

The nuclear Energy Density Functional formalism

Practice solutions

Deriving the EDF from the (simplified) two-body Skyrme pseudo-potential

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I. INTRODUCTION

The aim of the present practice is to derive the Energy Density Functional (EDF) from a simplified two-body Skyrme pseudo-potential v^{sk} . Such an example provides the base-line for more realistic EDF parameterizations. We derive in the second part, through functional derivatives of the EDF, the one-body field h that drives the effective single-particle shell structure. Finally, we apply the results thus obtained to the calculation of the equation of state (EOS) of infinite nuclear matter.

A. Energy of the system

The key degree of freedom, i.e. variable, in the problem is given by the so-called one-body density matrix

$$\rho_{ij} \equiv \frac{\langle \Phi | c_j^\dagger c_i | \Phi \rangle}{\langle \Phi | \Phi \rangle} , \quad (1)$$

where $\{c_j^\dagger, c_j\}$ denote creation and annihilation operators in an arbitrary single-particle basis $\{\varphi_i\}$ whereas $|\Phi\rangle$ is the reference product-state. In the present case where pairing correlations are omitted, such a product state takes the form of a Slater determinant

$$|\Phi\rangle \equiv \prod_{\alpha=1}^N a_\alpha^\dagger |0\rangle , \quad (2)$$

where $\{a_\alpha^\dagger, a_\alpha\}$ denote creation and annihilation operators in the basis $\{\psi_\alpha\}$ making ρ diagonal. Derivations below are performed in the arbitrary basis of reference $\{\varphi_i\}$ but that results can eventually be written in basis $\{\psi_\alpha\}$ (see Sec. IV for an example).

We start from a (effective) Hamilton operator

$$H_{\text{eff}} = \sum_{ij} t_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{ijkl} v_{ijkl}^{\text{sk}} c_i^\dagger c_j^\dagger c_l c_k , \quad (3)$$

where $t_{ij} \equiv \langle i | t | j \rangle$ and $v_{ijkl}^{\text{sk}} \equiv \langle 1 : i ; 2 : j | v^{\text{sk}} | 1 : k ; 2 : l \rangle$ denote matrix elements of the kinetic energy operator and of the two-body Skyrme pseudo-potential, i.e. the effective interaction, in basis $\{\varphi_i\}$. Given H_{eff} and using Wick's theorem [1, 2], the energy computed as an *effective* Hartree-Fock expression

$$\mathcal{E}[\rho] \equiv E_{\text{eff}}^{\text{HF}} = \frac{\langle \Phi | H_{\text{eff}} | \Phi \rangle}{\langle \Phi | \Phi \rangle} , \quad (4)$$

reads as a *functional* of the one-body density matrix taking the form

$$\mathcal{E}[\rho] = \mathcal{E}_{\text{kin}}^\rho + \mathcal{E}_{\text{sk}}^{\rho\rho} = \sum_{ij} t_{ij} \rho_{ji} + \frac{1}{2} \sum_{ijkl} \bar{v}_{ijkl}^{\text{sk}} \rho_{ki} \rho_{lj} , \quad (5)$$

where $\bar{v}_{ijkl}^{\text{sk}} \equiv v_{ijkl}^{\text{sk}} - v_{ijlk}^{\text{sk}}$ such that the direct and exchange contributions are grouped together. In the following, we omit spin and isospin degrees of freedom, except otherwise specified. Such an omission simplifies the analytical computation tremendously without preventing one from understanding the key steps of the derivation.

B. Coordinate-space matrix elements

The one-body kinetic energy operator is defined through its coordinate-space matrix elements

$$\langle \vec{r} | t | \vec{r}' \rangle = \langle \vec{r} | \frac{\vec{p}^2}{2m} | \vec{r}' \rangle = -\frac{\hbar^2}{2m} \delta(\vec{r} - \vec{r}') \Delta . \quad (6)$$

The simplified two-body Skyrme pseudo-potential v^{sk} used presently neglects tensor, spin-orbit and Coulomb components. It is defined through its non-antisymmetrized coordinate-space matrix elements

$$\langle 1 : \vec{r}_1 ; 2 : \vec{r}_2 | v^{\text{sk}} | 1 : \vec{r}_1 ; 2 : \vec{r}_2 \rangle \equiv \left(t_0 \delta(\vec{r}) + t_2 \overleftarrow{k}' \cdot \delta(\vec{r}) \overrightarrow{k} \right) \delta(\vec{r}_1 - \vec{r}_1) \delta(\vec{r}_2 - \vec{r}_2) \quad (7)$$

where $\vec{r} \equiv \vec{r}_1 - \vec{r}_2$, whereas \vec{k} and \overleftarrow{k}' are relative momentum operators acting on the wave-functions located to their right and to their left, respectively

$$\vec{k} \equiv -\frac{i}{2}(\vec{\nabla}_1 - \vec{\nabla}_2) \quad ; \quad \overleftarrow{k}' \equiv +\frac{i}{2}(\overleftarrow{\nabla}'_1 - \overleftarrow{\nabla}'_2) . \quad (8)$$

It is to be noted that the simplified Skyrme pseudo-potential defined in Eq. 7 is a very schematic local, quasi-zero-range, two-body interaction that is neither supposed to provide an approximation of a realistic vacuum two-nucleon interaction V^{NN} , nor meant to provide a satisfactory energy density functional through expression 5. It is thus essential to understand that (i) Skyrme or Gogny "effective interactions" are merely intermediate theoretical objects, with no clear connection to basic nuclear interactions, whose only goal is to provide a good enough empirical EDF parameterization through Eq. 5 and that (ii) what is derived below is to be understood as a baseline for a more complete Skyrme energy density functional.

