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Scaling and virial theorems in current-density-functional theory

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Starting from a constrained-search formulation of current-density-functional theory, we obtain rigorous scaling and virial relations for the kinetic, exchange, and correlation energy functionals of electronic systems in strong magnetic fields.

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The current-density-functional theory (CDFT) of Vignale and Rasolt [1–5] has proven to be a powerful tool for describing inhomogeneous electronic systems in magnetic fields of arbitrary strength. Atoms, molecules [6,7] and mesoscopic systems [5,8], electron-hole droplets [5,9,10], as well as the Wigner crystallization [5,11] in strong magnetic fields have been successfully treated and, most recently, a two-dimensional electron gas in the quantum Hall regime [12,13] has been studied.

In CDFT, the quantum many-body problem in the presence of magnetic fields is formulated in terms of two basic variables: the particle density $n(\mathbf{r})$ and the *paramagnetic* current density $\mathbf{j}(\mathbf{r})$. The heart of the theory is the exchange-correlation energy $E_{\rm xc}$, which is a functional of the two basic variables n and $\mathbf{j}$. The *exact* functional $E_{\rm xc}[n,\mathbf{j}]$ can be defined in terms of the (unknown) *exact* many-body wave function. In actual calculations, however, one has to resort to approximate forms [14] of this functional.

In ordinary density-functional theory, the knowledge of rigorous properties of the exact exchange-correlation functional [15–30] has provided valuable guidelines in the construction of such approximate functionals. In CDFT, very little is known about the exact functionals. The purpose of the present article is to deduce rigorous virial and scaling relations for the functionals appearing in CDFT.

We start from the Hamiltonian for a system of N interacting electrons subject to external scalar and vector potentials $v(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$:

$$\hat{H}=\hat{T}+\hat{W}+\hat{V} \tag{1}$$

with

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

$$\hat{W}=\frac{1}{2}\sum_{i=1}^{N}\sum_{j(\neq i)=1}^{N}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|}, \tag{3}$$

$$\hat{V}=\int d^3r\ \hat{n}(\mathbf{r})\left(v(\mathbf{r})+\frac{e^2}{2mc^2}\mathbf{A}^2(\mathbf{r})\right)+\frac{e}{c}\int d^3r\ \hat{\mathbf{j}}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r}), \tag{4}$$

where $\hat{n}(\mathbf{r})$ denotes the density operator and $\hat{\mathbf{j}}(\mathbf{r})$ the *paramagnetic* current density operator. By virtue of the Rayleigh-Ritz principle the ground-state energy E_0 of the system can be expressed as

$$E_0=\inf_{\chi}\langle\chi|\hat{H}|\chi\rangle=\inf_{\chi}\langle\chi|\hat{T}+\hat{W}+\hat{V}|\chi\rangle, \tag{5}$$

where the infimum is performed over all normalized antisymmetric N-particle wave functions χ.

The starting point of our derivation is a constrained-search formulation of CDFT. Following the constrained-search procedure [15] of ordinary density-functional theory, we split the infimum in Eq. (5) into two consecutive infima:

$$\begin{aligned}E_0&=\inf_{\chi}\langle\chi|\hat{T}+\hat{W}+\hat{V}|\chi\rangle=\inf_{(n,\mathbf{j})}\left[\inf_{\chi\to(n,\mathbf{j})}\langle\chi|\hat{T}+\hat{W}+\hat{V}|\chi\rangle\right]\\&=\inf_{(n,\mathbf{j})}\left[F[n,\mathbf{j}]+\int d^3r\ n(\mathbf{r})\left(v(\mathbf{r})+\frac{e^2}{2mc^2}\mathbf{A}^2(\mathbf{r})\right)\right.\\&\qquad\left.+\frac{e}{c}\int d^3r\ \mathbf{j}(\mathbf{r})\cdot\mathbf{A}(\mathbf{r})\right],\end{aligned} \tag{6}$$

with

$$F[n,\mathbf{j}]=\inf_{\chi\to(n,\mathbf{j})}\langle\chi|\hat{T}+\hat{W}|\chi\rangle=\langle\Psi|\hat{T}+\hat{W}|\Psi\rangle. \tag{7}$$

In Eq. (7) the infimum is taken over all normalized antisymmetric N-particle wave functions χ that yield the given densities $(n,\mathbf{j})$. In the following we shall assume that, for given $(n,\mathbf{j})$, a minimizing wave function Ψ exists (which need not be unique). The functional $F[n,\mathbf{j}]$ is *universal* in the sense that it does not depend on the external potentials v and $\mathbf{A}$ of the particular system considered.

