The relationship between the density functional Hartree-plus-exchange-correlation potential for an integer $N$-electron and $(N - 1)$ electron system.

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It is shown that the Hartree-plus-exchange-correlation density functional potential for an integer $N$-electron system differs by a constant form the corresponding potential for an $(N - 1)$-electron system if the densities are determined from the same external potential.

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I. INTRODUCTION

In the early 1980’s it was discovered that the density functional exchange correlation potential has a derivative discontinuity when the particle number crosses and integer $1, 2$. In this paper a relationship between the potentials of systems with different particle numbers is proven. It will be shown that the Hartree-plus-exchange-correlation potential for an integer $N$-electron ($N > 2$) system differs by a constant from the corresponding potential of an $(N - 1)$-electron system if the densities are determined from the same external potential. As a corollary it follows that the functional derivative of the independent particle kinetic energy functional of the $N$ and $(N - 1)$-electron systems also differ by a constant.

II. PROOF

In the adiabatic connection approach\textsuperscript{3–6} of the constrained minimization formulation of density functional theory\textsuperscript{7–10} the Hamiltonian $\hat{H}^\gamma$ for a system of $N$ electrons is given by

$$\hat{H}^\gamma_N = \hat{T}^N + \gamma \hat{V}_{ee}^N + \hat{v}_{N,\text{ext}}^\gamma [\rho_N].$$

(1)

Atomic units, $\hbar = e = m = 1$ are used throughout. $\hat{T}$ is the kinetic energy operator,

$$\hat{T}^N = -\frac{1}{2} \sum_{i=1}^{N} \nabla_i^2,$$

(2)

and $\gamma \hat{V}_{ee}$ is a scaled electron-electron interaction,

$$\gamma \hat{V}_{ee}^N = \gamma \sum_{i<j}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}.$$  

(3)

The the external potential

$$\hat{v}_{N,\text{ext}}^\gamma [\rho_N] = \sum_{i=1}^{N} v_{\text{ext}}^\gamma ([\rho_N] ; \mathbf{r}_i),$$

(4)

is constructed to keep the charge density fixed at $\rho_N (\mathbf{r})$, the ground state charge density of the fully interacting system ($\gamma = 1$), for all values of the coupling constant $\gamma$. It has the form\textsuperscript{10,11}

$$v_{\text{ext}}^\gamma ([\rho_N] ; \mathbf{r}) = (1 - \gamma) v_{\text{ux}} ([\rho_N] ; \mathbf{r})$$

$$+ \frac{1}{2} [v_{\text{ext}}^\gamma ([\rho_N] ; \mathbf{r}) + v_{\text{ext}}^\gamma ([\rho_N] ; \mathbf{r})],$$

(5)
where \( v_{\text{ext}}^1(\rho_N; \mathbf{r}) = v_{\text{ext}}(\mathbf{r}) \) is the external potential at full coupling strength, \( \gamma = 1 \), and \( v_{\text{ext}}^0(\rho_N; \mathbf{r}) \) is non-interacting Kohn-Sham potential. The exchange plus Hartree potential \( v_{\text{ex}}(\rho_N; \mathbf{r}) \), is independent of \( \gamma \), while the correlation potential \( v_{\text{c}}(\rho_N; \mathbf{r}) \) depends in the scaling parameter \( \gamma \).

The chemical potential

\[
\mu = E_N^\gamma - E_{N-1}^\gamma
\]

depends on the asymptotic decay of the charge density\(^{12-14}\), and hence is independent of the coupling constant \( \gamma \). In Eq. (6) \( E_{N-1}^\gamma \) is the groundstate energy of the \((N - 1)\)-electron system with the same single-particle external potential \( v_{\text{ext}}^\gamma(\rho_N; \mathbf{r}) \) as the \(N\)-electron system:

\[
\hat{H}_{N-1}^\gamma \left| \Psi_{\rho_{N-1}}^\gamma \right\rangle = E_{N-1}^\gamma \left| \Psi_{\rho_{N-1}}^\gamma \right\rangle \\
\hat{H}_{N-1}^\gamma = \hat{T}^{N-1} + \gamma \hat{V}_{ee}^{N-1} + \hat{v}_{N-1,\text{ext}}^\gamma(\rho_N) \\
\hat{v}_{N-1,\text{ext}}^\gamma(\rho_N) = \sum_{i=1}^{N-1} v_{\text{ext}}^\gamma(\rho_N; \mathbf{r}_i)
\]

Note that by construction of \( v_{\text{ext}}^\gamma(\rho_N; \mathbf{r}) \), Eq. (5) \( \rho_N \) is independent of \( \gamma \), but the groundstate density of the \((N - 1)\)-electron system \( \rho_{N-1}^\gamma \), is a function of \( \gamma \).