C. Densities

1. Density matrix in coordinate representation

A complete orthonormal set of single-particle wave functions is defined, in coordinate representation, by

$$\langle \vec{r} | i \rangle \equiv \varphi_i(\vec{r}) , \quad (9)$$

where spin σ and isospin τ have been omitted as already stated above. The operators creating and annihilating a particle at position \vec{r} are obtained through

$$c_{\vec{r}} = \sum_i \varphi_i(\vec{r}) c_i \quad ; \quad c_{\vec{r}}^\dagger = \sum_i \varphi_i^*(\vec{r}) c_i^\dagger , \quad (10)$$

such that the density matrix in coordinate space reads, using the basis φ_i as a reference, as

$$\rho_{\vec{r}\vec{r}'} \equiv \langle \Phi | c_{\vec{r}'}^\dagger c_{\vec{r}} | \Phi \rangle = \sum_{ij} \varphi_j^*(\vec{r}') \varphi_i(\vec{r}) \rho_{ij} . \quad (11)$$

2. Local densities

Given the specific operator structure of the Skyrme pseudo-potential (Eq. 7), the EDF $\mathcal{E}[\rho]$ derived below will be a functional of the three local densities¹

$$\rho_{\vec{r}\vec{r}'} \Big|_{\vec{r}=\vec{r}'} \equiv \rho(\vec{r}) = \sum_{ij} \varphi_j^*(\vec{r}) \varphi_i(\vec{r}) \rho_{ij} \quad (12)$$

$$\vec{\nabla}_{\vec{r}} \cdot \vec{\nabla}_{\vec{r}'} \rho_{\vec{r}\vec{r}'} \Big|_{\vec{r}=\vec{r}'} \equiv \tau(\vec{r}) = \sum_{ij} [\vec{\nabla} \varphi_j^*(\vec{r})] \cdot [\vec{\nabla} \varphi_i(\vec{r})] \rho_{ij} \quad (13)$$

$$-\frac{i}{2} (\nabla_\mu - \nabla'_\mu) \rho_{\vec{r}\vec{r}'} \Big|_{\vec{r}=\vec{r}'} \equiv j_\mu(\vec{r}) = -\frac{i}{2} \sum_{ij} \left\{ \varphi_j^*(\vec{r}) [\nabla_\mu \varphi_i(\vec{r})] - [\nabla_\mu \varphi_j^*(\vec{r})] \varphi_i(\vec{r}) \right\} \rho_{ij} , \quad (14)$$

where $\rho(\vec{r})$ denotes the matter density, $\tau(\vec{r})$ the so-called kinetic density and $\vec{j}(\vec{r})$ the so-called current density.

¹ Using a more realistic Skyrme pseudo potential, $\mathcal{E}[\rho]$ is a functional of a larger set of local densities, notably due to the inclusion of spin and isospin degrees of freedom.

3. *Useful identities*

In the following we make use of the identities²

$$\left(\vec{\nabla} \cdot \vec{\nabla} + \vec{\nabla}' \cdot \vec{\nabla}' \right) \rho_{\vec{r}\vec{r}'} \Big|_{\vec{r}=\vec{r}'} = \Delta \rho(\vec{r}) - 2\tau(\vec{r}) , \quad (15)$$

$$\vec{\nabla} \rho_{\vec{r}\vec{r}'} \Big|_{\vec{r}=\vec{r}'} = \frac{1}{2} \vec{\nabla} \rho(\vec{r}) + i \vec{j}(\vec{r}) , \quad (16)$$

$$\vec{\nabla}' \rho_{\vec{r}\vec{r}'} \Big|_{\vec{r}=\vec{r}'} = \frac{1}{2} \vec{\nabla} \rho(\vec{r}) - i \vec{j}(\vec{r}) , \quad (17)$$

where $\vec{\nabla}$ acts on coordinate \vec{r} while $\vec{\nabla}'$ acts on coordinate \vec{r}' .

² Proofs are given in Appendix A.

