# Exact properties of the Pauli potential for the square root of the electron density and the kinetic energy functional

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It is known that the square root of the electron density satisfies $\{-\frac{1}{2}\nabla^2+v_\theta([n];\mathbf{r})+v_s([n];\mathbf{r})\}n^{1/2}(\mathbf{r})=\varepsilon_M n^{1/2}(\mathbf{r})$, where $v_s$ is the Kohn-Sham potential and $\varepsilon_M$ is its highest-occupied orbital energy. The Pauli potential $v_\theta$ is defined as the functional derivative of the difference between the noninteracting kinetic energy $T_s[n]$ and the full von Weizsäcker kinetic energy. It has already been proven that $v_\theta([n];\mathbf{r})\geq 0$ for all $\mathbf{r}$. By starting primarily with a slightly modified version of an equation of Bartolotti and Acharya, new exact properties of $v_\theta([n];\mathbf{r})$ are derived for the purpose of approximating it. The gradient expansion for $T_s[n]$ gives a $v_\theta([n];\mathbf{r})$ that is found to violate several of the exact conditions. For instance, $v_\theta\geq 0$ is violated unless the full von Weizsäcker term is employed. A new approximate form for $v_\theta([n];\mathbf{r})$ is proposed.

## I. INTRODUCTION

Consider a system of electrons for which

$$\hat{H}=\sum_{i=1}^{N}-\tfrac{1}{2}\nabla_i^2+\sum_{i=1}^{N}v(\mathbf{r}_i)+\sum_{i}\sum_{j(>i)}|\mathbf{r}_i-\mathbf{r}_j|^{-1}, \tag{1}$$

where, for simplicity of discussion, we shall assume that $N$ is even. According to the Kohn-Sham partitioning[1] of density-functional theory, the exact ground-state energy for external potential $v$ may be obtained from

$$E=\min_n\left[T_s[n]+\int v(\mathbf{r})n(\mathbf{r})d\mathbf{r}+\tfrac{1}{2}\int\int n(\mathbf{r}_1)n(\mathbf{r}_2)|\mathbf{r}_1-\mathbf{r}_2|^{-1}d\mathbf{r}_1d\mathbf{r}_2+E_{xc}[n]\right], \tag{2}$$

where $E_{xc}[n]$ is the exchange-correlation functional of trial electron density $n$ and $T_s[n]$ is its noninteracting kinetic energy. The latter may be defined according to the "constrained-search" formulation by[2]

$$T_s[n]=\langle\Phi_n^{\min}|\hat{T}|\Phi_n^{\min}\rangle, \tag{3}$$

where $\Phi_n^{\min}$ is that single determinant which yields $n$ and minimizes $\langle\hat{T}\rangle$, where $\hat{T}=\sum_{i=1}^{N}-\frac{1}{2}\nabla_i^2$. (Again for simplicity, we shall restrict each $\Phi_n$ to consist of only doubly occupied orbitals, and we shall concern ourselves only with the density here and not with spin densities.)

The optimum doubly occupied space orbitals in $\Phi_n^{\min}$ satisfy the following Kohn-Sham equations:[1]

$$\{-\tfrac{1}{2}\nabla^2+v_s([n];r)\}\phi_i(\mathbf{r})=\varepsilon_i\phi_i(\mathbf{r}),\quad i=1,2,\ldots,M \tag{4}$$

with $\varepsilon_1\leq\varepsilon_2\leq\ldots\leq\varepsilon_M$, $\langle\phi_i|\phi_j\rangle=\delta_{ij}$, and

$$v_s(\mathbf{r})=v(\mathbf{r})+\int n(\mathbf{r}_2)|\mathbf{r}-\mathbf{r}_2|^{-1}d\mathbf{r}_2+\delta E_{xc}[n]/\delta n(\mathbf{r}), \tag{5}$$

where $M=N/2$. In addition, it has been proven[3] that either the occupied $\{\phi_i\}$ correspond to the lowest $M$ states of $v_s$ or at least one of the lowest $M$ states will be unoccupied. In any case, the $\phi_i$'s are eigenfunctions of the *same*[3] local potential, $v_s$, and the $T_s[n]$ of Eq. (3) is given in terms of the $\phi_i$ by

$$T_s[n]=2\sum_{i=1}^{M}\int\phi_i^*(-\tfrac{1}{2}\nabla^2)\phi_i d\mathbf{r}. \tag{6}$$

