

Exact differential equation for the density and ionization energy of a many-particle system

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The ground-state density n of a many-electron system obeys a Schrödinger-like differential equation for $n^{1/2}(\vec{r})$, which may be solved by standard Kohn-Sham programs. The exact local effective (nonexternal) potential, $v_{\text{eff}}(\vec{r})$, is displayed explicitly in terms of wave-function expectation values, from which $v_{\text{eff}}(\vec{r}) \geq 0$ for all \vec{r} . A derivation for n as $|\vec{r}| \rightarrow \infty$ implies that this new effective potential tends asymptotically to zero, as does the exact Kohn-Sham potential, with the highest occupied eigenvalue as the exact ionization energy. A new exact expression is also presented for the exchange-correlation hole density $\rho_{xc}(\vec{r}, \vec{r}')$ about an electron at \vec{r} , as $|\vec{r}| \rightarrow \infty$.

The electron density $n(\vec{r})$ determines the properties of a ground-state many-electron system.^{1,2} We show that the correct differential equation for the density, as dictated by density-functional theory, is

$$h_{\text{eff}}(\vec{r})n^{1/2}(\vec{r}) = \mu n^{1/2}(\vec{r}) \quad (1)$$

$$h_{\text{eff}} = -\frac{1}{2}\nabla^2 + v(\vec{r}) + v_{\text{eff}}(\vec{r}) \quad (2)$$

where $v(\vec{r})$ is the external (electron-nuclear) potential and $v_{\text{eff}}(\vec{r})$ a local or multiplicative effective potential. The eigenvalue μ is the chemical potential,³ which is⁴ the negative of the ionization energy in the exact density-functional theory.¹⁻⁴ We point out that, given the functional dependence of $v_{\text{eff}}(\vec{r})$ on $n(\vec{r})$, Eqs. (1) and (2) may be iterated to self-consistency by any Kohn-Sham² computer program; no special techniques are required to solve any approximate or exact Euler equation for $n(\vec{r})$. The exact $v_{\text{eff}}(\vec{r})$ is expressed here for the first time in terms of wave-function expectation values, from which we deduce that

$$v_{\text{eff}}(\vec{r}) \geq 0 \text{ for all } \vec{r} \quad (3)$$

$$\lim_{|\vec{r}| \rightarrow \infty} v_{\text{eff}}(\vec{r}) = 0 \quad (4)$$

As a step in the derivation of Eq. (4), we present a convincing proof of the long-range exponential decay⁵⁻¹⁵ of the square root of the electron density with an inverse length equal to $\sqrt{-2\mu}$. We have recently proved^{4,15} that the highest occupied orbital energy of the traditional Kohn-Sham formalism² is

$$\epsilon_{\text{max}}^{\text{KS}} = \mu \quad (5)$$

Although the exact Kohn-Sham potential $v_{\text{eff}}^{\text{KS}}(\vec{r})$ is not the

same as our exact $v_{\text{eff}}(\vec{r})$ of Eq. (2), we prove here rigorously that both have the same $|\vec{r}| \rightarrow \infty$ limit,^{4,15} i.e.,

$$v_{\text{eff}}^{\text{KS}}(\infty) = 0 \quad (6)$$

These conclusions apply not only to electrons but also to other nonrelativistic particles, including bosons; Eq. (3) is valid if the interaction is repulsive, while Eqs. (4) and (6) hold if the interaction vanishes as the interparticle separation tends to infinity.

Let $E_v[n]$ be any exact or approximate energy functional. The density which minimizes $E_v[n]$, subject to the constraint $\int d\vec{r} n(\vec{r}) = N$, is found by¹

$$\delta(E_v[n] - \mu N) = 0 \quad (7)$$

or

$$\delta E_v / \delta n(\vec{r}) = \mu \quad (8)$$

We shall assume that the functional derivative is taken from that direction such that, in the exact theory, the chemical potential μ is the negative of the ionization energy.⁴