II. DERIVATION OF THE SKYRME ENERGY DENSITY FUNCTIONAL

To perform the derivations below, use the following the set of steps

1. Start from the energy expressed in configuration space (Eq. 5)
2. Insert one-body and/or two-body completeness relations in coordinate space
3. Write the energy in terms of coordinate-space matrix elements of t and v^{sk} and of single-particle wave-functions
4. Apply derivatives coming from momentum operators onto single-particle wave functions
5. Perform operations, e.g. integration by part, to express the result in terms of local densities of interest

A. Kinetic energy

Inserting twice the completeness relation on \mathcal{H}_1 in coordinate representation (omitting spin and isospin)

$$1 = \int d\vec{r} |\vec{r}\rangle \langle \vec{r}| , \quad (18)$$

into the first term of Eq. 5 and using coordinate-space matrix elements of the one-body kinetic energy operator (Eq. 6), the kinetic energy becomes

$$\begin{aligned} \mathcal{E}_{\text{kin}}^\rho &= \sum_{ij} t_{ij} \rho_{ji} \\ &= \sum_{ij} \iint d\vec{r} d\vec{r}' \varphi_j^*(\vec{r}) \langle \vec{r} | t | \vec{r}' \rangle \varphi_i(\vec{r}') \rho_{ji} \\ &= -\frac{\hbar^2}{2m} \sum_{ij} \int d\vec{r} \varphi_j^*(\vec{r}) \Delta \varphi_i(\vec{r}) \rho_{ji} \\ &= +\frac{\hbar^2}{2m} \sum_{ij} \int d\vec{r} \vec{\nabla} \varphi_j^*(\vec{r}) \cdot \vec{\nabla} \varphi_i(\vec{r}) \rho_{ji} \\ &= +\frac{\hbar^2}{2m} \int d\vec{r} \tau(\vec{r}) , \end{aligned} \quad (19)$$

where one integration by parts was performed between third and fourth lines.

B. Potential energy

1. General expression

Let us now proceed similarly for the potential energy coming from the simplified Skyrme pseudo-potential. Inserting twice the completeness relation on the two-body Hilbert space \mathcal{H}_2

$$1 = \iint d\vec{r}_1 d\vec{r}_2 |1 : \vec{r}_1; 2 : \vec{r}_2\rangle \langle 1 : \vec{r}_1; 2 : \vec{r}_2| , \quad (20)$$

in the second term of Eq. 5, the interaction energy becomes (first and second steps of the procedure)

$$\begin{aligned} \mathcal{E}_{\text{sk}}^{\rho\rho} &= \frac{1}{2} \sum_{ijkl} \bar{v}_{ijkl}^{\text{sk}} \rho_{ki} \rho_{lj} \\ &= \frac{1}{2} \sum_{ijkl} \iiint d\vec{r}_1' d\vec{r}_2' d\vec{r}_1 d\vec{r}_2 \varphi_i^*(\vec{r}_1') \varphi_j^*(\vec{r}_2') \langle 1 : \vec{r}_1'; 2 : \vec{r}_2' | v^{\text{sk}} | 1 : \vec{r}_1; 2 : \vec{r}_2 \rangle \left(\varphi_k(\vec{r}_1) \varphi_l(\vec{r}_2) - \varphi_l(\vec{r}_1) \varphi_k(\vec{r}_2) \right) \rho_{ki} \rho_{lj} , \end{aligned} \quad (21)$$

where one clearly identifies direct and exchange contributions.

2. Computational rules

We now need to go through steps 4 and 5, i.e. take the explicit form of $\langle 1 : \vec{r}_1'; 2 : \vec{r}_2' | v^{\text{sk}} | 1 : \vec{r}_1; 2 : \vec{r}_2 \rangle$, apply derivative operators onto single-particle wave-functions and identify local densities $\rho(\vec{r})$, $\tau(\vec{r})$ and $\vec{j}(\vec{r})$. Although step 4 is not too difficult, making the local densities explicit can be difficult. For the kinetic energy, $\tau(\vec{r})$ appeared almost immediately at the price of performing one integration by parts. For the potential energy however, it is not the case in general, in particular when keeping spin and isospin and considering components of the interaction that couple spatial derivatives and spin Pauli matrices, e.g. the tensor force.

To reach the targeted objective, it is best to first express the potential energy (Eq. 21) in terms of the non-local density matrix in coordinate space (Eq. 11) and apply derivatives on the latter using specific computational rules derived once and for all (see below). Thus, one first need to go through the step³

$$\begin{aligned} \mathcal{E}_{\text{sk}}^{\rho\rho} &= \frac{1}{2} \int d\vec{r} \sum_{ijkl} \varphi_i^*(\vec{r}_1') \varphi_j^*(\vec{r}_2') f(\vec{\nabla}_1, \vec{\nabla}_2, \vec{\nabla}'_1, \vec{\nabla}'_2) \varphi_k(\vec{r}_1) \varphi_l(\vec{r}_2) \rho_{ki} \rho_{lj} \Big|_{\vec{r}} \\ &= \frac{1}{2} \int d\vec{r} f(\vec{\nabla}_1, \vec{\nabla}_2, \vec{\nabla}'_1, \vec{\nabla}'_2) \rho_{\vec{r}_1', \vec{r}_1} \rho_{\vec{r}_2', \vec{r}_2} \Big|_{\vec{r}} , \end{aligned} \quad (22)$$

where f denotes a certain function to be determined of derivative operators coming from the skyrme pseudo-potential, while the notation $|_{\vec{r}}$ indicates that one must take $\vec{r}_1' = \vec{r}_1 = \vec{r}_2' = \vec{r}_2 = \vec{r}$ after derivative operators have been applied on non-local density matrices. Having such an expression at hand, one needs to apply general computational rules that takes us from gradient operators acting on the non-local density matrix to an expression given in terms the local densities of interest. Given the simplified form of the Skyrme pseudo-potential used, as well as the fact that we omit spin and isospin degrees of freedom, the only computation rules needed are those given in Sec. IC3.