The use of the popular Kohn-Sham Euler equations, Eqs. (4), has been found to yield widespread success in recent years. Moreover, when these equations are employed, $T_s[n]$ is evaluated exactly by means of Eq. (6). However, since $v_s([n];\mathbf{r})$ is density dependent, Eqs. (4) must be solved iteratively to self-consistency, which causes some difficulty for very large molecules with little symmetry, even though $v_s$ is extremely attractive in that it is a local potential.

As an alternative to the Kohn-Sham equations, there exists an exact *single* Euler equation for $n^{1/2}$, namely, the following Schrodinger equation has recently been derived:[4–7]

$$\{-\tfrac{1}{2}\nabla^2+v_\theta([n];\mathbf{r})+v_s([n];\mathbf{r})\}n^{1/2}(\mathbf{r})=\varepsilon_M n^{1/2}(\mathbf{r}), \tag{7}$$

where $\varepsilon_M$ is the highest-occupied Kohn-Sham orbital energy in Eqs. (4). The presence of $\varepsilon_M$ in Eq. (7) results from[8] the fact that $n^{1/2}(\mathbf{r})$ decays assymptotically as $\phi_M$. It is assumed in Eq. (7), and shall be assumed for the remainder of the paper, that $v_s([n];|\mathbf{r}|\rightarrow\infty)=0$ and $v_\theta([n];|\mathbf{r}|\rightarrow\infty)=0$. This may always be accomplished if $|n^{-1/2}(-\frac{1}{2}\nabla^2)n^{1/2}|<\infty$ as $|\mathbf{r}|\rightarrow\infty$. Simply add constants, if necessary, to $v_s$ and $v_\theta$.

Equation (7) arises from expressing $T_s$ as[4–7]

$$T_s[n]=\int n^{1/2}(\mathbf{r})(-\tfrac{1}{2}\nabla^2)n^{1/2}(\mathbf{r})+T_\theta[n]=\tfrac{1}{8}\int|\nabla n(\mathbf{r})|^2n^{-1}d\mathbf{r}+T_\theta[n] \tag{8}$$

 

and by noting that

$$\frac{\delta T_s[n]}{\delta n(\mathbf{r})}=n^{-1/2}(\mathbf{r})(-\tfrac{1}{2}\nabla^2)n^{1/2}(\mathbf{r})+v_\theta([n];\mathbf{r}) , \quad (9)$$

with

$$v_\theta([n];\mathbf{r})=\delta T_\theta[n]/\delta n(\mathbf{r}) , \quad (10)$$

and by utilizing

$$\frac{\delta T_s[n]}{\delta n(\mathbf{r})}+v_s([n];\mathbf{r})=\varepsilon_M , \quad (11)$$

which arises from the minimization in Eq. (2). Observe that the first term in Eq. (8) is the full von Weizsäcker kinetic energy.

Eq. (7) is attractive, compared to Eqs. (4), because solution of Eq. (7) requires iteration to self-consistency for only one equation while Eqs. (4) require self-consistency for $M$ equations. Moreover, as brought out by Levy, Perdew, and Sahni,[5] any commonly employed Kohn-Sham program may be used to solve Eq. (7); simply extract only its lowest eigenfunction ($n^{1/2}$) and eigenvalue ($\varepsilon_M$). On the other hand, for practical calculations, $T_\theta[n]$ must be *approximated* as an explicit functional of $n$, which has proven a formidable task as far as accurate quantitative predictions are concerned.[9] In essence, $v_\theta$ must be made to embody all the effects of the Pauli principle (antisymmetry requirement). For this reason $v_\theta$ has been labeled the Pauli potential by March,[6] and $T_\theta$ is aptly referred to as the Pauli kinetic energy.