The correlation energy \( E_{\text{c}}^\gamma \left[ \rho_{N-1}^\gamma \right] \) is defined as\(^{10}\)

\[
E_{\text{c}}^\gamma \left[ \rho_{N-1}^\gamma \right] = \left\langle \Psi_{\rho_{N-1}}^\gamma \left| \hat{T}^{N-1} + \gamma \hat{V}_{ee}^{N-1} \right| \Psi_{\rho_{N-1}}^\gamma \right\rangle - \left\langle \Psi_{\rho_{N-1}}^0 \left| \hat{T}^{N-1} + \gamma \hat{V}_{ee}^{N-1} \right| \Psi_{\rho_{N-1}}^0 \right\rangle,
\]

where \( \left| \Psi_{\rho_{N-1}}^0 \right\rangle \) is the Kohn-Sham \((N - 1)\) independent particle groundstate wavefunction that yields the same density as the interacting \((N - 1)\)-electron system at coupling strength \( \gamma \). Since the correlation part of the kinetic energy is given by

\[
T_{\text{c}}^\gamma \left[ \rho_{N-1}^\gamma \right] \\
= \left\langle \Psi_{\rho_{N-1}}^\gamma \left| \hat{T}^{N-1} \right| \Psi_{\rho_{N-1}}^\gamma \right\rangle - \left\langle \Psi_{\rho_{N-1}}^0 \left| \hat{T}^{N-1} \right| \Psi_{\rho_{N-1}}^0 \right\rangle,
\]

and hence

\[
E_{\text{c}}^\gamma \left[ \rho_{N-1}^\gamma \right] - T_{\text{c}}^\gamma \left[ \rho_{N-1}^\gamma \right] \\
= \left\langle \Psi_{\rho_{N-1}}^\gamma \left| \hat{V}_{ee}^{N-1} \right| \Psi_{\rho_{N-1}}^\gamma \right\rangle - \left\langle \Psi_{\rho_{N-1}}^0 \left| \hat{V}_{ee}^{N-1} \right| \Psi_{\rho_{N-1}}^0 \right\rangle,
\]
the derivative of $E^\gamma_c[\rho^\gamma_{N-1}]$ with respect to $\gamma$ can be expressed as

$$\frac{\partial}{\partial \gamma} E^\gamma_c[\rho^\gamma_{N-1}] = E^\gamma_c[\rho^\gamma_{N-1}] - T^\gamma_c[\rho^\gamma_{N-1}]$$

$$= \frac{1}{\gamma} \left[ \left\langle \frac{\partial}{\partial \gamma} \left| \Psi_{\rho^\gamma_{N-1}}^\gamma \right| \hat{T}^{N-1} + \gamma \hat{V}_e^{N-1} \right| \Psi_{\rho^\gamma_{N-1}}^\gamma \rightangle + \left\langle \Psi_{\rho^\gamma_{N-1}}^\gamma \left| \hat{T}^{N-1} + \gamma \hat{V}_e^{N-1} \right| \frac{\partial}{\partial \gamma} \Psi_{\rho^\gamma_{N-1}}^\gamma \right\rangle + c.c\right] +$$

$$- \left\langle \frac{\partial}{\partial \gamma} \Psi_{\rho^0_{N-1}} \left| \hat{U}_{N-1,ext} \right| \Psi_{\rho^0_{N-1}}^0 \right\rangle - \left\langle \Psi_{\rho^0_{N-1}} \left| \hat{U}_{N-1,ext} \right| \frac{\partial}{\partial \gamma} \Psi_{\rho^0_{N-1}}^0 \right\rangle + c.c\right)$$

and utilizing the normalization of the wavefunctions which implies that

$$\frac{\partial}{\partial \gamma} \left\langle \Psi_{\rho^\gamma_{N-1}}^\gamma \left| \Psi_{\rho^\gamma_{N-1}}^\gamma \right\rangle = 0, \right\rangle \left(13\right)$$