Let us now illustrate such a procedure by computing the contribution of the two terms of the simplified Skyrme interaction (Eq. 7) to $\mathcal{E}_{\text{sk}}^{\rho\rho}$ (Eq. 21).

3. t_0 term

The contribution of the first term of the Skyrme pseudo-potential can be directly expressed as a function of $\rho(\vec{r})$ without the need for further manipulations. Indeed, one has for the direct term

$$\begin{aligned} \mathcal{E}_{t_0, \text{direct}}^{\rho\rho} &= \frac{1}{2} \sum_{ijkl} \int \int d\vec{r}_1 d\vec{r}_2 \varphi_i^*(\vec{r}_1) \varphi_j^*(\vec{r}_2) t_0 \delta(\vec{r}_1 - \vec{r}_2) \varphi_k(\vec{r}_1) \varphi_l(\vec{r}_2) \rho_{ki} \rho_{lj} \\ &= \frac{1}{2} \sum_{ijkl} \int d\vec{r} \varphi_i^*(\vec{r}) \varphi_j^*(\vec{r}) t_0 \varphi_k(\vec{r}) \varphi_l(\vec{r}) \rho_{ki} \rho_{lj} \\ &= \int d\vec{r} \frac{t_0}{2} \left[\sum_{ik} \varphi_i^*(\vec{r}) \varphi_k(\vec{r}) \rho_{ki} \right] \left[\sum_{jl} \varphi_j^*(\vec{r}) \varphi_l(\vec{r}) \rho_{lj} \right] \\ &= \int d\vec{r} \frac{t_0}{2} \rho(\vec{r}) \rho(\vec{r}) , \end{aligned} \quad (23)$$

whereas the exchange term gives exactly the opposite contribution. Overall, the contribution of the t_0 term to the EDF is zero. This should not come as a surprise given that such a term is a pure contact term requiring the two fermions to be at the same location in space, which is forbidden by the Pauli principle unless the two fermions can occupy different spin and/or isospin states. As the latter degrees of freedom have been omitted here, the two fermions cannot be at the same location in space and the t_0 term cannot contribute to the nuclear potential energy.

4. t_2 term

The t_2 term is a derivative terms that acts simultaneously to the left and to the right. It can be shown that such a term only acts in the $L = 1$ partial wave of relative motion of the two interacting nucleons, i.e. it is a P -wave

³ This is technically more involved when keeping spin and isospin but the overall idea is the same.

interaction. Such an odd- L interaction provides correlation energy whenever the two fermions are not at the same location in space. In spite of our omission of spin and isospin degrees of freedom, the t_2 term thus contributes to the correlation energy. As a matter of fact, one can easily realize that direct and exchange contributions are equal, which allows us to simply calculate one of the two and multiply it by a factor of two. Using the definitions of \vec{k} and \vec{k}' (Eq. 8), one has

$$\mathcal{E}_{t_2, \text{direct}}^{\rho\rho} = \frac{1}{2} \sum_{ijkl} \int d\vec{r} \varphi_i^*(\vec{r}_{1'}) \varphi_j^*(\vec{r}_{2'}) \frac{t_2}{4} \left(\vec{\nabla}_1 \cdot \vec{\nabla}'_1 + \vec{\nabla}_2 \cdot \vec{\nabla}'_2 - \vec{\nabla}_1 \cdot \vec{\nabla}'_2 - \vec{\nabla}_2 \cdot \vec{\nabla}'_1 \right) \varphi_k(\vec{r}_1) \varphi_l(\vec{r}_2) \rho_{ki} \rho_{lj} \Big|_{\vec{r}},$$

where one takes $\vec{r}_1 = \vec{r}_2 = \vec{r}_{1'} = \vec{r}_{2'} = \vec{r}$ after the derivatives have been applied on the appropriate wave functions. One notices that the first and second terms in the parenthesis are symmetric under the simultaneous exchanges $1 \leftrightarrow 2$ and $(i, k) \leftrightarrow (j, l)$. Using a proper renaming of running indices, one thus obtains identical contributions from both terms. The same situation occurs with the third and fourth terms. Identifying the non-local density matrices as explained in Sec. II B 2, one thus obtains

$$\mathcal{E}_{t_2, \text{direct}}^{\rho\rho} = \int d\vec{r} \frac{t_2}{4} \left(\vec{\nabla}_1 \cdot \vec{\nabla}'_1 - \vec{\nabla}_1 \cdot \vec{\nabla}'_2 \right) \rho_{\vec{r}_1 \vec{r}_1'} \rho_{\vec{r}_2 \vec{r}_2'} \Big|_{\vec{r}}. \quad (24)$$