In order to approximate $T_\theta$ and $v_\theta$ adequately, it is necessary to have knowledge of the exact properties of $T_\theta$ and $v_\theta$. It is the purpose of this article to first derive several of the important properties of $T_\theta$ and $v_\theta$ and then to examine existing commonly employed approximate $T_s[n]$ functionals in terms of these properties.

## II. DERIVATION OF EXACT PROPERTIES OF $v_\theta$ AND $t_\theta$

Following Bartolotti and Acharya,[10] multiply Eqs. (4) by $2\phi_i^*$ and sum to get

$$2\sum_{i=1}^{M}\phi_i^*(-\tfrac{1}{2}\nabla^2)\phi_i+v_s n=2\sum_{i=1}^{M}\varepsilon_i\phi_i^*\phi_i , \quad (12)$$

where

$$n(\mathbf{r})=\sum_{i=1}^{M}2\phi_i^*\phi_i . \quad (13)$$

Next, divide Eq. (12) by $n^{1/2}$ and manipulate the resultant equation to obtain

$$\left[-\tfrac{1}{2}\nabla^2+v_s+n^{-1}\left[2\sum_i\phi_i^*(-\tfrac{1}{2}\nabla^2)\phi_i-n^{1/2}(-\tfrac{1}{2}\nabla^2)n^{1/2}\right]+\sum_{i=1}^{M}(\varepsilon_M-\varepsilon_i)(2\phi_i^*\phi_i n^{-1})\right]n^{1/2}=\varepsilon_M n^{1/2} . \quad (14)$$

Now, with some algebra it can be shown that

$$n^{-1}\left[\sum_{i=1}^{M}2\phi_i^*(-\tfrac{1}{2}\nabla^2)\phi_i-n^{1/2}(-\tfrac{1}{2}\nabla^2)n^{1/2}\right]=\sum_{i=1}^{M}\nabla(\phi_i n^{-1/2})^*\cdot\nabla(\phi_i n^{-1/2})\geq 0 . \quad (15)$$

Comparison of Eqs. (7), (14), and (15) gives the desired exact formal expression for $v_\theta$:

$$v_\theta([n];\mathbf{r})=\sum_{i=1}^{M}\nabla(\phi_i n^{-1/2})^*\cdot\nabla(\phi_i n^{-1/2})+\sum_{i=1}^{M}(\varepsilon_M-\varepsilon_i)2\phi_i^*\phi_i n^{-1} . \quad (16)$$

Equation (16) is a slightly modified version of Eq. (14) of Bartolotti and Acharaya.[10] The $v_\theta$ of Eq. (16) is cast here in a form which renders certain properties of $v_\theta$ quite transparent.

Since no term in Eq. (16) is negative, it follows that

$$v_\theta([n];\mathbf{r})\geq 0 , \quad (17)$$

with $v_\theta([n];|\mathbf{r}|\rightarrow\infty)=0$. Equation (17) is an important result that was obtained previously[5,11] by a different method than employed in the present paper. Next, Eqs. (6) and (8) define $T_\theta$ by

$$T_\theta[n]=2\sum_{i=1}^{M}\int\phi_i^*(-\tfrac{1}{2}\nabla^2)\phi_i d\mathbf{r}-\int n^{1/2}(-\tfrac{1}{2}\nabla^2)n^{1/2}dr \quad (18)$$

or

$$T_\theta[n]=\sum_{i=1}^{M}\int\nabla\phi_i^*\cdot\nabla\phi_i d\mathbf{r}-\tfrac{1}{2}\int\nabla n^{1/2}\cdot\nabla n^{1/2}d\mathbf{r} \quad (19)$$

or

$$T_\theta[n]=\sum_{i=1}^{M}\nabla\phi_i^*\cdot\nabla\phi_i-\tfrac{1}{8}\int(\nabla n\cdot\nabla n)n^{-1}dr . \quad (20)$$