If the wave function $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ yields the densities n and $\mathbf{j}$ and minimizes $\langle\hat{T}+\hat{W}\rangle$, then the scaled function $\Psi_\lambda(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\lambda^{3N/2}\Psi(\lambda\mathbf{r}_1,\ldots,\lambda\mathbf{r}_N)$, $\lambda>0$, obviously generates the scaled densities $n_\lambda(\mathbf{r})\equiv\lambda^3 n(\lambda\mathbf{r})$ and $\mathbf{j}_\lambda(\mathbf{r})\equiv\lambda^4\mathbf{j}(\lambda\mathbf{r})$ and leads to

$$\langle\Psi_\lambda|\hat{T}|\Psi_\lambda\rangle=\lambda^2\langle\Psi|\hat{T}|\Psi\rangle \tag{8}$$

and

$$\langle\Psi_\lambda|\hat{W}|\Psi_\lambda\rangle=\lambda\langle\Psi|\hat{W}|\Psi\rangle. \tag{9}$$

In analogy to the case without magnetic fields [16] the scaled wave function $\Psi_\lambda(\mathbf{r}_1,\ldots,\mathbf{r}_N)$, which yields the scaled densities n_λ and $\mathbf{j}_\lambda$, is easily seen to minimize $\langle\hat{T}+\lambda\hat{W}\rangle$ and thus differs from the wave function $\Psi^\lambda(\mathbf{r}_1,\ldots,\mathbf{r}_N)$, which also yields n_λ and $\mathbf{j}_\lambda$ but minimizes $\langle\hat{T}+\hat{W}\rangle$. This gives the following inequalities:

$$\begin{aligned}T[n_\lambda,\mathbf{j}_\lambda]+W[n_\lambda,\mathbf{j}_\lambda]&=\langle\Psi^\lambda|\hat{T}+\hat{W}|\Psi^\lambda\rangle\\&<\langle\Psi_\lambda|\hat{T}+\hat{W}|\Psi_\lambda\rangle\\&=\lambda^2T[n,\mathbf{j}]+\lambda W[n,\mathbf{j}],\end{aligned} \tag{10}$$

$$T[n_\lambda,\mathbf{j}_\lambda]+\lambda W[n_\lambda,\mathbf{j}_\lambda]=\langle\Psi^\lambda|\hat{T}+\lambda\hat{W}|\Psi^\lambda\rangle$$
$$>\langle\Psi_\lambda|\hat{T}+\lambda\hat{W}|\Psi_\lambda\rangle$$
$$=\lambda^2T[n,\mathbf{j}]+\lambda^2W[n,\mathbf{j}] \qquad (11)$$

for $\lambda\neq1$. Combining (10) and (11) we obtain

$$T[n_\lambda,\mathbf{j}_\lambda]>\lambda^2T[n,\mathbf{j}] \quad \text{for } \lambda<1, \qquad (12)$$

$$T[n_\lambda,\mathbf{j}_\lambda]<\lambda^2T[n,\mathbf{j}] \quad \text{for } \lambda>1, \qquad (13)$$

$$W[n_\lambda,\mathbf{j}_\lambda]<\lambda W[n,\mathbf{j}] \quad \text{for } \lambda<1, \qquad (14)$$

$$W[n_\lambda,\mathbf{j}_\lambda]>\lambda W[n,\mathbf{j}] \quad \text{for } \lambda>1. \qquad (15)$$