Using the definition of $\tau(\vec{r})$ to deal with the first term in the parenthesis and Eqs. 16-17 to deal with the second, one has

$$\begin{aligned} \mathcal{E}_{t_2, \text{direct}}^{\rho\rho} &= \int d\vec{r} \frac{t_2}{4} \left(\rho_{\vec{r}_2 \vec{r}_2'} \vec{\nabla}_1 \cdot \vec{\nabla}'_1 \rho_{\vec{r}_1 \vec{r}_1'} \Big|_{\vec{r}} - \vec{\nabla}_1 \rho_{\vec{r}_1 \vec{r}_1'} \cdot \vec{\nabla}'_2 \rho_{\vec{r}_2 \vec{r}_2'} \Big|_{\vec{r}} \right) \\ &= \int d\vec{r} \frac{t_2}{4} \left(\rho(\vec{r}) \tau(\vec{r}) - \left[\frac{1}{2} \vec{\nabla} \rho(\vec{r}) + i \vec{j}(\vec{r}) \right] \cdot \left[\frac{1}{2} \vec{\nabla} \rho(\vec{r}) - i \vec{j}(\vec{r}) \right] \right) \\ &= \int d\vec{r} \frac{t_2}{4} \left(\rho(\vec{r}) \tau(\vec{r}) - \vec{j}(\vec{r}) \cdot \vec{j}(\vec{r}) - \frac{1}{4} \vec{\nabla} \rho(\vec{r}) \cdot \vec{\nabla} \rho(\vec{r}) \right) \\ &= \int d\vec{r} \frac{t_2}{4} \left(\rho(\vec{r}) \tau(\vec{r}) - \vec{j}(\vec{r}) \cdot \vec{j}(\vec{r}) + \frac{1}{4} \rho(\vec{r}) \Delta \rho(\vec{r}) \right), \end{aligned} \quad (25)$$

where an integration by parts has been performed to obtain the last expression. Adding the equal contribution of the exchange term, one obtains

$$\mathcal{E}_{t_2}^{\rho\rho} = \int d\vec{r} \frac{t_2}{8} \left(\rho(\vec{r}) \Delta \rho(\vec{r}) + 4 \rho(\vec{r}) \tau(\vec{r}) - 4 \vec{j}(\vec{r}) \cdot \vec{j}(\vec{r}) \right). \quad (26)$$

5. Skyrme energy density functional

Summing kinetic (Eq. 19) and potential (Eq. 26) energies, the EDF obtained from the simplified Skyrme pseudo-potential used here, in the hypothesis that spin and isospin are omitted, finally reads

$$\mathcal{E}[\rho] = \int d\vec{r} \left[\frac{\hbar^2}{2m} \tau(\vec{r}) + A^{\rho\Delta\rho} \rho(\vec{r}) \Delta \rho(\vec{r}) + A^{\rho\tau} \left(\rho(\vec{r}) \tau(\vec{r}) - \vec{j}(\vec{r}) \cdot \vec{j}(\vec{r}) \right) \right], \quad (27)$$

with the two couplings

$$A^{\rho\Delta\rho} \equiv \frac{t_2}{8} \quad \text{and} \quad A^{\rho\tau} \equiv \frac{t_2}{2}. \quad (28)$$

The fact that the coefficients of the last two terms in Eq. 27 are the same is a necessity for the EDF to be Galilean invariant [3, 4], i.e. it ensures that the binding energy of the nucleus remains the same when translating it or when putting it in motion with a constant velocity.

III. ONE-BODY FIELDS

Having the Skyrme EDF at hand (Eq. 27), one can derive the one-body field h whose matrix elements are defined for $j \leq i$ by

$$h_{ji} \equiv \frac{\delta \mathcal{E}[\rho]}{\delta \rho_{ij}} = \int d\vec{r} \left\{ \frac{\delta \mathcal{E}}{\delta \rho(\vec{r})} \frac{\delta \rho(\vec{r})}{\delta \rho_{ij}} + \frac{\delta \mathcal{E}}{\delta \tau(\vec{r})} \frac{\delta \tau(\vec{r})}{\delta \rho_{ij}} + \sum_{\mu=x,y,z} \frac{\delta \mathcal{E}}{\delta j_\mu(\vec{r})} \frac{\delta j_\mu(\vec{r})}{\delta \rho_{ij}} \right\}, \quad (29)$$

where a chain rule has been used has $\mathcal{E}[\rho]$ is manifestly a functional of $\rho(\vec{r})$, $\tau(\vec{r})$ and $\vec{j}(\vec{r})$ but only implicitly a functional of ρ_{ij} . The functional derivative of the densities with respect to matrix elements of the density matrix reads, for $j \leq i$, as

$$\begin{aligned}\frac{\delta\rho(\vec{r})}{\delta\rho_{ij}} &= \varphi_j^*(\vec{r})\varphi_i(\vec{r}) , \\ \frac{\delta\tau(\vec{r})}{\delta\rho_{ij}} &= [\vec{\nabla}\varphi_j^*(\vec{r})] \cdot [\vec{\nabla}\varphi_i(\vec{r})] , \\ \frac{\delta j_\mu(\vec{r})}{\delta\rho_{ij}} &= -\frac{i}{2}\left\{\varphi_j^*(\vec{r})[\nabla_\mu\varphi_i(\vec{r})] - [\nabla_\mu\varphi_j^*(\vec{r})]\varphi_i(\vec{r})\right\} ,\end{aligned}$$