Eq. (11) becomes

$$\frac{\partial}{\partial \gamma} E^\gamma_c[\rho^\gamma_{N-1}] = E^\gamma_c[\rho^\gamma_{N-1}] - T^\gamma_c[\rho^\gamma_{N-1}]$$

$$= \frac{1}{\gamma} \left[ \left\langle \frac{\partial}{\partial \gamma} \left| \Psi_{\rho^\gamma_{N-1}}^\gamma \right| \hat{T}^{N-1} + \gamma \hat{V}_e^{N-1} \right| \Psi_{\rho^\gamma_{N-1}}^\gamma \rightangle + \left\langle \Psi_{\rho^\gamma_{N-1}}^\gamma \left| \hat{T}^{N-1} + \gamma \hat{V}_e^{N-1} \right| \frac{\partial}{\partial \gamma} \Psi_{\rho^\gamma_{N-1}}^\gamma \right\rangle + c.c\right] +$$

$$- \left\langle \frac{\partial}{\partial \gamma} \Psi_{\rho^0_{N-1}} \left| \hat{U}_{N-1,ext} \right| \Psi_{\rho^0_{N-1}}^0 \right\rangle - \left\langle \Psi_{\rho^0_{N-1}} \left| \hat{U}_{N-1,ext} \right| \frac{\partial}{\partial \gamma} \Psi_{\rho^0_{N-1}}^0 \right\rangle + c.c\right)$$

$$- \gamma \left\langle \frac{\partial}{\partial \gamma} \Psi_{\rho^0_{N-1}} \left| \hat{V}_e^{N-1} \right| \Psi_{\rho^0_{N-1}}^0 \right\rangle.$$

Now\textsuperscript{12,13}

$$\left\langle \Psi_{\rho^0_{N-1}}^0 \left| \hat{V}_e^{N-1} \right| \Psi_{\rho^0_{N-1}}^0 \right\rangle = E_x[\rho^\gamma_{N-1}] + U[\rho^\gamma_{N-1}]$$

$$= E_{ux}[\rho^\gamma_{N-1}] . \right\rangle \left(15\right)$$
is the sum of the exchange $E_x[\rho_{N-1}^\gamma]$ and mutual Coulomb interaction energy $U[\rho_{N-1}^\gamma]$ of the $(N - 1)$-electron system. The charge density $\rho_{N-1}^\gamma$ is a function of $\gamma$, therefore\cite{12}

\[
\frac{\partial}{\partial \gamma} \langle \Psi_{\rho_{N-1}}^0 | \hat{V}_{ee}^{N-1} | \Psi_{\rho_{N-1}}^0 \rangle = \int d^3r \frac{\partial \rho_{N-1}^\gamma(r)}{\partial \gamma} v_{ux} ([\rho_{N-1}^\gamma] ; r),
\]

(16)

where

\[
v_{ux} ([\rho_{N-1}^\gamma] ; r) = \frac{\delta}{\delta \rho_{N-1}^\gamma(r)} (E_x[\rho_{N-1}^\gamma] + U[\rho_{N-1}^\gamma])
\]

(17)

is the sum of the exchange and Hartree potentials for the $(N - 1)$-electron system. Using Eq. (16), Eq. (5) and the fact that $\langle \Psi_{\rho_{N-1}}^\gamma |$ and $\langle \Psi_{\rho_{N-1}}^0 |$ yield the same density $\rho_{N-1}^\gamma$, Eq. (14) can be cast as

\[
\frac{\partial}{\partial \gamma} E_c^\gamma [\rho_{N-1}^\gamma] = E_c^\gamma [\rho_{N-1}^\gamma] - T_c^\gamma [\rho_{N-1}^\gamma]
\]

\[
+ \int d^3r \frac{\partial \rho_{N-1}^\gamma(r)}{\partial \gamma} (v_{ux} ([\rho_N] ; r) + \gamma v_{ux} ([\rho_N] ; r) - \gamma v_{ux} ([\rho_{N-1}^\gamma] ; r))
\]

(18)

From the definition of $E_c^\gamma [\rho_{N-1}^\gamma]$, Eq. (8), the correlation energy can also be written as

\[
E_c^\gamma [\rho_{N-1}^\gamma] = \hat{T}^\gamma [\rho_{N-1}^\gamma] - \hat{T}^0 [\rho_{N-1}^\gamma] + \gamma \hat{V}_{ee} [\rho_{N-1}^\gamma] - \gamma E_{ux} [\rho_{N-1}^\gamma]
\]