In noninteracting systems let $\Phi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ be the wave function that minimizes $\langle\hat{T}\rangle$ and yields given densities n and $\mathbf{j}$. Then the wave function $\Phi^\lambda(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ that minimizes $\langle\hat{T}\rangle$ but yields the scaled densities n_λ and $\mathbf{j}_\lambda$ is identical to the scaled wave function $\Phi_\lambda(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\lambda^{3N/2}\Phi(\lambda\mathbf{r}_1,\ldots,\lambda\mathbf{r}_N)$. As a consequence, the functionals

$$T_s[n,\mathbf{j}]=\langle\Phi|\hat{T}|\Phi\rangle \qquad (16)$$

and

$$E_x[n,\mathbf{j}]=\langle\Phi|\hat{W}|\Phi\rangle-U[n], \qquad (17)$$

where $U[n]$ denotes the classical Coulomb energy

$$U[n]=\frac{e^2}{2}\int d^3r\int d^3r'\,\frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \qquad (18)$$

scale homogeneously, namely,

$$T_s[n_\lambda,\mathbf{j}_\lambda]=\langle\Phi^\lambda|\hat{T}|\Phi^\lambda\rangle=\langle\Phi_\lambda|\hat{T}|\Phi_\lambda\rangle=\lambda^2\langle\Phi|\hat{T}|\Phi\rangle$$
$$=\lambda^2T_s[n,\mathbf{j}], \qquad (19)$$

$$E_x[n_\lambda,\mathbf{j}_\lambda]=\langle\Phi^\lambda|\hat{W}|\Phi^\lambda\rangle-U[n_\lambda]=\langle\Phi_\lambda|\hat{W}|\Phi_\lambda\rangle-\lambda U[n]$$
$$=\lambda\langle\Phi|\hat{W}|\Phi\rangle-\lambda U[n]=\lambda E_x[n,\mathbf{j}]. \qquad (20)$$

The exchange-correlation energy functional defined by

$$E_{\mathrm{xc}}[n,\mathbf{j}]=T[n,\mathbf{j}]+W[n,\mathbf{j}]-T_s[n,\mathbf{j}]-U[n] \qquad (21)$$

does not scale homogeneously. It satisfies the following inequalities:

$$E_{\mathrm{xc}}[n_\lambda,\mathbf{j}_\lambda]<\lambda E_{\mathrm{xc}}[n,\mathbf{j}] \quad \text{for } \lambda<1,$$
$$E_{\mathrm{xc}}[n_\lambda,\mathbf{j}_\lambda]>\lambda E_{\mathrm{xc}}[n,\mathbf{j}] \quad \text{for } \lambda>1. \qquad (22)$$

The inequality for $\lambda<1$ is readily proven by the following chain of arguments:

$$E_{\mathrm{xc}}[n_\lambda,\mathbf{j}_\lambda]=T[n_\lambda,\mathbf{j}_\lambda]+W[n_\lambda,\mathbf{j}_\lambda]-T_s[n_\lambda,\mathbf{j}_\lambda]-U[n_\lambda]$$
$$<\lambda^2T[n,\mathbf{j}]+\lambda W[n,\mathbf{j}]-\lambda^2T_s[n,\mathbf{j}]-\lambda U[n]$$
$$=\lambda E_{\mathrm{xc}}[n,\mathbf{j}]+(\lambda^2-\lambda)(T[n,\mathbf{j}]-T_s[n,\mathbf{j}])$$
$$\leqslant\lambda E_{\mathrm{xc}}[n,\mathbf{j}]. \qquad (23)$$

Here the first inequality follows immediately from applying (10) and (19). The second one, on the other hand, is a consequence of $(\lambda^2-\lambda)<0$ for $0<\lambda<1$ and of the fact that $T-T_s$ is always non-negative (which follows from the observation that, among all wave functions yielding n and $\mathbf{j}$, Φ is the one that minimizes $\langle\hat{T}\rangle$ so that $T_s=\langle\Phi|\hat{T}|\Phi\rangle\leqslant\langle\Psi|\hat{T}|\Psi\rangle=T$). The inequality for $\lambda>1$ in (22) can be shown with a similar argument using (11) and (19). Owing to the homogeneous scaling of E_x, the inequalities (22) also hold for the correlation energy functional $E_c\equiv E_{\mathrm{xc}}-E_x$ alone.