Comparison of Eq. (18) with Eq. (15) yields

$$T_\theta[n]=\int t_\theta([n];\mathbf{r})n(\mathbf{r})d\mathbf{r} , \quad (21)$$

with

$$t_\theta([n];\mathbf{r})=\sum_{i=1}^{M}\nabla(\phi_i n^{-1/2})^*\cdot\nabla(\phi_i n^{-1/2}) , \quad (22)$$

so that

$$t_\theta([n];\mathbf{r})\geq 0 , \quad (23)$$

which is a result in the spirit of Tal and Bader.[12] Furthermore, Eq. (22) implies

$$t_\theta([n];|\mathbf{r}|\rightarrow\infty)=0 . \quad (24)$$

Previously, Tal and Bader[12] noted the weaker condition, $\{n(\mathbf{r})t_\theta([n];\mathbf{r})\}_{|\mathbf{r}|\rightarrow\infty}=0$.

Comparison of Eq. (16) with Eq. (22) gives another key expression:

$$v_\theta([n];\mathbf{r})=t_\theta([n];\mathbf{r})+\sum_{i=1}^{M}(\varepsilon_M-\varepsilon_i)2\phi_i^*\phi_i n^{-1}\ , \quad (25)$$

which implies

$$v_\theta([n];\mathbf{r})\geq t_\theta([n];\mathbf{r})\ , \quad (26)$$

$$\int v_\theta([n];\mathbf{r})n(\mathbf{r})d\mathbf{r}\geq T_\theta[n]\ , \quad (27)$$

$$v_\theta([n];\mathbf{r})-t_\theta([n];\mathbf{r})\leq(\varepsilon_M-\varepsilon_1)\leq\left[M\varepsilon_M-\sum_{i=1}^{M}\varepsilon_i\right]<\infty\ . \quad (28)$$

It is also clear that from Eqs. (25) and (28) that

$$\int v_\theta([n];\mathbf{r})n(\mathbf{r})d\mathbf{r}<\infty\ . \quad (29)$$

Equation (28) can be put in a form which is especially suitable for testing an approximate $T_\theta$. To accomplish this, multiply Eq. (25) by $n$ and integrate to get

$$\int n(\mathbf{r})\{v_\theta([n];\mathbf{r})-t_\theta([n];\mathbf{r})\}d\mathbf{r}=2\left[M\varepsilon_M-\sum_{i=1}^{M}\varepsilon_i\right]\ . \quad (30)$$

Comparison of Eq. (30) with Eq. (28) generates the desired following form which is equivalent to Eq. (28), but more useful:

$$\max_{\mathbf{r}}\{v_\theta([n];\mathbf{r})-t_\theta([n];\mathbf{r})\}\leq\tfrac{1}{2}\int n(\mathbf{r})\{v_\theta([n];\mathbf{r})-t_\theta([n];\mathbf{r})\}\ . \quad (31)$$

As with Eq. (17), Eq. (31) is especially appealing because knowledge of the exact $v_s(\mathbf{r})$, or its eigenvalues, is *not required* in order to employ Eq. (31) with a given $n$.

There are important equalities involving $v_\theta$ and $t_\theta$. For instance, it is obvious that

$$v_\theta([n];\mathbf{r})=t_\theta([n];\mathbf{r})=0,\quad N=2\ . \quad (32)$$

Moreover, Eq. (31) actually becomes

$$\max_{\mathbf{r}}\{v_\theta([n];\mathbf{r})-t_\theta([n];\mathbf{r})\}=\tfrac{1}{2}\int n(\mathbf{r})\{v_\theta([n];\mathbf{r})-t_\theta([n];\mathbf{r})\}d\mathbf{r} \quad (33)$$

for $N=4$. The *equality* in Eq. (33), for $N=4$, arises from the fact that

$$\sum_{i=1}^{M}(\varepsilon_M-\varepsilon_i)2\phi_i^*\phi_i n^{-1}=M\varepsilon_M-\sum_{i=1}^{M}\varepsilon_i$$

at the nodes of $\phi_2$ for $N=4$.

