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Scalar nature of the nuclear density functional

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Abstract

Because of the rotational invariance of the nuclear Hamiltonian, there exists a density functional (DF) for nuclei that depends only on two scalar densities. Practical calculations boil down to radial, one-dimensional ones.

Let $Z, N, A \equiv Z + N$ be the proton, neutron and mass numbers, respectively. The nuclear Hamiltonian H is known to be invariant under rotations. Therefore, besides Z and N , nuclear ground states (GSs) carry good quantum numbers, J and M , for the total angular momentum and its z -component. Two cases occur : either $J = 0$, hence the GS is not degenerate and its density is isotropic, or $J > 0$, hence one sees a trivial degeneracy for a magnetic multiplet of GSs, the densities of which, non isotropic, contain multipole components [1] [2] up to order $2J$, with the same monopole for all members of the multiplet.

In any case, the ensemble density operator for the GS(s) of a given nucleus,

$$\mathcal{B}_{ZN} = (2J + 1)^{-1} \sum_M |ZNJM\rangle \langle ZN JM|, \quad (1)$$

is a scalar under rotations. In any case also, the GS energy obtains by,

$$E_{ZN} = \text{Tr } \mathcal{B}_{ZN} H. \quad (2)$$

Every spherical harmonic function, except a monopole, integrates out to zero. Therefore, only the monopole components of the proton and neutron densities contribute to the density normalizations which identify a nucleus,

$$\int_0^\infty r^2 dr \rho_{p0}(r) = Z, \quad \int_0^\infty r^2 dr \rho_{n0}(r) = N, \quad (3)$$

the position r being here taken as a scalar rather than a vector. In the following, for conciseness, we omit the subscript 0 and often denote ρ the pair $\{\rho_p, \rho_n\}$.

Consider the “density constrained search” [3] [4] for a minimal energy,

$$\text{Inf}_{\rho \rightarrow \{Z, N\}} \left[(\text{Inf}_{\mathcal{B} \rightarrow \rho} \text{Tr } \mathcal{B} H) + \int_0^\infty r^2 dr [u_p(r) \rho_p(r) + u_n(r) \rho_n(r)] \right], \quad (4)$$

where it is understood that the many-body density operator \mathcal{B} is restricted to be a scalar under rotations. Also u_p and u_n are scalar. With two distinct densities ρ_p, ρ_n , two potentials are needed to represent the external potential used by the Hohenberg-Kohn [5] theorem as a functional Lagrange multiplier to constrain the density. Notice that now we do not put subscripts Z, N to \mathcal{B} , because the normalizations, Eqs. (3), are implemented at the stage of the “outer” minimization. At the “inner” stage, N and Z do not need to be integers.

This inner minimization, $\text{Inf}_{\mathcal{B} \rightarrow \rho}$, defines a density functional,

$$F[\rho] \equiv \text{Inf}_{\mathcal{B} \rightarrow \rho} \text{Tr } \mathcal{B} H, \quad (5)$$

and, in that sector defined by the additional constraints, Eqs. (3), with now Z and N physical integers, the GS energy of a nucleus results from,

$$E_{ZN} = \text{Inf}_{\rho} F[\rho], \quad \int_0^{\infty} r^2 dr \rho_p(r) = Z, \quad \int_0^{\infty} r^2 dr \rho_n(r) = N. \quad (6)$$

It seems, therefore, that Eqs. (5) and (6) provide the basis of a fulfilled nuclear DF theory (DFT) in radial space, a symmetrized theory *à la* Görling [6].

However, one must first remove an ambiguity in the definition of the degree of freedom r and the associated density $\rho(r)$. For A nucleons, the simplest set of degrees of freedom are the single nucleon coordinates $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A$ and the simplest definition of the density consists in integrating out all of them but one,

$$\rho(\vec{r}) = A \int d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_{A-1} |\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{A-1}, r)|^2. \quad (7)$$

But, as discussed by [7], it is more physical to use a density $\sigma(\vec{r} - \vec{R})$, measured from the center-of-mass (CM) coordinate $\vec{R} = (\vec{r}_1 + \dots + \vec{r}_A)/A$ of the nucleus, rather than the density $\rho(\vec{r})$, defined in the laboratory frame. Since H is also translation invariant, the wave function for A nucleons is rather an “internal” one, $\psi_{int}(\vec{\xi}_1, \dots, \vec{\xi}_{A-1})$, of $(A-1)$ Jacobi coordinates only, $\vec{\xi}_1 = \vec{r}_2 - \vec{r}_1$, $\vec{\xi}_2 = \vec{r}_3 - (\vec{r}_2 + \vec{r}_1)/2$, \dots , $\vec{\xi}_{A-1} = \vec{r}_A - (\vec{r}_{A-1} + \vec{r}_{A-2} + \dots + \vec{r}_1)/(A-1)$.

It turns out that the last Jacobi coordinate is proportional to $\vec{r}_A - \vec{R}$, namely, $\vec{\xi}_{A-1} = \frac{A}{A-1}(\vec{r}_A - \vec{R})$. Except for trivial scaling factors, the “internal” density appears naturally to be,

$$\sigma(\vec{\xi}) = A \int d\vec{\xi}_1 d\vec{\xi}_2 \dots d\vec{\xi}_{A-2} |\psi_{int}(\vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_{A-2}, \vec{\xi})|^2. \quad (8)$$

Strictly speaking, what we called $F[\rho]$ should rather be a functional of σ . Unfortunately, there is no need to stress that calculations with Jacobi coordinates are much more complicated than calculations in the laboratory frame.