Next, let us consider a homogeneously scaling functional $Q[n,\mathbf{j}]$ of degree k, i.e.,

$$Q[n_\lambda,\mathbf{j}_\lambda]=\lambda^kQ[n,\mathbf{j}]. \qquad (24)$$

Taking the derivative of this equation with respect to λ in the limit $\lambda\to1$, we find

$$kQ[n,\mathbf{j}]=\lim_{\lambda\to1}\frac{d}{d\lambda}Q[n_\lambda,\mathbf{j}_\lambda]=\lim_{\lambda\to1}\left(\int d^3r\,\frac{\delta Q[n_\lambda,\mathbf{j}_\lambda]}{\delta n_\lambda(\mathbf{r})}\frac{\partial n_\lambda(\mathbf{r})}{\partial\lambda}+\int d^3r\,\frac{\delta Q[n_\lambda,\mathbf{j}_\lambda]}{\delta\mathbf{j}_\lambda(\mathbf{r})}\frac{\partial\mathbf{j}_\lambda(\mathbf{r})}{\partial\lambda}\right)$$
$$=\int d^3r\,\frac{\delta Q[n,\mathbf{j}]}{\delta n(\mathbf{r})}\lim_{\lambda\to1}\frac{\partial}{\partial\lambda}[\lambda^3n(\lambda\mathbf{r})]+\int d^3r\,\frac{\delta Q[n,\mathbf{j}]}{\delta\mathbf{j}(\mathbf{r})}\lim_{\lambda\to1}\frac{\partial}{\partial\lambda}[\lambda^4\mathbf{j}(\lambda\mathbf{r})]$$
$$=\int d^3r\,\frac{\delta Q[n,\mathbf{j}]}{\delta n(\mathbf{r})}(3+\mathbf{r}\nabla)n(\mathbf{r})+\int d^3r\,\frac{\delta Q[n,\mathbf{j}]}{\delta\mathbf{j}(\mathbf{r})}(4+\mathbf{r}\nabla)\mathbf{j}(\mathbf{r}), \qquad (25)$$

where we have used the identity

$$\lim_{\lambda\to1}\frac{\partial}{\partial\lambda}f(\lambda\mathbf{r})=\mathbf{r}\nabla f(\mathbf{r}). \qquad (26)$$

If the densities $n(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$ vanish for $r\to\infty$, partial integration yields

$$kQ=-\int d^3r\;n(\mathbf{r})(\mathbf{r}\nabla)\frac{\delta Q}{\delta n(\mathbf{r})}+\int d^3r\;\mathbf{j}(\mathbf{r})(1-\mathbf{r}\nabla)\frac{\delta Q}{\delta\mathbf{j}(\mathbf{r})}. \qquad (27)$$

Applying this result to the homogeneously scaling functions T_s and E_x, we obtain

$$2T_s = -\int d^3r\, n(\mathbf{r})(\mathbf{r}\nabla)\frac{\delta T_s}{\delta n(\mathbf{r})} + \int d^3r\, \mathbf{j}(\mathbf{r})(1-\mathbf{r}\nabla)\frac{\delta T_s}{\delta \mathbf{j}(\mathbf{r})}, \tag{28}$$

$$E_x = -\int d^3r\, n(\mathbf{r})(\mathbf{r}\nabla)\frac{\delta E_x}{\delta n(\mathbf{r})} + \int d^3r\, \mathbf{j}(\mathbf{r})(1-\mathbf{r}\nabla)\frac{\delta E_x}{\delta \mathbf{j}(\mathbf{r})}. \tag{29}$$

