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

B. G. Giraud* and P. Moussa†

Institut de Physique Théorique, Direction des Sciences de la Matière, CEA-Saclay, F-91191 Gif-sur-Yvette, France

(Received 12 June 2009; revised manuscript received 10 May 2010; published 2 August 2010)

We generalize a "one-eigenstate" version of the density square root theorem 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, a consequence of the rotational invariance of the nuclear Hamiltonian; when nuclear ground states have a finite spin, the RDFT uses eigenmixture density operators to simplify predictions of ground-state energies into one-dimensional, radial calculations. We also study Schrödinger equations governing spin eigendensity matrices.

DOI: 10.1103/PhysRevC.82.024301 PACS number(s): 21.60.Jz, 31.15.E−, 71.15.Mb

I. INTRODUCTION

It has been noticed by many authors [1–8] that, when basic interactions are local, the square root of the density of an eigenstate can be driven by a Schrödinger equation. The theorem may be described as follows:

(i) Let H_A be a Hamiltonian for A identical particles, with individual mass m:

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

(ii) Consider a ground-state (g.s.) eigenfunction of H_A, $\psi(\vec{r}_1, \sigma_1, \vec{r}_2, \sigma_2, \ldots, \vec{r}_A, \sigma_A)$, 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,

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

(iv) Then there exists a local potential $v_{\text{eff}}(\vec{r})$ such that

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

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

Reasonings leading to such a theorem belong, schematically, to three complementary approaches, namely, (1) the consideration of density functionals related to von Weizsäcker's functional and then a change of unknown function from ρ to $\sqrt{\rho}$ [1,3,7], (2) interpretations of squared wave functions as probabilities (conditional, marginal, etc.) [2,6,8], and (3) more direct derivations [4,5,7], including that from the A-body Schrödinger equation [4,6]. In Ref. [8], an equation driving ρ, extending the Thomas-Fermi approach, is also obtained. The corresponding effective potential, incidentally, must not be confused with the Kohn-Sham potential; the latter rather drives those orbitals out of which ρ later results as a by-product; however, see Ref. [9] for a relation between the Kohn-Sham equations and the equation driving $\sqrt{\rho}$. Beyond these approaches, the quantal density functional theory [10] offers a detailed analysis of all the kinetic, potential, and correlation energies.

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 ground states ψ_n? Many authors [11–17] have been interested in mixtures of degenerate eigenstates or have also considered nondegenerate ones, if only for extensions of the Rayleigh-Ritz variational principle to calculation of excited energies. But the *simultaneous* consideration of (1) degenerate mixtures and (2) the square root of their density has not yet, to our knowledge, received explicit attention. The degeneracy situation is of wide interest in nuclear physics for doubly odd nuclei, the ground states 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 radial density functional theory (RDFT) [17] 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 ground states ψ_{JM}. More generally, it is easily seen that the argument that follows holds for a degenerate multiplet of excited states as well.

This article proves the generalization for the square root of the density of a mixture of degenerate eigenstates by closely following the argument used for one eigenstate only [4]. In Sec. II, the proof for generalization is given for the case where spins are summed upon. In Sec. III, the generalization is extended to mixtures that retain spin information by means of a spin-density matrix, the square root of which is shown to obey a matrix Schrödinger equation. A short discussion and conclusion make up Sec. IV.

*bertrand.giraud@cea.fr
†pierre.moussa@cea.fr

II. MIXTURES OF DEGENERATE EIGENSTATES

Given A particles and their Hamiltonian, a generalization for degenerate mixtures can be obtained without the 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 $\vec{r}_i$. We single out the Ath particle, with its degrees of freedom labeled $\vec{r}$ and $\vec{\sigma}$ rather than $\vec{r}_A$ and $\vec{\sigma}_A$. For a theorem of maximal generality, with distinct masses and one- and two-body potentials, our Hamiltonian may become $\mathcal{H}_A = \mathcal{H}_{A-1} + \mathcal{V}_A + h_A$, with

