Schrödinger equations for the square root density of an eigenmixture and the square root of an eigendensity spin matrix

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Abstract

We generalize a "one eigenstate" theorem of Levy, Perdew and Sahni (LPS) [1] to the case of densities coming from eigenmixture density operators. The generalization is of a special interest for the radial density functional theory (RDFT) for nuclei [2], a consequence of the rotational invariance of the nuclear Hamiltonian; when nuclear ground states (GSs) have a finite spin, the RDFT uses eigenmixture density operators to simplify predictions of GS energies into one-dimensional, radial calculations. We also study Schrödinger equations governing spin eigendensity matrices.

The theorem of Levy, Perdew and Sahni [1] may be described as follows:
i) let H_A be a Hamiltonian for A identical particles, with individual mass m,

$$H_A = \sum_{i=1}^{A} [-\hbar^2 \Delta_{\vec{r}_i}/(2m) + u(\vec{r}_i)] + \sum_{i>j=1}^{A} v(\vec{r}_i, \vec{r}_j), \qquad (1)$$

ii) consider a GS eigenfunction of H_A, $\psi(\vec{r}_1, \sigma_1, \vec{r}_2, \sigma_2, ..., \vec{r}_A, \sigma_A)$, where σ_i denotes the spin state of the particle with space coordinates $\vec{r}_i$,
iii) use a trace of $|\psi\rangle\langle\psi|$ upon all space coordinates but the last one, and upon all spins, to define the density,

$$\rho(\vec{r}) = A \sum_{\sigma_1...\sigma_A} \int d\vec{r}_1 d\vec{r}_2...d\vec{r}_{A-1} |\psi(\vec{r}_1, \sigma_1, \vec{r}_2, \sigma_2, ..., \vec{r}_{A-1}, \sigma_{A-1}, \vec{r}, \sigma_A)|^2, \quad (2)$$

iv) then there exists a local potential $v_{eff}(\vec{r})$ so that,

$$[-\hbar^2 \Delta_{\vec{r}}/(2m) + v_{eff}(\vec{r})] \sqrt{\rho(\vec{r})} = (E_A - E_{A-1}) \sqrt{\rho(\vec{r})}, \qquad (3)$$

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where the eigenvalue is the difference of the GS energy E_A of the A-particle system and that, E_{A-1}, of the $(A-1)$-particle one.

Can this theorem be generalized for densities derived from eigenoperators, $\mathcal{D} \propto \sum_{n=1}^{\mathcal{N}} w_n |\psi_n\rangle\langle\psi_n|$, corresponding to cases where H has several $(\mathcal{N} > 1)$ degenerate GSs ψ_n? The degeneracy situation is of a wide interest in nuclear physics for doubly odd nuclei, the GSs of which often have a finite spin, and, if only because of Kramer's degeneracy, for odd nuclei. In particular, because of the rotational invariance of the nuclear Hamiltonian, the density operator of interest for the RDFT [2] reads, $\mathcal{D} = \sum_M |\psi_{JM}\rangle\langle\psi_{JM}|/(2J+1)$, where J and M are the usual angular momentum numbers of a degenerate magnetic multiplet of GSs ψ_{JM}. Actually, more generally, it will easily be seen that the argument which follows holds for a degenerate multiplet of excited states as well.

This paper proves the generalization, by closely following the argument used for one eigenstate only [1]. Furthermore, there is no need to assume identical particles. No symmetry or antisymmetry assumption for eigenfunctions is needed. Let $\vec{p}_i$ and $\vec{\sigma}_i$ be the momentum and spin operators for the ith particle, at position $\vec{r}_i$. Single out the A-th particle, with its degrees of freedom labelled $\vec{r}$ and $\vec{\sigma}$ rather than $\vec{r}_A$ and $\vec{\sigma}_A$. For a theorem of maximal generality, with distinct masses, one-body and two-body potentials, our Hamiltonian may become, $\mathcal{H}_A = \mathcal{H}_{A-1} + \mathcal{V}_A + h_A$, with

$$
\mathcal{H}_{A-1} = \sum_{i=1}^{A-1}[-\hbar^2\Delta_{\vec{r}_i}/(2m_i) + u_i(\vec{r}_i, \vec{p}_i, \vec{\sigma}_i)] + \sum_{i>j=1}^{A-1} v_{ij}(\vec{r}_i, \vec{p}_i, \vec{\sigma}_i, \vec{r}_j, \vec{p}_j, \vec{\sigma}_j),
$$

$$
\mathcal{V}_A = \sum_{j=1}^{A-1} v_{Aj}(\vec{r}, \vec{r}_j, \vec{p}_j, \vec{\sigma}_j), \quad h_A = -\hbar^2\Delta_{\vec{r}}/(2m_A) + u_A(\vec{r}). \tag{4}
$$

The potentials acting upon the first $(A-1)$ particles may be non local and spin dependent, but, for a technical reason which will soon become obvious, those potentials acting upon the A-th particle in $\mathcal{V}_A$ and h_A must be strictly local and independent of the A-th spin. For notational simplicity, we choose units so that $\hbar^2/(2m_A) = 1$ from now on.

