungeneralized) gradient expansions of the exchange-correlation energy do not work nearly as well as the PC gradient expansion, probably because the gradient expansion of the exchange-correlation hole has a spurious long-range tail [16] which the PC hole does not. Even standard generalized-gradient approximations are not much better than the local-density approximation [the first term of Eq. (11)] in the strongly interacting limit [6].

In systems with two electrons, the PC GEA [Eq. (11)] can be compared with the probably exact SCE model. For He, the exponential and Gaussian two-electron densities, and  $\text{Ne}^{8+}$ , the values  $W_{\text{PC}}$  are very close to the corresponding

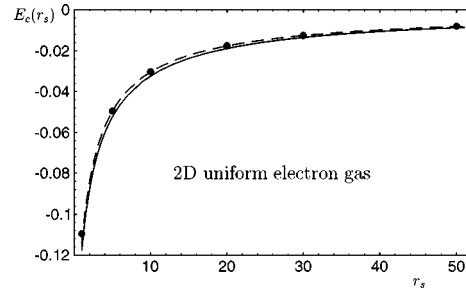


FIG. 1. Approximation (8) of the correlation energy per electron in the 2D uniform electron gas, using the PC model (solid line) or the Wigner-crystal energy (dashed line) for  $W_\infty$ . The dots represent quantum Monte Carlo results of Refs. [17] ( $r_s = 1, 5, 10, \text{ and } 20$ ) and [20]. Note that  $E_c^{\text{GL2}} = -0.19$  for all  $r_s$ . (All energies in hartree.)

values  $W_{\text{SCE}}$  in Table I. This provides further support for the PC approximation (11) which, in contrast to the SCE concept, applies straightforwardly to systems with more than two electrons. Table I also shows our results for the Be and Ne atoms, although our values for  $W'_0$  are less accurate for these atoms than for the two-electron systems.

The functional (8) does not directly apply to the three-dimensional (3D) uniform electron gas, which, in contrast to many real systems of interest, has no finite  $W'_0[\rho]$ . Therefore, we consider a 2D gas with constant density  $\rho = (\pi r_s^2)^{-1}$ , a system which is beyond the reach of standard density functionals. The exchange energy per electron is [17]  $W_0(r_s) = -4\sqrt{2}/(3\pi r_s)$ . The correlation energy is known exactly [18] in the high-density limit ( $r_s \rightarrow 0$ ),

$$E_c^{2\text{D}}(r_s) = -0.19 - 0.086 r_s \ln r_s + O(r_s). \quad (12)$$

It has the general scaling behavior [19]  $E_c^\alpha[\rho] = \alpha^2 E_c^{\alpha=1}[\rho_{1/\alpha}]$ , where, for a  $D$ -dimensional system,  $\rho_\lambda(\mathbf{r}) \equiv \lambda^D \rho(\lambda \mathbf{r})$ . Here  $E_c^\alpha = \int_0^\alpha d\beta (W_\beta - W_0)$  is the density functional for the correlation energy of electrons with coupling constant  $\alpha$ . Therefore, for small  $\alpha \ll 1$ , where  $\rho_{1/\alpha}$  is a high density, we obtain  $E_c^{2\text{D},\alpha}(r_s)$  by replacing  $r_s$  in Eq. (12) by  $\alpha r_s$  and multiplying the resulting expression by  $\alpha^2$ . Since  $W_\alpha - W_0 = dE_c^\alpha/d\alpha$ , we find  $W'_0(r_s) = -0.38$ .

To obtain  $W_\infty(r_s)$ , we apply the PC model: In two dimensions, the PC hole around the point electron becomes a flat circular disk of positive background. The electrostatic energy of such a charged disk with radius  $r_s$  and constant charge density  $(\pi r_s^2)^{-1}$  is  $8/(3\pi r_s)$ . A point electron, located in the plane of the disk at a small distance  $r \ll r_s$  from its center, has the electrostatic potential energy  $\phi(r) = -2r_s^{-1} + r^2/(2r_s^3)$ . Thus we can find the total energy per electron in the PC model (including the neutralizing positive background) to order  $r_s^{-3/2}$ , taking account of the 2D zero-point energy  $\frac{2}{5}\hbar\omega = r_s^{-3/2}$  of the electron in the oscillator-type potential  $\phi(r)$ . Subtracting the noninteracting kinetic energy  $T_s(r_s) = O(r_s^{-2})$  and the exchange energy  $W_0(r_s)$ , we obtain the PC model for the correlation energy in the low-density limit,

$$E_c^{2\text{D}}(r_s) = \left( \frac{8}{3\pi} - 2 + \frac{4\sqrt{2}}{3\pi} \right) r_s^{-1} + r_s^{-3/2} + O(r_s^{-2}). \quad (13)$$

To estimate  $E_c^{2D}(r_s)$  at intermediate densities, we could directly interpolate between Eqs. (12) and (13). In order to check our present approach, however, we will extract the quantity  $W_\infty(r_s)$  from Eq. (13).

Applying the general scaling behavior of the correlation energy to Eq. (13), in the same way as we did to Eq. (12) above, yields, for strong interaction,

$$W_\alpha(r_s) = \left( \frac{8}{3\pi} - 2 \right) r_s^{-1} + \frac{1}{2} r_s^{-3/2} \alpha^{-1/2} + O(\alpha^{-3/2}). \quad (14)$$

Therefore,  $W_\infty(r_s) = [(8/3\pi) - 2] r_s^{-1}$ . With this model and with the quantities  $W_0(r_s)$  and  $W'_0(r_s)$ , Eq. (8) yields a prediction for the correlation energy of the 2D uniform electron gas, shown in Fig. 1 as a solid curve. The close agreement with quantum Monte Carlo results [17,20] (dots in the figure) is very satisfying. Note that, at large  $\alpha \gg 1$ , the integrand (7) now becomes  $W_\alpha \rightarrow W_\infty + 0.47 r_s^{-3/2} \alpha^{-1/2}$ , with an  $\alpha^{-1/2}$  coefficient close to the one in Eq. (14).

We have used the PC model here. It is less accurate than the SCE model, which is not solved for a uniform electron gas. The SCE energy is expected to be close to the energy  $E_W^{2D}(r_s)$  of a 2D Wigner crystal [17], where the electronic positions are also strictly correlated. Using  $E_W^{2D}(r_s)$  instead of the PC model [i.e., replacing the number  $(8/3\pi) - 2 = -1.151$  by  $-1.106$ ] yields the dashed curve in Fig. 1.

We have presented an approach to the difficult problem of interacting electrons in actual physical systems by utilizing only the two relatively simple limits of weak and strong interaction. In the former limit, our approach might be extended to include third and higher-order terms in the perturbation expansion. The strict correlation that arises in the latter limit might be observed, for example in a quantum dot.

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