(19)

where

\[
\hat{T}^\gamma [\rho_{N-1}^\gamma] = \langle \Psi_{\rho_{N-1}}^\gamma | \hat{T}^{N-1} | \Psi_{\rho_{N-1}}^\gamma \rangle
\]

\[
\hat{T}^0 [\rho_{N-1}^\gamma] = \langle \Psi_{\rho_{N-1}}^0 | \hat{T}^{N-1} | \Psi_{\rho_{N-1}}^0 \rangle
\]

(20)

\[
\hat{V}_{ee} [\rho_{N-1}^\gamma] = \langle \Psi_{\rho_{N-1}}^\gamma | \hat{V}_{ee}^{N-1} | \Psi_{\rho_{N-1}}^\gamma \rangle
\]

(21)

It now follows that

\[
\frac{\partial}{\partial \gamma} E_c^\gamma [\rho_{N-1}^\gamma] = E_c^\gamma [\rho_{N-1}^\gamma] - T_c^\gamma [\rho_{N-1}^\gamma]
\]

\[
+ \int d^3r \frac{\partial \rho_{N-1}^\gamma(r)}{\partial \gamma} \left( \frac{\delta T_{N-1}^\gamma [\rho_{N-1}^\gamma]}{\delta \rho_{N-1}^\gamma(r)} - \frac{\delta T_{N-1}^0 [\rho_{N-1}^\gamma]}{\delta \rho_{N-1}^\gamma(r)} - \gamma \frac{\delta E_{ux} [\rho_{N-1}^\gamma]}{\delta \rho_{N-1}^\gamma(r)} \right)
\]

\[
+ \gamma \frac{\partial}{\partial \gamma} V_{ee} [\rho_{N-1}^\gamma]
\]

(22)
where use was made of the relation

$$\frac{E_{ee}^\gamma [\rho_{N-1}^\gamma]}{\gamma} - T_{ee}^\gamma [\rho_{N-1}^\gamma] \gamma = \hat{V}_{ee} [\rho_{N-1}^\gamma] - E_{ux} [\rho_{N-1}^\gamma].$$  \hfill (23)

The last term in Eq. (22) can be transformed as follows:

$$\frac{\partial}{\partial \gamma} V_{ee} [\rho_{N-1}^\gamma]$$

$$= \left\langle \frac{\partial}{\partial \gamma} \Psi_{\rho_{N-1}^\gamma} | V_{ee}^{N-1} | \Psi_{\rho_{N-1}^\gamma} \right\rangle + \left\langle \Psi_{\rho_{N-1}^\gamma} | \hat{V}_{ee}^{N-1} + \hat{v}_{N-1,ext} [\rho_N] \right\rangle \frac{\partial}{\partial \gamma} \Psi_{\rho_{N-1}^\gamma}$$

$$= \frac{1}{\gamma} \left\langle \frac{\partial}{\partial \gamma} \Psi_{\rho_{N-1}^\gamma} | \hat{T}^{N-1} + \gamma \hat{V}_{ee}^{N-1} + \hat{v}_{N-1,ext} [\rho_N] \right\rangle \frac{\partial}{\partial \gamma} \Psi_{\rho_{N-1}^\gamma}$$

$$- \frac{1}{\gamma} \left\langle \frac{\partial}{\partial \gamma} \Psi_{\rho_{N-1}^\gamma} | \hat{T}^{N-1} + \hat{v}_{N-1,ext} [\rho_N] \right\rangle \frac{\partial}{\partial \gamma} \Psi_{\rho_{N-1}^\gamma}$$

$$+ \left\langle \Psi_{\rho_{N-1}^\gamma} | \hat{T}^{N-1} + \hat{v}_{N-1,ext} [\rho_N] \right\rangle \frac{\partial}{\partial \gamma} \Psi_{\rho_{N-1}^\gamma}$$

$$= - \frac{1}{\gamma} \int d^3 \rho_{N-1} \gamma \frac{\partial}{\partial \gamma} \rho_{N-1} (r) \left( \frac{\delta T_{N-1}^{\gamma} [\rho_{N-1}^\gamma]}{\delta \rho_{N-1}^\gamma (r)} + v_{ex} (\rho_{N-1}^\gamma ; r) \right).$$  \hfill (24)