As in the one eigenstate case [1] we select situations where there exists a representation in which, simultaneously, the Hermitian Hamiltonian $\mathcal{H}_A$ and all the eigenfunctions $\psi(\vec{r}_1, \sigma_1, ..., \vec{r}_A, \sigma_A)$ under consideration are real. This reality condition does not seem to be restrictive, in view of time reversal invariance.

Let E_A be a degenerate eigenvalue of $\mathcal{H}_A$. The degeneracy multiplicity being larger than 1, select $\mathcal{N} \geq 2$ of the corresponding eigenfunctions ψ_n, orthonormalized. Their set may be either complete or incomplete in the eigensubspace. The density operators,

$$
\mathcal{D} = \sum_{n=1}^{\mathcal{N}} |\psi_n\rangle w_n \langle\psi_n|, \quad \sum_{n=1}^{\mathcal{N}} w_n = 1, \tag{5}
$$

with otherwise arbitrary, positive weights w_n, are normalized to unity, $\text{Tr}\,\mathcal{D} = 1$, in the A-body space. They are eigenoperators of $\mathcal{H}_A$, namely $\mathcal{H}_A\,\mathcal{D} = E_A\,\mathcal{D}$.

The partial trace of a $\mathcal{D}$ upon the first $(A-1)$ coordinates and all A spins,

$$\tau(\vec{r}) = \sum_{n=1}^{\mathcal{N}} w_n \sum_{\sigma_1...\sigma_{A-1}\sigma} \int d\vec{r}_1...d\vec{r}_{A-1} [\psi_n(\vec{r}_1, \sigma_1, ..., \vec{r}_{A-1}, \sigma_{A-1}, \vec{r}, \sigma)]^2, \quad (6)$$

defines a "density" τ, normalized so that $\int d\vec{r}\, \tau(\vec{r}) = 1$. Let now $\phi_{n\vec{r}\sigma}$ be, in the space of the first $(A-1)$ particles, an auxiliary wave function defined by,

$$\phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, ..., \vec{r}_{A-1}, \sigma_{A-1}) = \psi_n(\vec{r}_1, \sigma_1, ..., \vec{r}_{A-1}, \sigma_{A-1}, \vec{r}, \sigma)/\sqrt{\tau(\vec{r})}. \quad (7)$$

Note that this auxiliary wave function depends on the choice of the weights w_n.

Now the density operator in the space of the first $(A-1)$ particles, $\mathcal{D}'_{\vec{r}} = \sum_{n\sigma} |\phi_{n\vec{r}\sigma}\rangle w_n \langle\phi_{n\vec{r}\sigma}|$, is normalized, $\mathrm{Tr}'\,\mathcal{D}'_{\vec{r}} = 1$, where the symbol Tr' means integration upon the first $(A-1)$ coordinates and sum upon the first $(A-1)$ spins. Since this normalization of $\mathcal{D}'_{\vec{r}}$ in the $(A-1)$-particle space does not depend on $\vec{r}$, two trivial consequences read, $\nabla_{\vec{r}}\,\mathrm{Tr}'\,\mathcal{D}'_{\vec{r}} = 0$ and $\Delta_{\vec{r}}\,\mathrm{Tr}'\,\mathcal{D}'_{\vec{r}} = 0$. More explicitly, this gives,

$$\sum_{n\,\sigma\,\sigma_1...\sigma_{A-1}} \int d\vec{r}_1...d\vec{r}_{A-1} \quad w_n \; \phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, ..., \vec{r}_{A-1}, \sigma_{A-1}) \times$$
$$\nabla_{\vec{r}}\,\phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, ..., \vec{r}_{A-1}, \sigma_{A-1}) = 0, \quad (8)$$

and

$$\sum_{n\,\sigma\,\sigma_1...\sigma_{A-1}} \int d\vec{r}_1...d\vec{r}_{A-1} \; w_n \; \{ [\nabla_{\vec{r}}\phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, ..., \vec{r}_{A-1}, \sigma_{A-1})]^2 \quad +$$
$$\phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, ..., \vec{r}_{A-1}, \sigma_{A-1})\, \Delta_{\vec{r}}\phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, ..., \vec{r}_{A-1}, \sigma_{A-1}) \} \quad = \quad 0. (9)$$