$$\begin{aligned}\mathcal{H}_{A-1} &= \sum_{i=1}^{A-1}[-\hbar^2\Delta_{\vec{r}_i}/(2m_i) + u_i(\vec{r}_i, \vec{p}_i, \vec{\sigma}_i)] \\ &\quad + \sum_{i>j=1}^{A-1} v_{ij}(\vec{r}_i, \vec{p}_i, \vec{\sigma}_i, \vec{r}_j, \vec{p}_j, \vec{\sigma}_j), \\ \mathcal{V}_A &= \sum_{j=1}^{A-1} v_{Aj}(\vec{r}, \vec{r}_j, \vec{p}_j, \vec{\sigma}_j), \\ h_A &= -\hbar^2\Delta_{\vec{r}}/(2m_A) + u_A(\vec{r}).\end{aligned} \tag{4}$$

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

As in the one-eigenstate case [4], we select situations where there exists a representation in which, simultaneously, the Hermitian Hamiltonian $\mathcal{H}_A$ and all the eigenfunctions $\psi(\vec{r}_1, \sigma_1, \ldots, \vec{r}_A, \sigma_A)$ 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 $\mathcal{H}_A$. Because the degeneracy multiplicity is larger than 1, we select $\mathcal{N} \geqslant 2$ of the corresponding eigenfunctions ψ_n, orthonormalized. Their set may be either complete or incomplete in the eigensubspace. The density operators,

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

with otherwise arbitrary, positive weights w_n, are normalized to unity, $\mathrm{Tr}\,\mathcal{D} = 1$, 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,

$$\begin{aligned}\tau(\vec{r}) = \sum_{n=1}^{\mathcal{N}} w_n \sum_{\sigma_1\ldots\sigma_{A-1}\sigma} \int d\vec{r}_1 \cdots d\vec{r}_{A-1} \\ \times [\psi_n(\vec{r}_1, \sigma_1, \ldots, \vec{r}_{A-1}, \sigma_{A-1}, \vec{r}, \sigma)]^2,\end{aligned} \tag{6}$$

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

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

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 over the first $A-1$ coordinates and sum upon the first $A-1$ spins. Because 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

$$\begin{aligned}&\sum_{n\,\sigma\,\sigma_1\cdots\sigma_{A-1}} \int d\vec{r}_1 \cdots d\vec{r}_{A-1} w_n\ \phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, \ldots, \vec{r}_{A-1}, \sigma_{A-1}) \\ &\quad \times \nabla_{\vec{r}}\,\phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, \ldots, \vec{r}_{A-1}, \sigma_{A-1}) = 0\,,\end{aligned} \tag{8}$$

and

$$\begin{aligned}&\sum_{n\,\sigma\,\sigma_1\cdots\sigma_{A-1}} \int d\vec{r}_1 \cdots d\vec{r}_{A-1} w_n \\ &\quad \times \{[\nabla_{\vec{r}}\,\phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, \ldots, \vec{r}_{A-1}, \sigma_{A-1})]^2 \\ &\quad + \phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, \ldots, \vec{r}_{A-1}, \sigma_{A-1}) \\ &\quad \times \Delta_{\vec{r}}\,\phi_{n\vec{r}\sigma}(\vec{r}_1, \sigma_1, \ldots, \vec{r}_{A-1}, \sigma_{A-1})\} = 0.\end{aligned} \tag{9}$$

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

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

This also reads

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

The right-hand side (rhs) of Eq. (11) occurs because the Laplacian, $\Delta_{\vec{r}}$, present in h_A, also acts 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, avoiding 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:

$$\begin{aligned}\langle\langle\Psi_{n\vec{r}\sigma}\rangle\rangle = \sum_{\sigma_1\cdots\sigma_{A-1}} \int d\vec{r}_1 \cdots d\vec{r}_{A-1} \\ \times \Psi_{n\vec{r}\sigma}(r_1, \sigma_1, \ldots, r_{A-1}, \sigma_{A-1}).\end{aligned} \tag{12}$$