Further scaling relations can be derived for the functional derivatives $q([n,\mathbf{j}],\mathbf{r}) \equiv \delta Q[n,\mathbf{j}]/\delta n(\mathbf{r})$ and $\mathbf{q}([n,\mathbf{j}],\mathbf{r}) \equiv \delta Q[n,\mathbf{j}]/\delta \mathbf{j}(\mathbf{r})$. Taking the functional derivatives with respect to $n_\lambda(\mathbf{r})$ and $\mathbf{j}_\lambda(\mathbf{r})$, respectively, on both sides of Eq. (24) we find

$$\begin{aligned} q([n_\lambda,\mathbf{j}_\lambda],\mathbf{r}) &= \frac{\delta Q[n_\lambda,\mathbf{j}_\lambda]}{\delta n_\lambda(\mathbf{r})} = \lambda^k \frac{\delta Q[n,\mathbf{j}]}{\delta n_\lambda(\mathbf{r})} \\ &= \lambda^k \int d^3z\, \frac{\delta Q[n,\mathbf{j}]}{\delta n(\mathbf{z})}\frac{\delta n(\mathbf{z})}{\delta n_\lambda(\mathbf{r})}. \end{aligned} \tag{30}$$

Using

$$\frac{\delta n(\mathbf{z})}{\delta n_\lambda(\mathbf{r})} = \frac{1}{\lambda^3}\frac{\delta n_\lambda(\mathbf{z}/\lambda)}{\delta n_\lambda(\mathbf{r})} = \frac{1}{\lambda^3}\,\delta(\mathbf{z}/\lambda - \mathbf{r}) = \delta(\mathbf{z}-\lambda\mathbf{r}), \tag{31}$$

we obtain

$$q([n_\lambda,\mathbf{j}_\lambda],\mathbf{r}) = \lambda^k \frac{\delta Q[n,\mathbf{j}]}{\delta n(\lambda\mathbf{r})} = \lambda^k q([n,\mathbf{j}],\lambda\mathbf{r}). \tag{32}$$

In the same way we find

$$\mathbf{q}([n_\lambda,\mathbf{j}_\lambda],\mathbf{r}) = \lambda^{k-1}\mathbf{q}([n,\mathbf{j}],\lambda\mathbf{r}). \tag{33}$$

In order to derive a virial theorem for electronic systems in an external magnetic field we start from the equation

$$\lim_{\lambda\to 1}\frac{d}{d\lambda}\langle\Psi_\lambda|\hat{H}|\Psi_\lambda\rangle = 0, \tag{34}$$

which follows from the Rayleigh-Ritz principle if Ψ is the ground-state wave function of $\hat{H}$. Using relations (8) and (9) we find

$$\begin{aligned} \lim_{\lambda\to 1}\frac{d}{d\lambda}\langle\Psi_\lambda|\hat{H}|\Psi_\lambda\rangle &= \lim_{\lambda\to 1}\frac{d}{d\lambda}\left[\lambda^2\langle\Psi|\hat{T}|\Psi\rangle + \lambda\langle\Psi|\hat{W}|\Psi\rangle + \int d^3r\left(v(\mathbf{r}) + \frac{e^2}{2mc^2}\mathbf{A}^2(\mathbf{r})\right)n_\lambda(\mathbf{r}) + \frac{e}{c}\int d^3r\mathbf{A}(\mathbf{r})\mathbf{j}_\lambda(\mathbf{r})\right] \\ &= 2\langle\Psi|\hat{T}|\Psi\rangle + \langle\Psi|\hat{W}|\Psi\rangle + \int d^3r\left(v(\mathbf{r}) + \frac{e^2}{2mc^2}\mathbf{A}^2(\mathbf{r})\right)(3+\mathbf{r}\boldsymbol{\nabla})n(\mathbf{r}) + \frac{e}{c}\int d^3r\,\mathbf{A}(\mathbf{r})(4+\mathbf{r}\boldsymbol{\nabla})\mathbf{j}(\mathbf{r}) = 0, \end{aligned} \tag{35}$$

where the second equality follows from Eq. (26). Finally, partial integration yields

$$2\langle\Psi|\hat{T}|\Psi\rangle + \langle\Psi|\hat{W}|\Psi\rangle - \int d^3r\, n(\mathbf{r})(\mathbf{r}\nabla)\left(v(\mathbf{r}) + \frac{e^2}{2mc^2}\mathbf{A}^2(\mathbf{r})\right) - \frac{e}{c}\int d^3r\,\mathbf{j}(\mathbf{r})(\mathbf{r}\nabla - 1)\mathbf{A}(\mathbf{r}) = 0 \tag{36}$$