Express $E_v[n]$ by

$$E_v[n] = \int d\vec{r} n^{1/2}(\vec{r}) \left(-\frac{1}{2}\nabla^2 \right) n^{1/2}(\vec{r}) + G[n] + \int d\vec{r} v(\vec{r})n(\vec{r}) + \frac{1}{2} \int d\vec{r} \int d\vec{r}' n(\vec{r})n(\vec{r}')|\vec{r} - \vec{r}'|^{-1} \quad (9)$$

where $G[n]$ is the universal functional that in practice has to be approximated. Note that the first term in Eq. (9) is simply the kinetic energy of the ground state of noninteracting bosons of density $n(\vec{r})$. Hence, the Kohn-Sham formalism² is modified by utilizing the fact that any auxiliary

kinetic energy can be legitimately added to and subtracted from an interacting-fermion energy functional. In principle, we are free to choose the statistics of the auxiliary noninteracting particles, or even their masses and spins. The particular separation made in Eq. (9) is, however, a natural one, since it implies Eqs. (1)–(4) as we shall see.

Let us now apply Eq. (8) to the $E_v[n]$ given in Eq. (9). The result is the *single* Euler equation (1), with h_{eff} of the form (2) and

$$v_{\text{eff}}(\vec{r}) = \int d\vec{r}' n(\vec{r}') |\vec{r} - \vec{r}'|^{-1} + \delta G / \delta n(\vec{r}) . \quad (10)$$

$$G[n] = \frac{3}{5} C_k \int d\vec{r} n^{5/3} + \frac{3}{4} C_x \int d\vec{r} n^{4/3} + (\lambda - 1) \int n^{1/2} \left(-\frac{1}{2} \nabla^2 \right) n^{1/2} d\vec{r} \\ + C_4 \int d\vec{r} n^{1/3} \left[\left(\frac{\nabla^2 n}{n} \right)^2 - \frac{9}{8} \left(\frac{\nabla^2 n}{n} \right) \left(\frac{\nabla n}{n} \right)^2 + \frac{1}{3} \left(\frac{\nabla n}{n} \right)^4 \right] + \dots , \quad (11)$$

where C_k , C_x , C_4 , and λ are parameters. Specifically, for $\lambda = C_x = C_4 = 0$, this formalism attractively permits the solution of the Thomas-Fermi equation by the Kohn-Sham method, even though there is no ∇^2 in the Thomas-Fermi functional. Solutions of the extended Thomas-Fermi problem are interesting and useful in their own right, and can also serve to start the iteration of the more accurate Kohn-Sham approximation (in which the non-interacting-fermion kinetic energy is treated exactly).

Exact relationships between ground-state wave functions and their corresponding effective potentials in density-functional theory have been nonexistent. What is advantageous about the use of $n^{1/2}$ as a fundamental entity in density-functional theory is the fact that the exact v_{eff} of Eq. (2) can be displayed explicitly and simply in terms of components of the exact ground-state wave function as follows.

Begin with the N -electron ground-state problem

$$H(\bar{N})\psi(\bar{N}) = E_N\psi(\bar{N}) , \quad (12)$$

where \bar{M} signifies the space-spin coordinates of electrons $1 \cdots \bar{M}$. Now, partition the Hamiltonian as

$$H(\bar{N}) = H(N) + H(\overline{N-1}) + \sum_{i=1}^{N-1} r_{i\bar{N}}^{-1} , \quad (13)$$

$$v_{\text{eff}}(\vec{r}_N) = \int d\vec{r} \bar{n}(\vec{r}; \vec{r}_N) |\vec{r} - \vec{r}_N|^{-1} + \langle \phi(\overline{N-1}) | H(\overline{N-1}) - E_{N-1}^0 | \phi(\overline{N-1}) \rangle \\ + \frac{1}{2} \int \nabla_N \phi(\overline{N-1}) \cdot \nabla_N \phi(\overline{N-1}) d\vec{x}_1 \cdots d\vec{x}_{N-1} d\sigma_N , \quad (17)$$

where \vec{x} denotes a space-spin coordinate, σ a spin coordinate, and \bar{n} the electron density of that $\phi(\overline{N-1})$ associated with electron N at point \vec{r}_N .

It is important to point out and emphasize that the right-hand side of Eq. (17) is simply a *local* or multiplication operator. The nonlocal parts have vanished due to the fact that the normalization of $\phi(\overline{N-1})$, at each \vec{r}_N , dictates that

$$\nabla_N^2 \langle \phi(\overline{N-1}) | \phi(\overline{N-1}) \rangle = \nabla_N \langle \phi(\overline{N-1}) | \phi(\overline{N-1}) \rangle = 0 ,$$

even though $\nabla_N \phi(\overline{N-1}) \neq 0$ in general. (A much more complicated wave-function local potential relationship¹⁷ can be shown to exist in traditional Kohn-Sham theory.) Equation (17) is the first expression in the literature of density-

functional theory that displays the effective potential in terms of wave-function expectation values.