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

$$\begin{aligned}&\langle\langle\phi^2_{n\vec{r}\sigma}\rangle\rangle\big[E^{\mathrm{exc}}_{n\sigma}(\vec{r}) + E_{A-1} + U_{n\sigma}(\vec{r}) + u_A(\vec{r}) - E_A - \Delta_{\vec{r}}\big]\sqrt{\tau(\vec{r})} \\ &\quad = 2\,\langle\langle\phi_{n\vec{r}\sigma}\,(\nabla_{\vec{r}}\,\phi_{n\vec{r}\sigma})\rangle\rangle\cdot[\nabla_{\vec{r}}\sqrt{\tau(\vec{r})}] \\ &\qquad + \langle\langle\phi_{n\vec{r}\sigma}\,(\Delta_{\vec{r}}\,\phi_{n\vec{r}\sigma})\rangle\rangle\sqrt{\tau(\vec{r})},\end{aligned} \tag{13}$$

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

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

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

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

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 obtained explicitly as the sum of the g.s. energy E_{A-1} of $\mathcal{H}_{A-1}$ and a positive excitation energy $E^{\rm exc}_{n\sigma}(\vec{r})$. From Eq. (15), the Hartree nature of the potential $U_{n\sigma}(\vec{r})$ is transparent.

Keeping in mind that the density operator $\mathcal{D}'$ is normalized to unity $\forall\vec{r}$, 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

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

where the "mixture excitation potential"

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

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

$$U^{\rm Hart}(\vec{r})=\sum_{n\sigma} w_n\left\langle\left\langle\phi^2_{n\,\vec{r}\,\sigma}\right\rangle\right\rangle U_{n\sigma}(\vec{r}), \quad (18)$$

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 on the rhs of Eq. (16), $\sum_{n\sigma} w_n\langle\langle\phi_{n\,\vec{r}\,\sigma}\,(\nabla_{\vec{r}}\,\phi_{n\,\vec{r}\,\sigma})\rangle\rangle$, 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:

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

where, again, the symbol $\langle\langle\rangle\rangle$ denotes the trace Tr′, 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:

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

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

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

This is the expected generalization of the one-eigenstate theorem. Note that, if the $A-1$ particles are not identical, then E_{A-1}, the g.s. energy of $\mathcal{H}_{A-1}$, denotes 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} denotes the ground-state energy under such symmetries. For nuclear physics, this generalization can be used in two ways.

The first one consists of considering hypernuclei or mesonic nuclei, where the Ath particle is indeed distinct. Theoretical calculations with local interactions for the distinct particle may be attempted while nonlocal 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 respective neutron and proton 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 g.s. energy of the nucleus $\{N,Z\}$, a fermionic g.s. energy, rather than the absolute lower bound of the mathematical operator $\mathcal{H}_{A-1}$ in all subspaces.

The second one consists of setting all A particles to be nucleons, at the cost of restricting theoretical models to local interactions. Such models are indeed not without interest, although interactions that 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 Ath 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 denotes the fermionic g.s. of the nucleus $\{N-1,Z\}$, not that absolute, mathematical lower bound of operator $\mathcal{H}_{N-1,Z}$. Conversely, if the Ath coordinate is a proton one, then, with the respective differences having been considered, τ is the usual proton density, divided by Z, and E_{A-1} is the g.s. energy of the nucleus $\{N,Z-1\}$.

In both cases, the Hamiltonians to be used are scalars under the rotation group and, therefore [17], the density operators $\mathcal{D}$ considered by the RDFT are also scalars. Hence, all calculations defining $U^{\rm eff}$ reduce to calculations with a radial variable r only.

III. GENERALIZATION FOR A SPIN-DENSITY MATRIX

We 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 must also be considered. Hence, a generalization of our approach, which uses the spin-density matrix (SDM) formalism [18,19], is in order. The Hamiltonian may become

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

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 and 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 does 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 $v_{ppij}(\vec{r}_i, \sigma_i, \vec{r}_j, \sigma_j), \ldots$. (Of course, $v_{pn} = v_{np}$.) But nonlocalities of potentials and interactions, in the sense of explicit dependences upon momenta p_i, remain absent.