if the densities $n(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$ vanish for $r\to\infty$. The variational principle of CDFT, on the other hand, ensures that

$$\frac{\delta}{\delta n(\mathbf{r})}(T[n,\mathbf{j}] + W[n,\mathbf{j}]) + v(\mathbf{r}) + \frac{e^2}{2mc^2}\mathbf{A}^2(\mathbf{r}) = \mu, \tag{37}$$

$$\frac{\delta}{\delta \mathbf{j}(\mathbf{r})}(T[n,\mathbf{j}] + W[n,\mathbf{j}]) + \frac{e}{c}\mathbf{A}(\mathbf{r}) = \mathbf{0}. \tag{38}$$

Using these equations, the terms in Eq. (36) involving v or $\mathbf{A}$ can be eliminated, leading to

$$\begin{aligned} 2T + W &+ \int d^3r\, n(\mathbf{r})(\mathbf{r}\nabla)\frac{\delta(T+W)}{\delta n(\mathbf{r})} \\ &+ \int d^3\mathbf{r}\,\mathbf{j}(\mathbf{r})(\mathbf{r}\nabla - 1)\frac{\delta(T+W)}{\delta \mathbf{j}(\mathbf{r})} = 0. \end{aligned} \tag{39}$$

For noninteracting systems ($W\equiv 0$, $T\equiv T_s$) one immediately recovers Eq. (28). Subtracting (28) from (39) and replacing $T+W-T_s$ by $E_{\mathrm{xc}}+U$, we obtain the central result:

$$\begin{aligned} E_{\mathrm{xc}} + \int d^3r\, n(\mathbf{r})(\mathbf{r}\nabla)\frac{\delta E_{\mathrm{xc}}}{\delta n(\mathbf{r})} + \int d^3r\,\mathbf{j}(\mathbf{r})(\mathbf{r}\nabla - 1)\frac{\delta E_{\mathrm{xc}}}{\delta \mathbf{j}(\mathbf{r})} \\ = -T + T_s \equiv -T_{\mathrm{xc}}. \end{aligned} \tag{40}$$

In order to obtain an equation for the correlation energy alone we subtract Eq. (29) from Eq. (40), leading to

$$\begin{aligned} E_c + \int d^3r\, n(\mathbf{r})(\mathbf{r}\nabla)\frac{\delta E_c}{\delta n(\mathbf{r})} + \int d^3r\,\mathbf{j}(\mathbf{r})(\mathbf{r}\nabla)\frac{\delta E_c}{\delta \mathbf{j}(\mathbf{r})} \\ - \int d^3r\,\mathbf{j}(\mathbf{r})\frac{\delta E_c}{\delta \mathbf{j}(\mathbf{r})} = -T_{\mathrm{xc}}. \end{aligned} \tag{41}$$

As shown by Vignale and Rasolt [2], the gauge invariance of $E_{\mathrm{xc}}[n,\mathbf{j}]$ implies that the exchange-correlation energy functional only depends on the density and a new variable, the so-called vorticity, $\boldsymbol{\nu}(\mathbf{r}) = \nabla\times[\mathbf{j}(\mathbf{r})/n(\mathbf{r})]$, i.e., $E_{\mathrm{xc}}[n,\mathbf{j}] = E_{\mathrm{xc}}[n,\boldsymbol{\nu}]$. The same statement holds for E_{x} and for E_{c} separately. In contrast to the paramagnetic current density $\mathbf{j}(\mathbf{r})$, $\boldsymbol{\nu}(\mathbf{r})$ is a gauge-invariant quantity. In order to express Eq. (40) in terms of the variable $\boldsymbol{\nu}$ we use the following identities:

$$\frac{\delta E_{\rm xc}}{\delta n(\mathbf{r})}=\frac{\delta \bar{E}_{\rm xc}}{\delta n(\mathbf{r})}-\frac{\mathbf{j}(\mathbf{r})}{n^2(\mathbf{r})}\,\nabla\times\frac{\delta \bar{E}_{\rm xc}}{\delta \boldsymbol{\nu}(\mathbf{r})} \tag{42}$$

and

$$\frac{\delta E_{\rm xc}}{\delta \mathbf{j}(\mathbf{r})}=\frac{1}{n(\mathbf{r})}\,\nabla\times\frac{\delta \bar{E}_{\rm xc}}{\delta \boldsymbol{\nu}(\mathbf{r})}. \tag{43}$$

Substitution of (42) and (43) into (40) yields, after some straightforward algebra, the equation

$$\bar{E}_{\rm xc}+\int d^3r\; n(\mathbf{r})(\mathbf{r}\nabla)\,\frac{\delta \bar{E}_{\rm xc}}{\delta n(\mathbf{r})}+\int d^3r\;\boldsymbol{\nu}(\mathbf{r})(\mathbf{r}\nabla)\,\frac{\delta \bar{E}_{\rm xc}}{\delta \boldsymbol{\nu}(\mathbf{r})}+\int d^3r\;\boldsymbol{\nu}(\mathbf{r})\,\frac{\delta \bar{E}_{\rm xc}}{\delta \boldsymbol{\nu}(\mathbf{r})}=-T_{\rm xc}, \tag{44}$$

or, equivalently,

$$\bar{E}_{x}+\int d^3r\; n(\mathbf{r})(\mathbf{r}\nabla)\,\frac{\delta \bar{E}_{x}}{\delta n(\mathbf{r})}+\int d^3r\;\boldsymbol{\nu}(\mathbf{r})(\mathbf{r}\nabla)\,\frac{\delta \bar{E}_{x}}{\delta \boldsymbol{\nu}(\mathbf{r})}+\int d^3r\;\boldsymbol{\nu}(\mathbf{r})\,\frac{\delta \bar{E}_{x}}{\delta \boldsymbol{\nu}(\mathbf{r})}=0, \tag{45}$$

$$\bar{E}_{c}+\int d^3r\; n(\mathbf{r})(\mathbf{r}\nabla)\,\frac{\delta \bar{E}_{c}}{\delta n(\mathbf{r})}+\int d^3r\;\boldsymbol{\nu}(\mathbf{r})(\mathbf{r}\nabla)\,\frac{\delta \bar{E}_{c}}{\delta \boldsymbol{\nu}(\mathbf{r})}+\int d^3r\;\boldsymbol{\nu}(\mathbf{r})\,\frac{\delta \bar{E}_{c}}{\delta \boldsymbol{\nu}(\mathbf{r})}=-T_{\rm xc}. \tag{46}$$

These two equations are the central result of our analysis. Equation (45) [or, equivalently, Eq. (29)] is particularly useful if approximate expressions for the exchange *potentials* are employed without explicit knowledge of the corresponding (approximate) exchange *energy* functional. Given the exchange potentials and the corresponding self-consistent densities $(n,\mathbf{j})$, then Eq. (29) immediately yields the corresponding exchange-energy value.

Equations (28), (29), and (41), as well as (45) and (46) have been obtained under the assumption that the densities $n(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$ vanish for $r\to\infty$. Analogous equations for extended systems can easily be derived if Eqs. (25) and (35) are used directly [rather than the partially integrated Eqs. (27) and (36)].

We finally note that in arbitrary integer dimension d the scaled densities are given by $n_\lambda(\mathbf{r})=\lambda^d n(\lambda\mathbf{r})$, $\mathbf{j}_\lambda(\mathbf{r})=\lambda^{d+1}\mathbf{j}(\lambda\mathbf{r})$, and $\boldsymbol{\nu}_\lambda(\mathbf{r})=\lambda^{d-1}\boldsymbol{\nu}(\lambda\mathbf{r})$. The above relations (12)–(22), (27)–(33), (39)–(41), and (44)–(46) remain valid if all vectors and integrals are considered to be d-dimensional.

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