The wave-function connection enables us to understand and prove rigorously various aspects of $v_{\text{eff}}(\vec{r}_N)$. For instance, no term on the RHS of Eq. (17) is ever negative. Hence, $v_{\text{eff}}(\vec{r}_N) \geq 0$ for all \vec{r}_N .

The correct behavior of $v_{\text{eff}}(\vec{r})$ can be systematically studied. Given an accurate density $n(\vec{r})$, say from configuration-interaction calculations on a small atom or molecule, v_{eff} can be found simply by inverting Eqs. (1) and (2):

$$v_{\text{eff}}(\vec{r}) = \frac{1}{2} \frac{\nabla^2 n^{1/2}(\vec{r})}{n^{1/2}(\vec{r})} - v(\vec{r}) + \mu \geq 0 . \quad (18)$$

On the other hand, the exact Kohn-Sham² potential $v_{\text{eff}}^{\text{KS}}(\vec{r})$

where $H(N) = -\frac{1}{2} \nabla_N^2 + v(\vec{r}_N)$, and factor the normalized ground-state wave function as

$$\psi(\bar{N}) = N^{-1/2} n^{1/2}(\vec{r}_N) \phi(\overline{N-1}) . \quad (14)$$

Although antisymmetric in electrons $1 \cdots N-1$, $\phi(\overline{N-1})$ also depends parametrically on the position vector \vec{r}_N and spin σ_N of the N th electron. It is important to note, however, that by construction Eq. (14) dictates that $\langle \phi(\overline{N-1}) | \phi(\overline{N-1}) \rangle = 1$ for each \vec{r}_N , where the integrations and all future integrations, unless otherwise specified, are performed over the space-spin coordinates of electrons $1 \cdots N-1$ and over the spin coordinates of electron N .

Subtract $E_{N-1}^0 \psi(\bar{N})$ from both sides of Eq. (12), multiply by $[\phi(\overline{N-1})]^*$, and integrate. This gives

$$\langle \phi(\overline{N-1}) | H(\bar{N}) - E_{N-1}^0 | \psi(\bar{N}) \rangle = \mu \langle \phi(\overline{N-1}) | \psi(\bar{N}) \rangle \\ = \mu N^{-1/2} n^{1/2}(\vec{r}_N) . \quad (15)$$

Here,

$$\mu = E_N - E_{N-1}^0 , \quad (16)$$

where E_{N-1}^0 is the ground-state energy of that $(N-1)$ -electron system with the same $v(\vec{r})$ as the N -electron system. Algebraic manipulations of Eqs. (12)–(15) then yield the desired expression:

functional theory that displays the effective potential in terms of wave-function expectation values.

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The correct behavior of $v_{\text{eff}}(\vec{r})$ can be systematically studied. Given an accurate density $n(\vec{r})$, say from configuration-interaction calculations on a small atom or molecule, v_{eff} can be found simply by inverting Eqs. (1) and (2):

$$v_{\text{eff}}(\vec{r}) = \frac{1}{2} \frac{\nabla^2 n^{1/2}(\vec{r})}{n^{1/2}(\vec{r})} - v(\vec{r}) + \mu \geq 0 . \quad (18)$$

On the other hand, the exact Kohn-Sham² potential $v_{\text{eff}}^{\text{KS}}(\vec{r})$

can be found from $n(\bar{r})$ only by a more complex procedure, for more than two electrons.^{15,18}

It is well-known empirically that the ground-state density of an atom is a monotonically decreasing function of r , the distance from the nucleus. Hoffmann-Ostenhof and Hoffmann-Ostenhof¹¹ have presented a proof for a part of configuration space, using the latter part of Eq. (18), which they also derived as a "Schrödinger inequality": In the exterior region, where $v(\bar{r}) > \mu$, Eq. (18) dictates that $\nabla^2 n^{1/2}$ must be positive. Hence, in this region, $n^{1/2}$ cannot have a relative maximum or saddle point for a spherical atom, so $n(\bar{r})$ must be decreasing monotonically.