Then the Ath particle is again singled out, with degrees of freedom again labeled $\vec{r}$ 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 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 Ath nucleon, we represent eigenstates ψ_n as column vectors, $\overline{\psi}_n = [\begin{smallmatrix}\psi_{n+}\\ \psi_{n-}\end{smallmatrix}]$, and operators as matrices such as

$$\overline{\mathcal{W}} = \begin{bmatrix} \mathcal{W}_{++} & \mathcal{W}_{+-} \\ \mathcal{W}_{-+} & \mathcal{W}_{--} \end{bmatrix}, \quad \overline{k} = \begin{bmatrix} k_{++} & k_{+-} \\ k_{-+} & k_{--} \end{bmatrix},$$

$$\text{and} \quad \bar{u} = \begin{bmatrix} u_{A++} & u_{A+-} \\ u_{A-+} & u_{A--} \end{bmatrix}.$$

The matrix $\overline{\mathcal{K}} = [\begin{smallmatrix}\mathcal{K} & 0\\ 0 & \mathcal{K}\end{smallmatrix}]$ is a scalar in spin space, since $\mathcal{K}$ does not act upon the Ath 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:

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

It depends on the last coordinate, $\vec{r}$, and its matrix elements are labeled 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

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

Then the following property,

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

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

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

and

$$\sum_n w_n \left\langle\!\!\left\langle \left(\Delta_{\vec{r}} \begin{bmatrix} \phi_{n\vec{r}+} \\ \phi_{n\vec{r}-} \end{bmatrix} \right) \times [\phi_{n\vec{r}+} \quad \phi_{n\vec{r}-}] \right\rangle\!\!\right\rangle + 2 \sum_n w_n \left\langle\!\!\left\langle \left(\nabla_{\vec{r}} \begin{bmatrix} \phi_{n\vec{r}+} \\ \phi_{n\vec{r}-} \end{bmatrix} \right) \cdot (\nabla_{\vec{r}} [\phi_{n\vec{r}+} \quad \phi_{n\vec{r}-}]) \right\rangle\!\!\right\rangle + \sum_n w_n \left\langle\!\!\left\langle \begin{bmatrix} \phi_{n\vec{r}+} \\ \phi_{n\vec{r}-} \end{bmatrix} \times (\Delta_{\vec{r}} [\phi_{n\vec{r}+} \quad \phi_{n\vec{r}-}]) \right\rangle\!\!\right\rangle = 0, \quad \forall \vec{r}. \tag{27}$$

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

$$(\overline{\mathcal{K}} + \overline{\mathcal{W}} + \bar{u} - E_A\, \bar{\mathbf{1}})\, \bar{\theta}^{\frac{1}{2}}(\vec{r})\, \overline{\phi}_{n\vec{r}} - \left[\Delta_{\vec{r}}\, \bar{\theta}^{\frac{1}{2}}(\vec{r})\right] \overline{\phi}_{n\vec{r}} = 2\left[\nabla_{\vec{r}}\, \bar{\theta}^{\frac{1}{2}}(\vec{r})\right] \cdot (\nabla_{\vec{r}}\, \overline{\phi}_{n\vec{r}}) + \bar{\theta}^{\frac{1}{2}}(\vec{r})(\Delta_{\vec{r}}\, \overline{\phi}_{n\vec{r}}). \tag{28}$$

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 over n. Because of Eq. (25), the weighted sum of averages over the $A-1$ space simplifies to

$$[\overline{\mathcal{U}}^{\text{exc}}(\vec{r}) + (E_{A-1} - E_A)\, \bar{\mathbf{1}} + \overline{\mathcal{U}}^{\text{Hart}}(\vec{r}) + \bar{u}(\vec{r}) - \Delta_{\vec{r}}]\, \bar{\theta}^{\frac{1}{2}}(\vec{r}) = \sum_n w_n \left\{ 2\left[\nabla_{\vec{r}}\, \bar{\theta}^{\frac{1}{2}}(\vec{r})\right] \cdot \left\langle\!\!\left\langle (\nabla_{\vec{r}}\, \overline{\phi}_{n\vec{r}}) \times \overline{\phi}_{n\vec{r}}^T \right\rangle\!\!\right\rangle + \bar{\theta}^{\frac{1}{2}}(\vec{r}) \left\langle\!\!\left\langle (\Delta_{\vec{r}}\, \overline{\phi}_{n\vec{r}}) \times \overline{\phi}_{n\vec{r}}^T \right\rangle\!\!\right\rangle \right\}, \tag{29}$$