Then one can rewrite the eigenstate property, $(\mathcal{H}_A - E_A)\,\psi_n = 0$, into,

$$(\mathcal{H}_{A-1} + \mathcal{V}_A + h_A - E_A)\,\sqrt{\tau}\,\phi_{n\vec{r}\sigma} = 0. \quad (10)$$

This also reads,

$$\sqrt{\tau}\,(\mathcal{H}_{A-1} + \mathcal{V}_A + u_A - E_A)\,\phi_{n\vec{r}\sigma} - (\Delta_{\vec{r}}\sqrt{\tau})\,\phi_{n\vec{r}\sigma} =$$
$$2\,(\nabla_{\vec{r}}\sqrt{\tau}) \cdot (\nabla_{\vec{r}}\phi_{n\vec{r}\sigma}) + \sqrt{\tau}\,(\Delta_{\vec{r}}\phi_{n\vec{r}\sigma}). \quad (11)$$

The right-hand side (rhs) of Eq. (11) occurs because the Laplacian, $\Delta_{\vec{r}}$, present in h_A, acts also upon the parameter, $\vec{r}$, of $\phi_{n\vec{r}\sigma}$. This is where the local, multiplicative nature of u_A and v_{Aj} in the last particle space is used and avoids the occurrence of further terms, that would induce a somewhat unwieldy theory.

Define, for any integrand $\Psi_{n\vec{r}\sigma}$, the following expectation value in the first $(A-1)$-particle space,

$$\langle\langle\Psi_{n\vec{r}\sigma}\rangle\rangle = \sum_{\sigma_1...\sigma_{A-1}} \int d\vec{r}_1...d\vec{r}_{A-1}\,\Psi_{n\vec{r}\sigma}(r_1, \sigma_1, ..., r_{A-1}, \sigma_{A-1}). \quad (12)$$

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Multiply Eq. (11) by $\phi_{n\vec{r}\sigma}$ and integrate out the first $(A-1)$ coordinates and spins, to obtain,

$$\langle\langle\phi^2_{n\vec{r}\sigma}\rangle\rangle\left[E^{exc}_{n\sigma}(\vec{r})+E_{A-1}+U_{n\sigma}(\vec{r})+u_A(\vec{r})-E_A-\Delta_{\vec{r}}\right]\sqrt{\tau(\vec{r})}$$
$$=2\,\langle\langle\,\phi_{n\vec{r}\sigma}\left(\nabla_{\vec{r}}\phi_{n\vec{r}\sigma}\right)\,\rangle\rangle\cdot\left[\nabla_{\vec{r}}\sqrt{\tau(\vec{r})}\right]+\langle\langle\,\phi_{n\vec{r}\sigma}\left(\Delta_{\vec{r}}\phi_{n\vec{r}\sigma}\right)\,\rangle\rangle\sqrt{\tau(\vec{r})},\ (13)$$

where $E^{exc}_{n\sigma}(\vec{r})$ is defined from,

$$\langle\langle\phi^2_{n\vec{r}\sigma}\rangle\rangle\left[E^{exc}_{n\sigma}(\vec{r})+E_{A-1}\right]=\sum_{\sigma_1...\sigma_{A-1}}\int d\vec{r}_1...d\vec{r}_{A-1}$$
$$\phi_{n\vec{r}\sigma}(r_1,\sigma_1,...,r_{A-1},\sigma_{A-1})\left[\mathcal{H}_{A-1}\,\phi_{n\vec{r}\sigma}\right](r_1,\sigma_1,...,r_{A-1},\sigma_{A-1}),\quad(14)$$

and $U_{n\sigma}(\vec{r})$ results from,

$$\langle\langle\phi^2_{n\vec{r}\sigma}\rangle\rangle\,U_{n\sigma}(\vec{r})=\sum_{j=1}^{A-1}\sum_{\sigma_1...\sigma_{A-1}}\int d\vec{r}_1...d\vec{r}_{A-1}$$
$$\phi_{n\vec{r}\sigma}(r_1,\sigma_1,...,r_{A-1},\sigma_{A-1})v_{Aj}(\vec{r},\vec{r}_j,\vec{p}_j,\vec{\sigma}_j)\phi_{n\vec{r}\sigma}(r_1,\sigma_1,...,r_{A-1},\sigma_{A-1}).(15)$$

The square norm of $\phi_{n\vec{r}\sigma}$ in the $(A-1)$-particle space results from Eq. (12) with $\Psi=\phi^2$. In Eq. (14) the expectation value of $\mathcal{H}_{A-1}$ is explicited as the sum of the GS energy E_{A-1} of $\mathcal{H}_{A-1}$ and a positive, excitation energy $E^{exc}_{n\sigma}(\vec{r})$. From Eq. (15), the Hartree nature of the potential $U_{n\sigma}(\vec{r})$ is transparent.