The decay of the electron density toward the vacuum has been the subject of recent theoretical interest,⁵⁻¹⁵ and may have implications for the interaction between a low-energy rare-gas atom and a crystalline surface.¹⁹ What is the exact behavior of $n(\bar{r})$ and $v_{\text{eff}}(\bar{r})$ in an atom as $r \rightarrow \infty$? Equations (1) and (2) give simply that

$$n(\bar{r}) \rightarrow e^{-2\alpha r}, \quad (19)$$

where $\alpha = \{-2[\mu - v_{\text{eff}}(\infty)]\}^{1/2}$, and Eq. (3) reveals that^{7,11}

$$\alpha \geq \sqrt{-2\mu}. \quad (20)$$

Further, Eq. (17) dictates that $v_{\text{eff}}(\infty) = 0$ and hence $\alpha = \sqrt{-2\mu}$ if and only if $\phi(\bar{N}-1)$ collapses as $|\bar{r}_N| \rightarrow \infty$ to

$$\delta_{\sigma_N, 1} C \psi_1(\bar{N}-1) + \delta_{\sigma_N, 1} (1 - |C|^2)^{1/2} \psi_1(\bar{N}-1),$$

where C is a constant ($|C| \leq 1$) and ψ_1, ψ_1 are degenerate (or identical) ground states of the $(N-1)$ -electron system. Under this condition, not only do the first two terms of Eq. (17) vanish, but so also does $\nabla_N \phi(\bar{N}-1)$, because $\phi(\bar{N}-1)$ becomes independent of \bar{r}_N .

The universal result $\alpha = \sqrt{-2\mu}$ has been asserted by several groups,^{5,9,13,15} but it has generally been assumed that an infinite series of exponentials decays asymptotically as the term which decays slowest, an assumption which has been criticized.^{10,14} By direct use of $n^{1/2}$, we shall now prove $\alpha = \sqrt{-2\mu}$, without recourse to an infinite expansion: Multiply Eq. (12) by the eigenstate $\psi_i^*(\bar{N}-1)$, employ Eqs. (13) and (14), and integrate over the first $N-1$ spatial coordinates to obtain^{5,13,15}

$$\begin{aligned} & \left[-\frac{1}{2} \nabla_N^2 + v(\bar{r}_N) + (N-1)/r_N - \epsilon_l \right] g_l(\bar{r}_N, \sigma_N) \\ &= -n^{1/2}(\bar{r}_N) (N-1) \langle \psi_i(\bar{N}-1) | (r_{iN}^{-1} - r_N^{-1}) | \phi(\bar{N}-1) \rangle, \end{aligned} \quad (21)$$

where $\epsilon_l = E_N - E_{N-1}^l$ and

$$g_l(\bar{r}_N, \sigma_N) = n^{1/2}(\bar{r}_N) \langle \psi_i(\bar{N}-1) | \phi(\bar{N}-1) \rangle. \quad (22)$$

The general solution of Eq. (21) is $g_l = g_l(h) + g_l(p)$, where $g_l(h)$ is the homogeneous solution and $g_l(p)$ is the particular solution. Thus, for $l=0$, Eq. (22) becomes

$$g_0(h) + g_0(p) = n^{1/2}(\bar{r}_N) \langle \psi_0(\bar{N}-1) | \phi(\bar{N}-1) \rangle. \quad (23)$$

Asymptotically, $g_0(h) \sim e^{-(-2\mu)^{1/2} r_N}$ and $n^{1/2} \sim e^{-\alpha r_N}$. Now, since $|\langle \psi_0(\bar{N}-1) | \phi(\bar{N}-1) \rangle| \leq 1$ by the Schwartz inequality, $|\langle \psi_0(\bar{N}-1) | \phi(\bar{N}-1) \rangle|$ cannot increase exponentially. Consequently, Eq. (23) dictates that

$$\alpha \leq \sqrt{-2\mu} \quad (24)$$

[unless $\psi_0(\bar{N}-1)$ is "inaccessible," i.e., unless $\langle \psi_0(\bar{N}-1) | \phi(\bar{N}-1) \rangle = 0$ at all \bar{r}_N for symmetry reasons¹³]. On the other hand, Eq. (20) gives the inequality in the opposite direction: $\alpha \geq \sqrt{-2\mu}$. Hence, only the equality can hold:

$$\alpha = \sqrt{-2\mu}. \quad (25)$$

The conclusion is that, if $\psi_0(\bar{N}-1)$ is "accessible," then $\alpha = \sqrt{-2\mu}$, $v_{\text{eff}}(\infty) = 0$, and $\phi(\bar{N}-1)$ collapses asymptotically to $\psi_0(\bar{N}-1)$. Compatible results within optimized finite basis sets have been obtained by Silverstone.¹⁴