with

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

and

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

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

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

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,

$$\sum_n w_n \langle\!\langle (\Delta_{\vec r}\,\overline{\phi}_{n\vec r}) \times \overline{\phi}^T_{n\vec r} \rangle\!\rangle$$
$$= -\sum_n w_n \left\langle\!\!\left\langle \left(\nabla_{\vec r} \begin{bmatrix} \phi_{n\vec r+} \\ \phi_{n\vec r-} \end{bmatrix}\right) \cdot (\nabla_{\vec r}[\phi_{n\vec r+}\ \ \phi_{n\vec r-}]) \right\rangle\!\!\right\rangle$$
$$+ \frac{1}{2}\sum_n w_n \left\langle\!\!\left\langle \left[\left(\Delta_{\vec r} \begin{bmatrix} \phi_{n\vec r+} \\ \phi_{n\vec r-} \end{bmatrix}\right) \times [\phi_{n\vec r+}\ \ \phi_{n\vec r-}] \right.\right.$$
$$\left.\left. - \begin{bmatrix} \phi_{n\vec r+} \\ \phi_{n\vec r-} \end{bmatrix} \times (\Delta_{\vec r}[\phi_{n\vec r+}\ \ \phi_{n\vec r-}]) \right]\right\rangle\!\!\right\rangle. \tag{33}$$

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

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

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

and

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

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

$$[\overline{\mathcal{U}}^{\rm exc} + \overline{\mathcal{U}}^{\rm Hart} + \bar u + \overline{\mathcal{U}}^{\rm kin} - \overline{\mathcal{U}}^{\rm ant} - \Delta]\,\bar\theta^{\frac12} - \overline{\mathcal{U}}^{\rm grd} \cdot \nabla\bar\theta^{\frac12} = (E_A - E_{A-1})\,\bar\theta^{\frac12}. \tag{37}$$

IV. DISCUSSION AND CONCLUSION

We found two generalizations of the one-eigenstate 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 one-eigenstate equation. On the other hand, at the cost of a slightly less simple result, we also obtained [see Eq. (37)] a somewhat similar equation to drive the square root of the spin-density matrix.

One may ask whether the densities, or spin densities, obtained from degenerate mixtures are v representable and, for that matter, whether their Kohn-Sham v [20] is finite everywhere, shows cusps, etc. [9]. This representability question was raised for electronic densities [21,22], with the result that interacting v representability does not hold, but ensemble v representability is satisfied. See Ref. [23] for the topologies relevant to ensemble v representability. Similar issues can be raised for nuclear densities, and have not yet been investigated. Anyhow, representability questions are not very relevant in the context of the present work, because (1) of the very existence of that "$v_{\rm eff}$ driver of $\rho^{\frac12}$," directly derived from the many-body Schrödinger equation through the proofs offered by this paper, and (2) it is indeed $\rho^{\frac12}$ that is being studied here, not ρ.

The formal derivations used in this paper seem to be too unwieldy to guide actual implementations of effective potentials for $\rho^{\frac12}$ and $\bar\theta^{\frac12}$. The quantal density functional theory [10] offers a possible construction (see Ref. [24]). In addition, nuclear physics is also familiar with empirical approaches, such as the parametrization of optical potentials. Because of the presence of a Hartree-like term, $U^{\rm Hrt}$ or $\mathcal{U}^{\rm Hrt}$, in the elementary proofs shown here, a connection of such Hartree-like terms with optical potentials, or rather their real parts, is likely. The nuclear literature about optical potentials for nucleon-nucleus collisions, involving spin terms if necessary, is very rich. Extended parametrizations can be tested with models of already-known densities. Among many possible papers on the subject of nuclear optical potentials, we can quote a review [25] of those for low-energy nucleon-nucleus scattering, for the obvious reason that bound orbitals are dominated by low- or moderate-energy components.

This article opens a completely new zoology of nuclear, local, effective potentials. Little of them is known at present, but their interest is obvious, because they drive a reasonably easily measurable observable, the square root of an eigenmixture density. The latter depends on one degree of freedom, $r = |\vec r|$, only. It can be stressed again that the radial, one-dimensional formalism of the RDFT holds for deformed as well as spherical nuclei. This should bring a considerable simplification for practical calculations.

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