whereas the local potentials defined through

$$U(\vec{r}) \equiv \frac{\delta\mathcal{E}}{\delta\rho(\vec{r})} , \quad (31a)$$

$$B(\vec{r}) \equiv \frac{\delta\mathcal{E}}{\delta\tau(\vec{r})} , \quad (31b)$$

$$A_\mu(\vec{r}) \equiv \frac{\delta\mathcal{E}}{\delta j_\mu(\vec{r})} , \quad (31c)$$

read for the simplified Skyrme EDF (Eq. 27) as

$$U(\vec{r}) = A^{\rho\tau}\tau(\vec{r}) + 2A^{\rho\Delta\rho}\Delta\rho(\vec{r}) , \quad (32a)$$

$$B(\vec{r}) = \frac{\hbar^2}{2m} + A^{\rho\tau}\rho(\vec{r}) , \quad (32b)$$

$$A_\mu(\vec{r}) = -2A^{\rho\tau}j_\mu(\vec{r}) . \quad (32c)$$

Finally, matrix elements of the field can be written as

$$h_{ji} \equiv \int d\vec{r}\varphi_j^*(\vec{r})h(\vec{r})\varphi_i(\vec{r}) , \quad (33)$$

such that the one-body field h is local and expressed in coordinate space as

$$h(\vec{r}) = -\vec{\nabla} \cdot B(\vec{r})\vec{\nabla} + U(\vec{r}) - \frac{i}{2}\left[\vec{A}(\vec{r}) \cdot \vec{\nabla} + \vec{\nabla} \cdot \vec{A}(\vec{r})\right] , \quad (34)$$

where gradients act to their right on both the potentials and the wave-function h is eventually applied to.

IV. INFINITE NUCLEAR MATTER

A. Introduction

Having the energy functional at hand (Eq. (27)), one can calculate the so-called equation of state of infinite nuclear matter. Symmetric infinite nuclear matter is an idealized system characterized by the following properties

1. It is infinite and translational invariant, with a constant density $\rho = N/V$
2. It is made of an equal number of neutrons and protons
3. It omits the Coulomb interaction between protons
4. It possesses an equilibrium point characterized by
 - The density $\rho_{\text{sat}} = 0.16 \text{ fm}^{-3}$
 - The energy per nucleon $e_{\text{sat}} = -16 \text{ MeV}$
 - The compressibility $K_\infty \approx 230 \text{ MeV}$
 - The symmetry energy $a_{\text{sym}} \approx 32 \text{ MeV}$

One is interested in computing the equation of state (EOS) of such a system, i.e. its energy per nucleon as a function of its density. The total energy per nucleon of infinite matter is given by

$$\frac{\mathcal{E}}{N}[\rho] = \frac{V}{N}\epsilon[\rho] = \frac{\epsilon[\rho]}{\rho} \quad , \quad (35)$$

where $\mathcal{E}[\rho] \equiv \int d\vec{r} \epsilon[\rho] = V\epsilon[\rho]$. The EOS displays a minimum at ρ_{sat} , i.e.

$$\left. \frac{\partial \epsilon[\rho]/\rho}{\partial \rho} \right|_{\rho=\rho_{\text{sat}}} = 0 \quad , \quad (36)$$

such that the pressure of the system

$$P \equiv - \left. \frac{\partial \mathcal{E}}{\partial V} \right|_N = \frac{N}{V^2} \left. \frac{\partial \mathcal{E}}{\partial \rho} \right|_N = \rho^2 \left. \frac{\partial \epsilon[\rho]/\rho}{\partial \rho} \right|_N \quad , \quad (37)$$

is zero at saturation density $P(\rho_{\text{sat}}) = 0$. The incompressibility K_∞ that provides the curvature of the equation of state around its minimum is defined as

$$K_\infty \equiv 9\rho_{\text{sat}}^2 \left. \frac{\partial^2 \epsilon[\rho]/\rho}{\partial \rho^2} \right|_{\rho=\rho_{\text{sat}}} \quad . \quad (38)$$

Note that in the present case where spin and isospin are omitted throughout, the equation of state will not provide a realistic description of symmetric nuclear matter. To obtain a realistic equation of state, one must start from a realistic Skyrme EDF and consider spin and isospin explicitly.

B. Local densities

In a translational invariant medium, the reference Slater determinant is built from single-particle wave-functions that are eigenstates of a translational invariant field h . Consequently, those single-particle states are necessarily plane-waves of the form

$$\psi_{\vec{k}}(\vec{r}) \equiv \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} \quad . \quad (39)$$