Keeping in mind that, $\forall\vec{r}$, the density operator $\mathcal{D}'$ is normalized to unity, namely, that $\sum_{n\sigma}w_n\langle\langle\phi^2_{n\vec{r}\sigma}\rangle\rangle=1$, multiply Eq. (13) by w_n and perform the sum upon n and σ. This gives,

$$\left[U^{exc}(\vec{r})+E_{A-1}+U^{Hrt}(\vec{r})+u_A(\vec{r})-E_A-\Delta_{\vec{r}}\right]\sqrt{\tau}=$$
$$\sum_{n\sigma}w_n\left[2\langle\langle\phi_{n\vec{r}\sigma}\left(\nabla_{\vec{r}}\phi_{n\vec{r}\sigma}\right)\rangle\rangle\cdot(\nabla_{\vec{r}}\sqrt{\tau})+\langle\langle\phi_{n\vec{r}\sigma}\left(\Delta_{\vec{r}}\phi_{n\vec{r}\sigma}\right)\rangle\rangle\sqrt{\tau}\right],(16)$$

where the "mixture excitation potential",

$$U^{exc}(\vec{r})=\sum_{n\sigma}w_n\,\langle\langle\phi^2_{n\vec{r}\sigma}\rangle\rangle\,E^{exc}_{n\sigma}(\vec{r}),\qquad(17)$$

is local and positive and the "mixture Hartree-like potential",

$$U^{Hrt}(\vec{r})=\sum_{n\sigma}w_n\,\langle\langle\phi^2_{n\vec{r}\sigma}\rangle\rangle\,U_{n\sigma}(\vec{r}),\qquad(18)$$

is also local. Because of the frequent dominance of attractive terms in v_{Aj}, it may show more negative than positive signs. Then notice that, because of Eqs. (8), and Eq. (12) with $\Psi=\phi\nabla\phi$, the sum in the rhs of Eq. (16), $\sum_{n\sigma}w_n\langle\langle\phi_{n\vec{r}\sigma}\left(\nabla_{\vec{r}}\phi_{n\vec{r}\sigma}\right)\rangle\rangle$, vanishes. Note also, from Eqs. (9), and Eq. (12) with $\Psi=\phi\Delta\phi$, that, again for the rhs of Eq. (16), the following equality holds,

$$-\sum_{n\sigma}w_n\,\langle\langle\phi_{n\vec{r}\sigma}\left(\Delta_{\vec{r}}\phi_{n\vec{r}\sigma}\right)\rangle\rangle=\sum_{n\sigma}w_n\,\langle\langle\left(\nabla_{\vec{r}}\phi_{n\vec{r}\sigma}\right)\cdot\left(\nabla_{\vec{r}}\phi_{n\vec{r}\sigma}\right)\rangle\rangle,\quad(19)$$

where, again, the symbol $\langle\langle\ \rangle\rangle$ denotes the trace $\mathrm{T}r'$, an integration upon the first $(A-1)$ coordinates together with summation upon their spins. The rhs of this equation, Eq. (19), defines a positive, local potential,

$$U^{kin}(\vec{r})=\sum_{n\sigma}w_n\,\langle\langle\left(\nabla_{\vec{r}}\phi_{n\vec{r}\sigma}\right)\cdot\left(\nabla_{\vec{r}}\phi_{n\vec{r}\sigma}\right)\rangle\rangle.\qquad(20)$$

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Finally, according to Eq. (16), the sum of local potentials, $U^{eff} = U^{exc} + U^{Hrt} + U^{kin} + u_A$, drives a Schrödinger equation for $\sqrt{\tau}$,

$$[-\Delta_{\vec{r}} + U^{eff}(\vec{r})]\sqrt{\tau(\vec{r})} = (E_A - E_{A-1})\sqrt{\tau(\vec{r})}. \qquad (21)$$

This is the expected generalization of the LPS theorem. Note that, if the $(A-1)$ particles are not identical, then E_{A-1}, the GS energy of $\mathcal{H}_{A-1}$, means here the mathematical, absolute lower bound of the operator in all subspaces of arbitrary symmetry or lack of symmetry. In practice, however, most cases imply symmetries in the $(A-1)$-space, and E_{A-1} means the ground state energy under such symmetries.