By the collapse of $\phi(\bar{N}-1)$ to $\psi_0(\bar{N}-1)$ as $|\bar{r}_N| \rightarrow \infty$, Eq. (17) implies that

$$v_{\text{eff}}(\bar{r}) \rightarrow (N-1)/r, \quad (26)$$

and thus by Eq. (1)

$$n^{1/2}(\bar{r}) \rightarrow r^\beta e^{-\alpha r}, \quad (27)$$

as $r \rightarrow \infty$, where¹² $\beta = (Z - N + 1)/\alpha - 1$, and Z is the nuclear charge [$v(r) = -Z/r$]. While our discussion here is specifically for the electron density in an atom, it is clear that the inverse decay length of Eq. (25) is truly universal.

We now connect our results to the traditional exact Kohn-Sham theory,² in which $n(\bar{r})$ is constructed as a sum of squares of N orbitals. Each orbital is an eigenvector of a Hamiltonian like Eq. (2), but with the effective potential

$$v_{\text{eff}}^{\text{KS}}(\bar{r}) = \int d\bar{r}' n(\bar{r}') |\bar{r} - \bar{r}'|^{-1} + \delta E_{\text{xc}}/\delta n(\bar{r}). \quad (28)$$

E_{xc} is the exchange-correlation energy, and we assume as always in this paper that the functional derivative is taken from the electron-deficient side⁴ of integer electron number N . Except in two-electron systems, $v_{\text{eff}}^{\text{KS}}(\bar{r})$ is different from our $v_{\text{eff}}(\bar{r})$. However, for $|\bar{r}| \rightarrow \infty$, $n(\bar{r})$ is dominated by those occupied orbitals which have the highest^{15,18,20} eigenvalue $\epsilon_{\text{max}}^{\text{KS}}$ which is⁴ precisely the chemical potential μ of Eq. (16) or minus the ionization energy. It follows at once that $v_{\text{eff}}^{\text{KS}}(\infty) = v_{\text{eff}}(\infty)$, and then Eq. (6) follows from Eq. (4).

The results of this paper are readily extended to spin-density functional theory.¹⁷ In partial summary, unless prevented by reasons of symmetry (spin), the inverse decay length α equals $\sqrt{-2\mu}$ by Eq. (25), the eigenvalue $\epsilon_{\text{max}}^{\text{KS}}$ of the highest occupied Kohn-Sham orbital equals μ of Eq. (16) or minus the ionization energy, and the long-range limit $v_{\text{eff}}^{\text{KS}}(\infty)$ of the Kohn-Sham potential equals zero.

We close by observing that the wave-function collapse (when an electron is far out) implies that

$$\begin{aligned} & \lim_{|\bar{r}'| \rightarrow \infty} \rho_{\text{xc}}(N; \bar{r}, \bar{r}') \\ &= \int_0^1 d\lambda [n_\lambda(N; \bar{r}') |_{N-1} - n_\lambda(N; \bar{r}') |_N], \end{aligned} \quad (29)$$

where $\rho_{\text{xc}}(N; \bar{r}, \bar{r}')$ is the density at \bar{r}' of the exchange-correlation hole²¹ about an electron at \bar{r} in an N -electron system. Here, $n_\lambda(N; \bar{r})|_M$ is the ground-state density for M electrons with electron-electron interaction $\lambda e^2/r$ in the presence of the external potential $v_\lambda(N; \bar{r})$, constructed so that $n_\lambda(N; \bar{r})|_N$ is independent of λ and equal to the ground-state density of the fully interacting ($\lambda=1$) N -electron system or its Kohn-Sham noninteracting ($\lambda=0$) counterpart.

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