Given basis $\{\psi_{\vec{k}}\}$, one can now compute local densities introduced in Sec. (I C 2) for infinite nuclear matter. The density matrix $\rho_{\vec{k}\vec{k}'}$ is diagonal in the plane-wave basis, with diagonal elements given by a heavyside function $\Theta(k_F - |\vec{k}|)$, such that all states with $|\vec{k}|$ up to the Fermi momentum k_F are occupied in the slater determinant⁴. In the definition of the densities, the sum over single-particle states becomes an integral over the sphere of radius k_F in momentum space, such that the local density ρ finally reads

$$\begin{aligned} \rho(\vec{r}) &= \int_{|\vec{k}|\leq k_F} d\vec{k} \psi_{\vec{k}}^*(\vec{r}) \psi_{\vec{k}}(\vec{r}) \\ &= \frac{1}{(2\pi)^3} \int_{|\vec{k}|\leq k_F} d\vec{k} e^{-i\vec{k}\cdot\vec{r}} e^{i\vec{k}\cdot\vec{r}} \\ &= \frac{1}{(2\pi)^3} \int_0^{k_F} dk k^2 \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \\ &= \frac{1}{(2\pi)^3} \frac{4\pi}{3} k_F^3 \\ &= \frac{k_F^3}{6\pi^2} \quad , \end{aligned} \quad (40)$$

⁴ When considering spin and isospin, there are in fact four such Fermi momenta $k_F^{\sigma\tau}$, one for each combination of spin and isospin projections. Symmetric nuclear matter corresponds to the system for which the four Fermi momenta $k_F^{\sigma\tau}$ are equal. Otherwise, one talks about isospin asymmetric and/or spin-polarized infinite nuclear matter.

where we have used spherical coordinates to work out the integral. As expected from translational invariance, the local density is constant over space. The τ density reads

$$\begin{aligned}
\tau(\vec{r}) &= \int_{|\vec{k}| \leq k_F} d\vec{k} [\vec{\nabla} \psi_{\vec{k}}^*(\vec{r})] \cdot [\vec{\nabla} \psi_{\vec{k}}(\vec{r})] \\
&= \frac{1}{(2\pi)^3} \int_{|\vec{k}| \leq k_F} d\vec{k} (-i\vec{k}) e^{-i\vec{k} \cdot \vec{r}} (i\vec{k}) e^{i\vec{k} \cdot \vec{r}} \\
&= \frac{1}{(2\pi)^3} \int_0^{k_F} dk k^4 \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \\
&= \frac{1}{(2\pi)^3} \frac{4\pi}{5} k_F^5 \\
&= \frac{k_F^5}{10\pi^2} .
\end{aligned} \tag{41}$$

Given the two previous results, one sees that the matter density and the kinetic density are trivially related in this case

$$\tau = \frac{3}{5} \rho k_F^2 = \frac{3}{5} (6\pi^2)^{2/3} \rho^{5/3} . \tag{42}$$

The \vec{j} density gives

$$\begin{aligned}
\vec{j}(\vec{r}) &= -\frac{i}{2} \int_{|\vec{k}| \leq k_F} d\vec{k} \left\{ \psi_{\vec{k}}^*(\vec{r}) [\vec{\nabla} \psi_{\vec{k}}(\vec{r})] - [\vec{\nabla} \psi_{\vec{k}}^*(\vec{r})] \psi_{\vec{k}}(\vec{r}) \right\} \\
&= -\frac{i}{2} \frac{1}{(2\pi)^3} \int_{|\vec{k}| \leq k_F} d\vec{k} \left\{ e^{-i\vec{k} \cdot \vec{r}} (i\vec{k}) e^{i\vec{k} \cdot \vec{r}} - (-i\vec{k}) e^{-i\vec{k} \cdot \vec{r}} e^{i\vec{k} \cdot \vec{r}} \right\} \\
&= \frac{1}{(2\pi)^3} \int_{|\vec{k}| \leq k_F} d\vec{k} \vec{k} \\
&= \frac{1}{(2\pi)^3} \int_0^{k_F} \int_0^\pi \int_0^{2\pi} k^2 dk \sin \theta d\theta d\phi k (\sin \theta \cos \phi \vec{u}_x + \sin \theta \sin \phi \vec{u}_y + \cos(\phi) \vec{u}_z) \\
&= \frac{1}{(2\pi)^3} \int_0^{k_F} k^3 dk \left[\int_0^\pi \sin^2 \theta d\theta \int_0^{2\pi} \cos \phi d\phi \vec{u}_x + \int_0^\pi \sin^2 \theta d\theta \int_0^{2\pi} \sin \phi d\phi \vec{u}_y + \int_0^\pi \sin \theta \cos \theta d\theta \int_0^{2\pi} d\phi \vec{u}_z \right] \\
&= \vec{0} ,
\end{aligned} \tag{43}$$

as each of the three terms inside the bracket is zero.

C. Equation of state

Finally, the EOS provided by the simplified Skyrme EDF can be calculated by inserting Eqs. ?? into Eq. 27. This gives

$$\begin{aligned}
\frac{\epsilon[\rho]}{\rho} &= \frac{\hbar^2}{2m} \frac{\tau}{\rho} + A^{\rho\tau} \frac{\rho\tau}{\rho} \\
&= \frac{3}{10} \frac{\hbar^2}{m} (6\pi^2)^{2/3} \rho^{2/3} + \frac{3}{5} A^{\rho\tau} (6\pi^2)^{2/3} \rho^{5/3} ,
\end{aligned} \tag{44}$$

providing for the pressure

$$P[\rho] = \rho \left(\frac{1}{5} \frac{\hbar^2}{m} (6\pi^2)^{2/3} \rho^{2/3} + A^{\rho\tau} (6\pi^2)^{2/3} \rho^{5/3} \right) , \tag{45}$$

and finally for the incompressibility

$$K_\infty = -\frac{3}{5} \frac{\hbar^2}{m} (6\pi^2)^{2/3} \rho_{\text{sat}}^{2/3} + 6A^{\rho\tau} (6\pi^2)^{2/3} \rho_{\text{sat}}^{5/3} . \tag{46}$$