For nuclear physics, this generalization can be used in two ways:
i) The first one consists in considering hypernuclei or mesonic nuclei, where the A-th particle is indeed distinct. Theoretical calculations with local interactions for the distinct particle may be attempted while non local and/or spin dependent interactions for the $A-1$ nucleons are useful, if not mandatory. Then, obviously, the density τ refers to the hyperon or the meson and, given the neutron and proton respective numbers N and Z, wave functions ψ_n and $\phi_{n\,\vec{r},\,\sigma}$ belong to both N- and Z-antisymmetric subspaces. The energy E_{A-1} is the GS energy of nucleus $\{N, Z\}$, a fermionic GS energy, rather than the absolute lower bound of the mathematical operator $\mathcal{H}_{A-1}$ in all subspaces.
ii) The second one consists in setting all A particles to be nucleons, at the cost of restricting theoretical models to local interactions. Such models are not without interest indeed, although interactions which are spin dependent are certainly more realistic. The antisymmetric properties of the functions ψ_n are requested in both N- and Z-spaces. If the singled out, A-th coordinate is a neutron one, the density τ defined by Eq. (6) is the usual neutron density, divided by N; the functions $\phi_{n\,\vec{r}\sigma}$ are antisymmetric in the $(N-1)$-neutron space and the Z-proton space; the energy E_{A-1} now means the fermionic GS of nucleus $\{N-1, Z\}$, not that absolute, mathematical lower bound of operator $\mathcal{H}_{N-1,Z}$. Conversely, if the A-th coordinate is a proton one, then, *mutatis mutandis*, τ is the usual proton density, divided by Z, and E_{A-1} is the GS energy of nucleus $\{N, Z-1\}$.

In both cases, the Hamiltonians to be used are scalars under the rotation group, and, therefore [2], the density operators $\mathcal{D}$ considered by the RDFT are also scalars. Hence, all calculations defining U^{eff} reduce to calculations with a radial variable r only.

We shall now extend our previous results to the case where we allow spin dependence for all interactions, a most useful feature if all A particles are nucleons. Polarized eigenmixtures are also interesting and need also be considered. Hence, a generalisation of our approach, which uses the "spin-density matrix" (SDM) formalism [3] [4], is in order. The Hamiltonian may become,

$$\sum_{i=1}^{A}[-\hbar^2\Delta_{\vec{r}_i}/(2m_i) + u_i(\vec{r}_i, \vec{\sigma}_i)] + \sum_{i>j=1}^{A} v_{ij}(\vec{r}_i, \vec{\sigma}_i, \vec{r}_j, \vec{\sigma}_j). \qquad (22)$$

It allows subtle differences between neutrons and protons, besides the Coulomb interactions between protons. More explicitly, there can be two distinct one-

body potentials, u_n, u_p, namely one for neutrons and one for protons, but within the neutron space the function $u_n(\vec{r}_i, \sigma_i)$ obviously will not read $u_{ni}(\vec{r}_i, \sigma_i)$. Similarly in the proton space, the Hamiltonian contains terms $u_p(\vec{r}_i, \sigma_i)$ rather than $u_{pi}(\vec{r}_i, \sigma_i)$. The same subtlety allows terms $v_{pp}(\vec{r}_i, \sigma_i, \vec{r}_j, \sigma_j)$, $v_{pn}(\vec{r}_i, \sigma_i, \vec{r}_j, \sigma_j)$, $v_{np}(\vec{r}_i, \sigma_i, \vec{r}_j, \sigma_j)$ and $v_{pp}(\vec{r}_i, \sigma_i, \vec{r}_j, \sigma_j)$, rather than $v_{ppij}(\vec{r}_i, \sigma_i, \vec{r}_j, \sigma_j)$, ... etc. (Of course, $v_{pn} = v_{np}$.) But non localities of potentials and interactions, in the sense of explicit dependences upon momenta p_i, remain absent.

Then the A-th particle is again singled out, with degrees of freedom again labelled $\vec{r}$ and $\vec{\sigma}$, and the Hamiltonian is split as a sum, $\mathcal{K}_{A-1} + \mathcal{W}_A + k_A$, somewhat similar to the split described by Eqs. (4). For simplicity, we shall use short notations, $\mathcal{K}$, $\mathcal{W}$ and k, rather than $\mathcal{K}_{A-1}$, $\mathcal{W}_A$ and k_A. With two spin states, $\sigma = \pm 1/2$, for the A-th nucleon, we represent eigenstates ψ_n as column vectors, $\overline{\psi}_n = \begin{bmatrix} \psi_{n+} \\ \psi_{n-} \end{bmatrix}$, and operators as matrices such as, $\overline{\mathcal{W}} = \begin{bmatrix} \mathcal{W}_{++} & \mathcal{W}_{+-} \\ \mathcal{W}_{-+} & \mathcal{W}_{--} \end{bmatrix}$, $\overline{k} = \begin{bmatrix} k_{++} & k_{+-} \\ k_{-+} & k_{--} \end{bmatrix}$ and $\bar{u} = \begin{bmatrix} u_{A++} & u_{A+-} \\ u_{A-+} & u_{A--} \end{bmatrix}$. The matrix, $\overline{\mathcal{K}} = \begin{bmatrix} \mathcal{K} & 0 \\ 0 & \mathcal{K} \end{bmatrix}$, is a scalar in spin space, since $\mathcal{K}$ does not act upon the A-th particle.