As far as coordinate scaling equalities are concerned, we already know that[13–16]

$$T_s[n_\lambda]=\lambda^2T_s[n]\ , \quad (34)$$

where $n_\lambda(\mathbf{r})=\lambda^2n(\mathbf{r})$. Equations (34) and (8) dictate that

$$T_\theta[n_\lambda]=\lambda^2T_\theta[n]\ . \quad (35)$$

Equation (35), in turn, implies

$$T_\theta[n]=\tfrac{1}{2}\int d\mathbf{r}\,n(\mathbf{r})\mathbf{r}\cdot\nabla v_\theta([n];\mathbf{r})\ . \quad (36)$$

Equation (36) follows from combination of Eq. (35) with

$$(\partial T_\theta[n_\lambda]\partial\lambda)_{\lambda=1}=\int d\mathbf{r}\,n(\mathbf{r})\cdot\nabla v_\theta([n];\mathbf{r})\ . \quad (37)$$

Equation (37) is the Ghosh-Parr relation[17] as applied to $T_\theta$ and $v_\theta$.

By the definition of $v_\theta$, knowledge of $T_\theta$ is sufficient to give $v_\theta$. But Eq. (36) reveals that one may actually go the other way as well; knowledge of $v_\theta$ implies knowledge of $T_\theta$. This is a significant point because it is entirely possible that the universal structure of $v_\theta$ is going to become clearer, with time, than is the universal structure of $T_\theta$.

We now reveal an exact *local* coordinate scaling condition that is shared by the exact $v_\theta$, $t_\theta$, $t_s$, and $v_s$. The condition is[18]

$$v_\theta([n_\lambda];\mathbf{r}=\mathbf{r}_0)=\lambda^2v_\theta([n];\mathbf{r}=\lambda\mathbf{r}_0)\ , \quad (38)$$

$$t_\theta([n_\lambda];\mathbf{r}=\mathbf{r}_0)=\lambda^2t_\theta([n];\mathbf{r}=\lambda\mathbf{r}_0)\ , \quad (39)$$

$$t_s([n_\lambda];\mathbf{r}=\mathbf{r}_0)=\lambda^2t_s([n];\mathbf{r}=\lambda\mathbf{r}_0)\ , \quad (40)$$

$$v_s([n_\lambda];\mathbf{r}=\mathbf{r}_0)=\lambda^2v_s([n];\mathbf{r}=\lambda\mathbf{r}_0)\ . \quad (41)$$

In Eq. (38), $v_\theta([n_\lambda];\mathbf{r}=\mathbf{r}_0)$ signifies that $\lambda^3n(\lambda\mathbf{r})$ is inserted into the universal form of $v_\theta$, and $v_\theta$ is evaluated at the point $\mathbf{r}=\mathbf{r}_0$, while $v_\theta([n];\mathbf{r}=\lambda\mathbf{r}_0)$ signifies that $n(\mathbf{r})$ is inserted into the universal form of $v_\theta$, and $v_\theta$ is evaluated at the point $\mathbf{r}=\lambda\mathbf{r}_0$. It is straightforward to verify that Eqs. (38)–(41) arise directly from Eqs. (4) and (7) with utilization of the fact, as shown by Levy and Perdew,[15] that $\lambda^{3/2}\phi_i(\lambda\mathbf{r})$ and $\lambda^2\varepsilon_i$ are the Kohn-Sham orbitals and eigenvalues corresponding to $n_\lambda$. Finally, note that Eqs. (39) and (40) yield[18] Eqs. (34) and (35).

We conclude this section by asserting the following conditions which are so stringent that they would be satisfied by only the very best approximations to the true $v_\theta$ and $t_\theta$:

If any $n_q$ is adjusted to be related to any $n_p$ by

$$n_p^{-1/2}(-\tfrac{1}{2}\nabla^2)n_p^{1/2}-n_q^{-1/2}(-\tfrac{1}{2}\nabla^2)n_q^{1/2}(\mathbf{r})+v_\theta([n_p];\mathbf{r})-v_\theta([n_q];\mathbf{r})=c\ , \quad (42)$$

where $\int n_p(\mathbf{r})d\mathbf{r}=p$, $\int n_q(\mathbf{r})d\mathbf{r}=q$, and where $p=q+2$, then $n_p$ and $n_q$ belong to the same $v_s$, so that

$$c\geq 0 \quad (43)$$

by Eqs. (4). Moreover, by Eq. (16)

$$n_p(\mathbf{r})\{v_\theta([n_p];\mathbf{r})-t_\theta([n_p];\mathbf{r})\}=n_q(\mathbf{r})\{v_\theta([n_q];\mathbf{r})-t_\theta([n_q];\mathbf{r})\}+(n_p-n_q)c\ , \quad (44)$$

where $c$ is a constant in Eqs. (43)–(44). (The constant $c$ is, of course, equal to $\varepsilon_p-\varepsilon_q$.)

## III. EXACT CONDITIONS AND THE GRADIENT EXPANSION

The Hodges gradient expansion through fourth order, $T_s = T_0 + T_2 + T_4$, is[19,20]

$$T_s[n] = C_0 \int n^{5/3} d\mathbf{r} + C_2 \int \tfrac{1}{8} \frac{|\nabla n|^2}{n} dr + C_4 \int d\mathbf{r}\, n^{1/3} \left[ \left| \frac{\nabla^2 n}{n} - \left| \frac{3}{4} \frac{\nabla n}{n} \right|^2 \right|^2 + \frac{13}{768} \left| \frac{\nabla n}{n} \right|^4 \right], \tag{45}$$

so that its corresonding $t_\theta$ is

$$t_\theta[n] = C_0 n^{2/3} + (C_2 - 1) \left[ \frac{1}{8} \frac{|\nabla n|^2}{n^2} \right] + C_4 n^{-2/3} \left\{ \left| \frac{\nabla^2 n}{n} - \left[ \frac{3}{4} \frac{\nabla n}{n} \right]^2 \right|^2 + \frac{13}{768} \left[ \frac{\nabla n}{n} \right]^4 \right\}, \tag{46}$$

and its corresponding $v_\theta$, as shown through second order, is

$$v_\theta[n] = \tfrac{5}{3} C_0 n^{3/2} + (C_2 - 1) \left[ \frac{1}{8} \frac{|\nabla n|^2}{n^2} - \frac{1}{4} \frac{\nabla^2 n}{n} \right] + \cdots, \tag{47}$$

where $C_0 = \frac{3}{10}(3\pi^2)^{2/3}$, $C_2 = \frac{1}{9}$, and $C_4 = [540(3\pi^2)^{2/3}]^{-1}$. It is easy to verify that the local scaling conditions for $v_\theta$ and $t_\theta$, Eqs. (38) and (39), are satisfies by Eqs. (46) and (47).

$T_0 + T_2$ and $T_0 + T_2 + T_4$ have been found to give qualitatively reasonable kinetic energies for atoms[21] and molecules,[22] but these kinetic energies are outside the realm of quantitative accuracy for chemical binding.[9] Perhaps[9] these binding energies will be improved by applying the local asymptotic truncation of Pearson and Gordon[23] to the gradient expansion of the proper kinetic energy density as discussed by Perdew *et al.*[20] It would also be interesting to test, for binding-energy purposes, the new functionals of Herring and Chopra,[11,24] DePristo and Kress,[25] and Plumer and Stott.[26]

The exact $T_s$ satisfies the conditions of Sec. II for all valid $n$. It is impossible, however, to test the conditions on any approximate $T_s$ with respect to all $n$. For now, it is instructive to look at just $n(\mathbf{r}) = ae^{-br}$ for illustrative purposes. With the latter $n$, the $v_\theta$ corresponding to Eq. (45) diverges as $r \to \infty$ because of the presence of $T_4$. If $T_4$ is not present in Eq. (45), so that the expansion now consists of just the Thomas-Fermi $T_0$ or $T_0 + T_2$, then $v_\theta$ is still not properly behaved; it violates the condition $v_\theta \geq 0$, at small $r$, with $n = ae^{-br}$. Also, $t_\theta \geq 0$ is violated. It is noteworthy, therefore, that the recent nonlocal functional of Herring and Chopra[11,24] does satisfy $v_\theta \geq 0$.