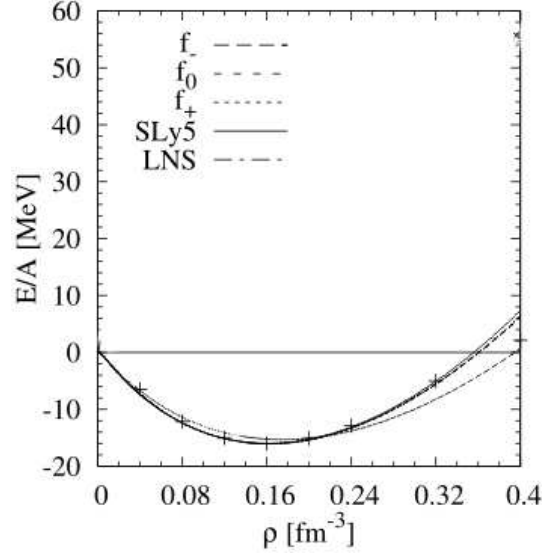


FIG. 1: Equation of state of symmetric nuclear matter calculated with a selection of realistic Skyrme energy density functionals [5].

It is important to note that the above formula are totally unrealistic as for describing symmetric nuclear matter. As a matter of fact, omitting spin and isospin correspond effectively to describing, for instance, spin-polarized neutron matter. Indeed, in such a system only one spin projection and one isospin projection are occupied, which effectively corresponds to our present description. Requiring the equation of state of spin-polarized neutron matter to have an extremum ($P = 0$) leads to a maximum characterized by $K_\infty < 0$. One can check that this is precisely what the above set of equations can deliver. This is not at all the situation encountered for symmetric nuclear matter which presents an equilibrium minimum, as the typical equation of state shown in Fig. 1 illustrates.

Annexe A: COMPUTATIONAL RULES

We start with

$$\begin{aligned}
(\Delta + \Delta') \rho_{\vec{r}\vec{r}'} \Big|_{\vec{r}=\vec{r}'} &= \sum_{ij} \left[\Delta \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) + \varphi_i^*(\vec{r}) \Delta \varphi_j(\vec{r}) \right] \rho_{ji} \\
&= \sum_{ij} \left[\Delta \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) + \varphi_i^*(\vec{r}) \Delta \varphi_j(\vec{r}) + 2 \vec{\nabla} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) - 2 \vec{\nabla} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) \right] \rho_{ji} \\
&= \sum_{ij} \vec{\nabla} \left[\vec{\nabla} \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) + \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) \right] \rho_{ji} - \left[2 \vec{\nabla} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) \right] \rho_{ji} \\
&= \Delta \rho(\vec{r}) - 2 \tau(\vec{r}) ,
\end{aligned} \tag{A1}$$

follow by

$$\begin{aligned}
\vec{\nabla} \rho_{\vec{r}\vec{r}'} \Big|_{\vec{r}=\vec{r}'} &= \sum_{ij} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) \rho_{ji} \\
&= \sum_{ij} \left[\frac{1}{2} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) + \frac{1}{2} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) + \frac{1}{2} \vec{\nabla} \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) - \frac{1}{2} \vec{\nabla} \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) \right] \rho_{ji} \\
&= \sum_{ij} \left[\frac{1}{2} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) + \frac{1}{2} \vec{\nabla} \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) + \frac{1}{2} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) - \frac{1}{2} \vec{\nabla} \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) \right] \rho_{ji} \\
&= \frac{1}{2} \vec{\nabla} \rho(\vec{r}) + i \vec{j}(\vec{r}) ,
\end{aligned} \tag{A2}$$

and terminate with

$$\begin{aligned}
\vec{\nabla}' \rho_{\vec{r}\vec{r}'} \Big|_{\vec{r}=\vec{r}'} &= \sum_{ij} \vec{\nabla} \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) \rho_{ji} \\
&= \sum_{ij} \left[\frac{1}{2} \vec{\nabla} \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) + \frac{1}{2} \vec{\nabla} \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) + \frac{1}{2} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) - \frac{1}{2} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) \right] \rho_{ji} \\
&= \sum_{ij} \left[\frac{1}{2} \vec{\nabla} \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) + \frac{1}{2} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) + \frac{1}{2} \vec{\nabla} \varphi_i^*(\vec{r}) \varphi_j(\vec{r}) - \frac{1}{2} \varphi_i^*(\vec{r}) \vec{\nabla} \varphi_j(\vec{r}) \right] \rho_{ji} \\
&= \frac{1}{2} \vec{\nabla} \rho(\vec{r}) - i \vec{j}(\vec{r}) .
\end{aligned} \tag{A3}$$

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