The spin density matrix, $\overline{\rho}_n$, results from an integration and spin sum over the $(A-1)$-space of the matrix, $\overline{\psi}_n \times \overline{\psi}_n^T$, where the superscript ^{T} denotes transposition,

$$\overline{\rho}_n(\vec{r}) = \langle\langle \begin{bmatrix} \psi_{n+} \\ \psi_{n-} \end{bmatrix} \times [\psi_{n+} \quad \psi_{n-}] \rangle\rangle = \langle\langle \begin{bmatrix} (\psi_{n+})^2 & \psi_{n+}\psi_{n-} \\ \psi_{n-}\psi_{n+} & (\psi_{n-})^2 \end{bmatrix} \rangle\rangle. \qquad (23)$$

It depends on the last coordinate, $\vec{r}$, and its matrix elements are labelled by two values, $\{\sigma, \sigma'\}$, of the last spin. For an eigenmixture one defines, obviously, $\bar{\theta}(\vec{r}) = \sum_n w_n \overline{\rho}_n(\vec{r})$, and the trace in the last spin space, $[\theta_{++}(\vec{r}) + \theta_{--}(\vec{r})]$, is that density, $\tau(\vec{r})$, defined by Eq. (6).

The SDM, $\bar{\theta}$, is symmetric and positive semidefinite, $\forall \vec{r}$. Except for marginal situations, it is also invertible, in which case there exists a unique inverse square root, also symmetric and positive. Define, therefore, a column vector $\overline{\phi}_{n\,\vec{r}}$ of states in the $(A-1)$-space according to,

$$\overline{\phi}_{n\,\vec{r}} = \bar{\theta}^{-\frac{1}{2}}(\vec{r})\, \overline{\psi}_n. \qquad (24)$$

Then the following property,

$$\sum_n w_n \langle\langle \overline{\phi}_{n\,\vec{r}} \times \overline{\phi}_{n\,\vec{r}}^T \rangle\rangle = \bar{\theta}^{-\frac{1}{2}}(\vec{r}) \left(\sum_n w_n \langle\langle \overline{\psi}_n \times \overline{\psi}_n^T \rangle\rangle \right) \bar{\theta}^{-\frac{1}{2}}(\vec{r}) = \bar{1}, \quad (25)$$

holds $\forall \vec{r}$. Here $\bar{1}$ denotes the identity matrix. Hence, the following gradient and Laplacian properties also hold,

$$\sum_n w_n \langle\langle \left(\nabla_{\vec{r}} \begin{bmatrix} \phi_{n\,\vec{r}+} \\ \phi_{n\,\vec{r}-} \end{bmatrix} \right) \times [\phi_{n\,\vec{r}+} \quad \phi_{n\,\vec{r}-}] \rangle\rangle \quad +$$

$$\sum_n w_n \langle\langle \begin{bmatrix} \phi_{n\,\vec{r}+} \\ \phi_{n\,\vec{r}-} \end{bmatrix} \times (\nabla_{\vec{r}} [\phi_{n\,\vec{r}+} \quad \phi_{n\,\vec{r}-}]) \rangle\rangle = 0, \quad \forall \vec{r}, \qquad (26)$$

and

$$\sum_n w_n \left\langle\!\left\langle \left(\Delta_{\vec{r}} \begin{bmatrix} \phi_{n\,\vec{r}+} \\ \phi_{n\,\vec{r}-} \end{bmatrix} \right) \times [\, \phi_{n\,\vec{r}+} \quad \phi_{n\,\vec{r}-} \,] \right\rangle\!\right\rangle +$$

$$2 \sum_n w_n \left\langle\!\left\langle \left(\nabla_{\vec{r}} \begin{bmatrix} \phi_{n\,\vec{r}+} \\ \phi_{n\,\vec{r}-} \end{bmatrix} \right) \cdot (\nabla_{\vec{r}} [\, \phi_{n\,\vec{r}+} \quad \phi_{n\,\vec{r}-} \,]) \right\rangle\!\right\rangle +$$

$$\sum_n w_n \left\langle\!\left\langle \begin{bmatrix} \phi_{n\,\vec{r}+} \\ \phi_{n\,\vec{r}-} \end{bmatrix} \times (\Delta_{\vec{r}} [\, \phi_{n\,\vec{r}+} \quad \phi_{n\,\vec{r}-} \,]) \right\rangle\!\right\rangle = 0, \quad \forall \vec{r} \quad . \tag{27}$$