The solution found in [8] to link internal density σ and laboratory density ρ consists in trapping the CM by a harmonic potential. The Hamiltonian becomes,

$$\mathcal{H} = \sum_{i=1}^A \frac{p_i^2}{2m} + \frac{Km}{2} \left(\sum_{i=1}^A \vec{r}_i \right)^2 + \sum_{i>j=1}^A v_{ij} + \sum_{i>j>k=1}^A w_{ijk}. \quad (9)$$

Here v is the usual two-body interaction, and one can also include a three-body interaction w or even the luxury of more-body ones. Except for the trap, Galilean invariance is requested; no density dependence in v, w, \dots is allowed.

The trap is parametrized by an arbitrary, but fixed constant K , to be chosen for maximum convenience of practical calculations. The term, $Km \left(\sum_{i=1}^A \vec{r}_i \right)^2$, can also be written as, $Am\omega^2 R^2$, with the CM coordinate $\vec{R} = A^{-1} \sum_{i=1}^A \vec{r}_i$ and $\omega = \sqrt{KA}$; the CM frequency depends on the mass number A . The same form also shows that the trap is the sum of a one-body and a two-body operators, representable in second quantization without coefficients depending on A ,

$$\frac{K m}{2} \left(\sum_{i=1}^A \vec{r}_i \right)^2 = \frac{K m}{2} \left(\sum_{i=1}^A r_i^2 + 2 \sum_{i>j=1}^A \vec{r}_i \cdot \vec{r}_j \right). \quad (10)$$

In each sector specified by integer Z and N , the GS(s) of \mathcal{H} factorize(s) as product(s) of a common Gaussian Γ for the CM and internal wave function(s) of the $(A-1)$ Jacobi coordinates,

$$\Psi(\vec{r}_1, \dots, \vec{r}_A) = \Gamma(R) \psi_{int}(\vec{\xi}_1, \dots, \vec{\xi}_{A-1}), \quad \Gamma(R) = \pi^{-\frac{3}{4}} b^{-\frac{3}{2}} \exp \left[-\frac{R^2}{2b^2} \right], \quad (11)$$

with $b = [\hbar/(Am\omega)]^{\frac{1}{2}}$. The Gaussian is rotation invariant. Its does not perturb the physical quantum numbers J, M when \mathcal{H} is substituted for H .

As shown in [8] the link between ρ and σ is a trivial, invertible convolution,

$$\rho(\vec{r}) = \frac{A^3}{(A-1)^3} \int d\vec{R} [\Gamma(R)]^2 \sigma \left[\frac{A}{A-1} (\vec{r} - \vec{R}) \right]. \quad (12)$$

This link is the same for any member of a magnetic multiplet. Hence it extends to the scalar densities ρ and σ provided by that kind of ensemble described by Eq. (1). The vector coordinates we used temporarily to handle the non isotropic densities of individual members of a magnetic multiplet can be reduced again to scalars. The convolution, $\rho = \Gamma^2 * \sigma$, see Eq. (12), actually becomes,

$$r \rho(r) = \frac{2 \pi^{-\frac{1}{2}} A^3}{(A-1)^3 b} \int_0^\infty ds \exp \left[-\frac{r^2 + s^2}{b^2} \right] \sinh \left[\frac{2rs}{b^2} \right] s \sigma \left[\frac{A}{A-1} s \right]. \quad (13)$$

Since it is easy to second quantize \mathcal{H} and use the laboratory proton and neutron densities, $\rho_p(r) = \text{Tr } \mathcal{B} c_{pr}^\dagger c_{pr}$, $\rho_n(r) = \text{Tr } \mathcal{B} c_{nr}^\dagger c_{nr}$, where, with obvious notations, we have introduced proton and neutron creation and annihilation operators at a scalar position r , traces upon scalar density operators can be calculated in Fock space. Then one only tunes Eqs. (6) into,

$$E_{ZN} + \frac{1}{2} \hbar \sqrt{KA} = \text{Inf}_\rho \mathcal{F}[\rho], \quad \int_0^\infty r^2 dr \rho_p(r) = Z, \quad \int_0^\infty r^2 dr \rho_n(r) = N. \quad (14)$$

We conclude by claiming that a DFT for nuclei energies (and every other scalar) is available with *scalar* densities. Practical designs of a nuclear DF,

$\mathcal{F}[\rho] \equiv \text{Inf}_{\mathcal{B} \rightarrow \rho} \text{Tr } \mathcal{B} \mathcal{H}$, simultaneously valid for doubly even, odd and doubly odd nuclei, can be attempted in the laboratory radial frame.

From a DFT, one expects densities and energies. At the cost of ignoring density multipoles¹ other than monopoles, our approach does provide formally *exact* energies, in a most simplified, one-dimensional theory. A major problem of nuclear physics is the prediction of exotic nuclei. Our result is of a special interest for the study of the neutron drip line, where neutron halos are notoriously difficult to describe. Dimensional reduction should make it easier to better focus the theory on the design² of the functional \mathcal{F} , a still formidable problem. Whether the same reduction to “radial pictures” might also simplify the non local [10] versions of the DFT, in particular the quasi-local versions derived from Skyrme force models and labelled “energy density” theories, is likely.

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¹The wave function multipoles, nonetheless, contribute to the density monopole.

²See [9] for expansions of densities in polynomials constrained by matter conservation.