Let's now free the coefficients in Eqs. (45)–(47). When $C_0 \geq 0$, $C_2 \geq 1$, and $C_4 \geq 0$, then the condition $t_\theta([n];\mathbf{r}) \geq 0$ is satisfied for all $n$. However, with these latter coefficients, the condition $t_\theta([n]; |\mathbf{r}| \to \infty) = 0$ is violated for $n = ae^{-br}$, unless $C_2 = 1$ and $C_4 = 0$. In fact, observe that the fourth-order contribution to $t_\theta$ actually goes to $\infty$ as $r \to \infty$. Moreover, for $C_0 > 0$, $C_2 < 1$, and $C_4 = 0$, $v_\theta$ violates the condition $v_\theta \geq 0$ at small $r$ when $n = ae^{-br}$. The condition $v_\theta \geq 0$ will also be violated for $C_2 > 1$ when densities other than $ae^{-br}$ are employed. Hence an argument is made for employment of the original full von Weizsäcker term ($C_2 = 1$). It should be noted, though, that $C_2 < 1$ arises naturally from the recent Feynman path integral results of Yang.[27,28]

The case of Acharya *et al.*, where $C_2 = 1$, where $C_4 = 0$, and where $C_0$ is considered as a function of $N$ has been found to yield fairly encouraging qualitative results[29–31] and is supported by information theory.[32] This simple functional actually satisfies $v_\theta \geq 0$, $t_\theta(|\mathbf{r}| \to \infty) = 0$, and $\int d\mathbf{r}\, n v_\theta \geq T_\theta[n]$, for all $n$. Equation (31), however, is not generally satisfied. For instance, Eq. (31) is not satisfied at small $r$ for $N < 8$ when $n = ae^{-br}$.

## IV. NEW EXPRESSION FOR $v_\theta[n]$.

The analysis in Sec. III on known approximations to $T_s$ reveals that the exact conditions of Sec. II are severe enough to be quite meaningful and useful. Also, the conditions may be tested with arbitrary $n$ because knowledge of the exact $v_s([n];\mathbf{r})$, or its eigenvalues, is not required. In other words, in order to test an $n$, we do not have to know its $v_s$.

Since none of the tested functionals obeyed all of the conditions, it is reasonable to assume that we should be able to improve upon existing approximations for $T_s[n]$ by modifying the functionals so that they are forced to satisfy the conditions as closely as possible.

Perhaps it would be fruitful to investigate working directly with a universal $v_\theta[n]$ in order to most easily satisfy the requisites of Sec. II and to satisfy other known requisites. For instance, a simple form for $v_\theta[n]$ such as

$$v_\theta[n] = \tfrac{5}{3} a(N) n^{2/3} + b(N) n^{-2/3} |\nabla n| + \cdots \tag{48}$$

will obey the local scaling requirement, Eq. (38), and will satisfy the condition $v_\theta([n];\mathbf{r}) \geq 0$ for all $n$, with $a(N) \geq 0$ and $b(N) \geq 0$. (Note that $v_\theta$ in Eq. (48) is constructed so that $v_\theta([n]; |\mathbf{r}| \to \infty) = 0$. It is thus not necessary to add a constant to this $v_\theta$ in order to make it vanish as $|\mathbf{r}| \to \infty$.)

From the $v_\theta$ in Eq. (48), $T_\theta$ may be formed from Eq. (36). This gives

$$T_\theta[n] = a(N) \int n^{5/3} d\mathbf{r} + \tfrac{1}{2} b(N) \int n\mathbf{r} \cdot \nabla [n^{-2/3} |\nabla n|] d\mathbf{r} + \cdots \tag{49}$$

so that

$$T_s[n] = \tfrac{1}{8} \int \frac{|\nabla n|^2}{n} d\mathbf{r} + a(N) \int n^{5/3} d\mathbf{r} + \tfrac{1}{2} b(N) \int n\mathbf{r} \cdot \nabla [n^{-2/3} |\nabla n|] d\mathbf{r} + \cdots. \tag{50}$$

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