The eigenvector property, $\left(\overline{\mathcal{K}} + \overline{\mathcal{W}} + \overline{k} - E_A\, \overline{\mathbf{1}} \right) \overline{\psi}_n = 0$, also reads,

$$\left(\overline{\mathcal{K}} + \overline{\mathcal{W}} + \bar{u} - E_A\, \overline{\mathbf{1}} \right) \bar{\theta}^{\frac{1}{2}}(\vec{r})\, \overline{\phi}_{n\,\vec{r}} - \left[\Delta_{\vec{r}}\, \bar{\theta}^{\frac{1}{2}}(\vec{r}) \right] \overline{\phi}_{n\vec{r}} =$$

$$2 \left[\nabla_{\vec{r}}\, \bar{\theta}^{\frac{1}{2}}(\vec{r}) \right] \cdot \left(\nabla_{\vec{r}}\, \overline{\phi}_{n\,\vec{r}} \right) + \bar{\theta}^{\frac{1}{2}}(\vec{r})\, \left(\Delta_{\vec{r}}\, \overline{\phi}_{n\,\vec{r}} \right) . \tag{28}$$

Right-multiply Eq. (28) by the row vector, $\overline{\phi}_{n\,\vec{r}}^{T}$, integrate and sum over the $(A-1)$-space, weigh the result by w_n and sum upon n. Because of Eq. (25), the weighted sum of averages over the $(A-1)$-space simplifies into,

$$\left[\overline{\mathcal{U}}^{exc}(\vec{r}) + (E_{A-1} - E_A)\, \overline{\mathbf{1}} + \overline{\mathcal{U}}^{Hrt}(\vec{r}) + \bar{u}(\vec{r}) - \Delta_{\vec{r}} \right] \bar{\theta}^{\frac{1}{2}}(\vec{r}) = \sum_n w_n \times$$

$$\left\{ 2 \left[\nabla_{\vec{r}}\, \bar{\theta}^{\frac{1}{2}}(\vec{r}) \right] \cdot \left\langle\!\left\langle \left(\nabla_{\vec{r}}\, \overline{\phi}_{n\,\vec{r}} \right) \times \overline{\phi}_{n\,\vec{r}}^{T} \right\rangle\!\right\rangle + \bar{\theta}^{\frac{1}{2}}(\vec{r}) \left\langle\!\left\langle \left(\Delta_{\vec{r}} \overline{\phi}_{n\,\vec{r}} \right) \times \overline{\phi}_{n\,\vec{r}}^{T} \right\rangle\!\right\rangle \right\} , \tag{29}$$

with

$$\overline{\mathcal{U}}^{exc}(\vec{r}) = \sum_n w_n\, \left\langle\!\left\langle \left(\overline{\mathcal{K}}\, \overline{\phi}_{n\,\vec{r}} \right) \times \overline{\phi}_{n\,\vec{r}}^{T} \right\rangle\!\right\rangle - E_{A-1}\, \overline{\mathbf{1}} , \tag{30}$$

and

$$\overline{\mathcal{U}}^{Hrt}(\vec{r}) = \sum_n w_n\, \left\langle\!\left\langle \left(\overline{\mathcal{W}}\, \overline{\phi}_{n\,\vec{r}} \right) \times \overline{\phi}_{n\,\vec{r}}^{T} \right\rangle\!\right\rangle . \tag{31}$$

The rhs of Eq. (29) can be simplified, but less than that of Eq. (16). Indeed Eq. (26) does not imply that the coefficient of $\nabla_{\vec{r}}\, \bar{\theta}^{\frac{1}{2}}(\vec{r})$ vanishes. In fact this coefficient is,

$$\sum_n w_n \left\langle\!\left\langle \left(\nabla_{\vec{r}}\, \overline{\phi}_{n\vec{r}} \right) \times \overline{\phi}_{n\vec{r}}^{T} \right\rangle\!\right\rangle = \sum_n w_n \begin{bmatrix} 0 & \left\langle\!\left\langle (\nabla_{\vec{r}} \phi_{n\vec{r}+}) \phi_{n\vec{r}-} \right\rangle\!\right\rangle \\ \left\langle\!\left\langle (\nabla_{\vec{r}} \phi_{n\vec{r}-})\, \phi_{n\vec{r}+} \right\rangle\!\right\rangle & 0 \end{bmatrix}, \tag{32}$$