Here use was made Eqs. (7) and (13). Combining Eqs. (22) and (24) leads to

$$\frac{\partial}{\partial \gamma} E_{ee}^\gamma [\rho_{N-1}^\gamma]$$

$$= E_{ee}^\gamma [\rho_{N-1}^\gamma] - T_{ee}^\gamma [\rho_{N-1}^\gamma]$$

$$\gamma + \int d^3 \rho_{N-1} \gamma \frac{\partial}{\partial \gamma} \rho_{N-1} (r) \left( -v_{ex}^\gamma (\rho_{N}; r) - \frac{\delta T_{N-1}^{\gamma}}{\delta \rho_{N-1}^\gamma (r)} - \gamma v_{ux} (\rho_{N-1}^\gamma ; r) \right).$$  \hfill (25)

At the solution point\textsuperscript{12,13} the following equation has to be satisfied for the \((N-1)\)-electron system:

$$\frac{\delta T_{N-1}^{\gamma}}{\delta \rho_{N-1}^\gamma (r)} + \gamma v_{ux} (\rho_{N-1}^\gamma ; r) + v_{ee}^\gamma (\rho_{N-1}^\gamma ; r) + v_{ex}^\gamma (\rho_{N}; r) = \mu_{N-1}^\gamma,$$  \hfill (26)

where \(\mu_{N-1}^\gamma\) is a constant, the chemical potential of the \((N-1)\)-electrons moving in the external potential \(v_{ex}^\gamma (\rho_{N}; r)\). Taking into account that the number of electrons is fixed at \((N-1)\) independent of \(\gamma\), it follows that

$$\int d^3 \rho_{N-1} \gamma \frac{\partial}{\partial \gamma} \rho_{N-1} (r) = \frac{\partial}{\partial \gamma} (N-1)$$

$$= 0,$$  \hfill (27)
where it is assumed that the order of the integration and derivative can be reversed. From Eqs. (25), (26) and (27)

$$\frac{\partial}{\partial \gamma} E_c \left[ \rho_{N-1}^\gamma \right]$$

$$= E_c^\gamma \left[ \rho_{N-1}^\gamma \right] - T_c^\gamma \left[ \rho_{N-1}^\gamma \right] + \int d^3 r \frac{\partial \rho_{N-1}^\gamma (r)}{\partial \gamma} v_c^\gamma \left( \left[ \rho_{N-1}^\gamma \right] ; r \right). \quad (28)$$

Comparing Eqs. (18) and (28) shows that

$$0 = \int d^3 r \frac{\partial \rho_{N-1}^\gamma (r)}{\partial \gamma} \left( v_{uxc}^\gamma ([\rho_N] ; r) - v_{uxc}^\gamma \left( \left[ \rho_{N-1}^\gamma \right] ; r \right) \right) \quad (29)$$

where

$$v_{uxc}^\gamma ([\rho] ; r) = v_c^\gamma ([\rho] ; r) + \gamma v_{ux} ([\rho] ; r) \quad (30)$$

is the Hartree plus exchange-correlation potential for a system with density $\rho$ and coupling strength $\gamma$.

The charge density $\rho_{N-1}^\gamma (r)$ is a function of the potential $v_{ext}^\gamma ([\rho_N] ; r)$ as can be seen from Eq. (7). Therefore

$$\frac{\partial \rho_{N-1}^\gamma (r)}{\partial \gamma} = \int d^3 r' \left. \frac{\delta \rho_{N-1}^\gamma (r)}{\delta v_{ext}^\gamma ([\rho_N] ; r')} \right|_{N-1} \frac{\partial v_{ext}^\gamma ([\rho_N] ; r)}{\partial \gamma} \quad (31)$$

Now

$$\left. \frac{\delta \rho_{N-1}^\gamma (r)}{\delta v_{ext}^\gamma ([\rho_N] ; r')} \right|_{N-1} = \chi_{N-1}^\gamma (r, r') \quad (32)$$

is the density response function of the $(N-1)$-particle system. From stability considerations $\chi_{N-1}^\gamma (r, r')$ is negative semi-definite and has one zero eigenvalue which corresponds to the invariance of the density when the potential is changed by a constant. This implies that

$$0 = \int d^3 r \frac{\partial \rho_{N-1}^\gamma (r)}{\partial \gamma} f (r)$$

$$= - \int d^3 r \int d^3 r' f (r) \chi_{N-1}^\gamma (r, r') \left( v_{ux} ([\rho_N] ; r') + \frac{\partial}{\partial \gamma} v_c^\gamma ([\rho_N] ; r') \right) \quad (33)$$

is only possible if $f (r) = \text{constant}$ since $v_{ux} ([\rho_N] ; r') + \frac{\partial}{\partial \gamma} v_c^\gamma ([\rho_N] ; r') \neq \text{constant}$. This proves the main point of this paper:

$$v_{uxc}^\gamma ([\rho_N] ; r) = v_{uxc}^\gamma \left( \left[ \rho_{N-1}^\gamma \right] ; r \right) + \text{constant} \quad (34)$$

when $\rho_N$ and $\rho_{N-1}$ are determined by the same external potential $v_{ext}^\gamma ([\rho_N] ; r)$. 