and Eq. (26) shows that the matrix on the rhs is antisymmetric. In turn, from Eq. (27), the "Laplacian induced coefficient" in the rhs of Eq. (29) may be listed as,

$$\sum_n w_n \left\langle\!\left\langle \left(\Delta_{\vec{r}} \overline{\phi}_{n\,\vec{r}} \right) \times \overline{\phi}_{n\,\vec{r}}^{T} \right\rangle\!\right\rangle =$$

$$-\sum_n w_n \left\langle\!\left\langle \left(\nabla_{\vec{r}} \begin{bmatrix} \phi_{n\,\vec{r}+} \\ \phi_{n\,\vec{r}-} \end{bmatrix} \right) \cdot (\nabla_{\vec{r}} [\, \phi_{n\,\vec{r}+} \quad \phi_{n\,\vec{r}-} \,]) \right\rangle\!\right\rangle + \tfrac{1}{2} \sum_n w_n \times$$

$$\left\langle\!\left\langle \left[\left(\Delta_{\vec{r}} \begin{bmatrix} \phi_{n\vec{r}+} \\ \phi_{n\vec{r}-} \end{bmatrix} \right) \times [\, \phi_{n\vec{r}+} \quad \phi_{n\vec{r}-} \,] - \begin{bmatrix} \phi_{n\vec{r}+} \\ \phi_{n\vec{r}-} \end{bmatrix} \times (\Delta_{\vec{r}} [\, \phi_{n\vec{r}+} \quad \phi_{n\vec{r}-} \,]) \right] \right\rangle\!\right\rangle \tag{33}$$

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In the rhs of Eq. (33), the similarity of its first term with potential U^{kin}, Eq. (19), is transparent. Also transparent is the antisymmetry of the second term. With the definitions,

$$\overline{\mathcal{U}}^{kin}(\vec{r}) = \sum_n w_n \left\langle\!\left\langle \left(\nabla_{\vec{r}} \overline{\phi}_{n\,\vec{r}}\right) \cdot \left(\nabla_{\vec{r}} \overline{\phi}^T_{n\,\vec{r}}\right) \right\rangle\!\right\rangle, \tag{34}$$

$$\overline{\mathcal{U}}^{ant}(\vec{r}) = \frac{1}{2} \sum_n w_n \left\langle\!\left\langle \left[\left(\Delta_{\vec{r}} \overline{\phi}_{n\,\vec{r}}\right) \times \overline{\phi}^T_{n\,\vec{r}} - \overline{\phi}_{n\,\vec{r}} \times \left(\Delta_{\vec{r}} \overline{\phi}^T_{n\,\vec{r}}\right)\right] \right\rangle\!\right\rangle, \tag{35}$$

and

$$\overline{\mathcal{U}}^{grd}(\vec{r}) = 2 \sum_n w_n \begin{bmatrix} 0 & \left\langle\!\left\langle \left(\nabla_{\vec{r}} \phi_{n\vec{r}+}\right) \phi_{n\vec{r}-} \right\rangle\!\right\rangle \\ \left\langle\!\left\langle \left(\nabla_{\vec{r}} \phi_{n\vec{r}-}\right) \phi_{n\vec{r}+} \right\rangle\!\right\rangle & 0 \end{bmatrix}, \tag{36}$$

the Schrödinger equation for the square root of the spin density matrix reads,

$$\left[\overline{\mathcal{U}}^{exc} + \overline{\mathcal{U}}^{Hrt} + \bar{u} + \overline{\mathcal{U}}^{kin} - \overline{\mathcal{U}}^{ant} - \Delta\right] \bar{\theta}^{\frac{1}{2}} - \overline{\mathcal{U}}^{grd} \cdot \nabla \bar{\theta}^{\frac{1}{2}} = (E_A - E_{A-1}) \bar{\theta}^{\frac{1}{2}}. \tag{37}$$

This concludes our generalizations of the LPS theorem. On the one hand, see Eq. (21), we obtained for the square root density of an eigenmixture a Schrödinger equation, most similar to the LPS equation. On the other hand, at the cost of a slightly less simple result, we also obtained, see Eq. (37), an LPS-like equation that drives the square root of the spin density matrix.

This opens a completely new zoology of local, effective potentials, of which very little is known, but the interest of which is obvious, since they drive a reasonably easily measurable observable, the square root of an eigenmixture density, which depends on one degree of freedom $\vec{r}$ only. A connection of such potentials with optical potentials, or rather their real parts, is likely, but yet remains an open problem.

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