III. PROOF OF COROLLARY

Let the energy functional $F_N^\gamma[\rho_N]^{12,13}$ be defined as

$$F_N^\gamma[\rho_N] = T_N^0[\rho_N] + \gamma U[\rho_N] + \gamma E_x[\rho_N] + E_N^\gamma[\rho_N].$$  \hspace{1cm} (35)

Then$^{12,13}$

$$\frac{\delta F_N^\gamma[\rho_N]}{\delta \rho_N(r)} + v_{\text{ext}}^\gamma([\rho_N]; r) = \mu$$  \hspace{1cm} (36)

and

$$\frac{\delta F_N^\gamma[\rho_{N-1}]}{\delta \rho_{N-1}^\gamma(r)} + v_{\text{ext}}^\gamma([\rho_N]; r) = \mu_{N-1}^\gamma.$$  \hspace{1cm} (37)

From the last two equations we find that

$$\frac{\delta F_N^\gamma[\rho_N]}{\delta \rho_N(r)} - \frac{\delta F_N^\gamma[\rho_{N-1}]}{\delta \rho_{N-1}^\gamma(r)} = \mu - \mu_{N-1}^\gamma$$  \hspace{1cm} (38)

and therefore, using Eqs. (34) and (35), it follows that

$$\frac{\delta T_N^0[\rho_N]}{\delta \rho_N(r)} - \frac{\delta T_N^0[\rho_{N-1}]}{\delta \rho_{N-1}^\gamma(r)} = \text{constant}$$  \hspace{1cm} (39)

IV. DISCUSSION AND SUMMARY

The relationship in Eq. (34) is valid for $N > 2$. This follows from the step in Eq. (28) where the correlation energy of the $N - 1$ electron system is taken as non-zero. In the proof use is made of the $N$ and $(N - 1)$ electron wave functions, hence the proof given here is valid for integer $N$. The proof for non-integer values of the electrons and will be presented in another paper.

In summary, it was shown that the Hartree-plus-exchange-correlation potential for an integer $N$-electron ($N > 2$) system differs by a constant form the corresponding potential for an $(N - 1)$-electron system if the densities are determined with the same external potential. As a corollary it was shown that the functional derivative of the independent particle kinetic energy functional of the $N$ and $(N - 1)$-electron systems also differ by a constant.
REFERENCES

1. J. Perdew, R. Parr, M. Levy, and J. Balduz, Phys. Rev. Lett. 49, 1691 (1982).
2. L. J. Sham and M. Schlüter, Phys. Rev. Lett. 51, 1888 (1983).
3. J. Harris and R. O. Jones, J. Phys. F 4, 1174 (1974).
4. D. C. Langreth and J. P. Perdew, Solid State Comm. 17, 1425 (1975).
5. D. C. Langreth and J. P. Perdew, Phys. Rev. B 15, 2884 (1977).
6. O. Gunnarson and B. I. Lundqvist, Phys. Rev. B 13, 4274 (1976).
7. P. Hohenberg and W. Kohn, Phys. Rev. B 136, 864 (1964).
8. W. Kohn and L. J. Sham, Phys. Rev. A 140, 1133 (1965).
9. M. Levy, Natl. Acad. Sci. USA 76, 6062 (1979).
10. M. Levy and J. P. Perdew, Phys. Rev. A 32, 2010 (1985).
11. A. Görling and M. Levy, Phys. Rev. B 47, 13105 (1993).
12. R. G. Parr and W. Yang, Density Functional Theory of Atoms and Molecules (Oxford University Press, New York, 1989).
13. R. M. Dreizler and E. K. U. Gross, Density Functional Theory (Springer-Verlag, Berlin, 1990).
14. R. Jones and O. Gunnarsson, Rev. Mod. Phys. 61, 689 (1989).
15. M. Levy and A. Görling, Phys. Rev. A 53, 3140 (1996).
16. M. Levy and A. Görling, Phys. Rev. B 53, 969 (1996).