The nuclear Energy Density Functional formalism

Practice session

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

$$\rho_{ij} \;\equiv\; \frac{\langle\Phi|c^\dagger_j c_i|\Phi\rangle}{\langle\Phi|\Phi\rangle} \;\; , \tag{1}$$

where $\{c^\dagger_j,\, c_j\}$ 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

$$|\Phi\rangle \equiv \prod_{\alpha=1}^{N} a^\dagger_\alpha |0\rangle \;\; , \tag{2}$$

where $\{a^\dagger_\alpha, a_\alpha\}$ 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

$$H_{\mathrm{eff}} \;=\; \sum_{ij} t_{ij}\, c^\dagger_i\, c_j + \frac{1}{2}\sum_{ijkl} v^{\mathrm{sk}}_{ijkl}\, c^\dagger_i\, c^\dagger_j\, c_l\, c_k \;\; , \tag{3}$$

where $t_{ij} \equiv \langle i|\, t\, |j\rangle$ and $v^{\mathrm{sk}}_{ijkl} \equiv \langle 1:i;2:j|\, v^{\mathrm{sk}}\, |1:k;2:l\rangle$ 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

$$\mathcal{E}[\rho] \;\equiv\; E^{HF}_{\mathrm{eff}} = \frac{\langle\Phi|\, H_{\mathrm{eff}}\, |\Phi\rangle}{\langle\Phi|\Phi\rangle} \;\; , \tag{4}$$

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

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

where $\bar{v}^{\mathrm{sk}}_{ijkl} \equiv v^{\mathrm{sk}}_{ijkl} - v^{\mathrm{sk}}_{ijlk}$ 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

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

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

$$\langle 1:\vec r_{1'};2:\vec r_{2'}|\, v^{\mathrm{sk}}\, |1:\vec r_1;2:\vec r_2\rangle \;\equiv\; \Big(t_0\, \delta(\vec r) + t_2\, \overleftarrow{k}\,' \cdot\, \delta(\vec r)\, \overrightarrow{k}\Big)\, \delta(\vec r_1 - \vec r_{1'})\, \delta(\vec r_2 - \vec r_{2'}) \tag{7}$$

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

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

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. Completeness relations

1. *One-body Hilbert space*

The completeness relation on the one-body Hilbert space $\mathcal{H}_1$ reads in coordinate representation (omitting spin and isospin) as

$$1 = \int d\vec{r}\, |\vec{r}\rangle\langle\vec{r}\,| \ . \tag{9}$$

2. *Two-body Hilbert space*

The completeness relation on the two-body Hilbert space $\mathcal{H}_2$ reads in coordinate representation (omitting spin and isospin) as

$$1 = \int\!\!\int d\vec{r}_1 d\vec{r}_2 \ \ |1:\vec{r}_1; 2:\vec{r}_2\rangle\langle 1:\vec{r}_1; 2:\vec{r}_2| \ . \tag{10}$$

D. Densities

1. *Density matrix in coordinate representation*

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

$$\langle\,\vec{r}\,|\,i\rangle \equiv \varphi_i(\vec{r}) \ , \tag{11}$$

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

$$c_{\vec{r}} = \sum_i \varphi_i(\vec{r})\; c_i \quad ; \quad c^\dagger_{\vec{r}} = \sum_i \varphi^*_i(\vec{r})\; c^\dagger_i \ , \tag{12}$$

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

$$\rho_{\vec{r}\vec{r}\,'} \equiv \langle\Phi|c^\dagger_{\vec{r}\,'} c_{\vec{r}}|\Phi\rangle = \sum_{ij} \varphi^*_j(\vec{r}\,')\, \varphi_i(\vec{r})\, \rho_{ij} \ . \tag{13}$$

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 densities[1]

$$\begin{aligned}
\rho_{\vec{r}\vec{r}\,'}\Big|_{\vec{r}=\vec{r}\,'} &\equiv \rho(\vec{r}) = \sum_{ij} \varphi^*_j(\vec{r})\,\varphi_i(\vec{r})\,\rho_{ij} && (14)\\
\vec{\nabla}_{\vec{r}}\cdot\vec{\nabla}_{\vec{r}\,'}\,\rho_{\vec{r}\vec{r}\,'}\Big|_{\vec{r}=\vec{r}\,'} &\equiv \tau(\vec{r}) = \sum_{ij}\left[\vec{\nabla}\varphi^*_j(\vec{r})\right]\cdot\left[\vec{\nabla}\varphi_i(\vec{r})\right]\rho_{ij} && (15)\\
-\frac{i}{2}\left(\nabla_\mu - \nabla'_\mu\right)\rho_{\vec{r}\vec{r}\,'}\Big|_{\vec{r}=\vec{r}\,'} &\equiv j_\mu(\vec{r}) = -\frac{i}{2}\sum_{ij}\Big\{\varphi^*_j(\vec{r})\left[\nabla_\mu\varphi_i(\vec{r})\right] - \left[\nabla_\mu\varphi^*_j(\vec{r})\right]\varphi_i(\vec{r})\Big\}\,\rho_{ij}\ , && (16)
\end{aligned}$$

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.

3. Useful identities

In the following we will make use of the identities

$$\begin{aligned}
\left(\vec{\nabla}\cdot\vec{\nabla} + \vec{\nabla}'\cdot\vec{\nabla}'\right)\rho_{\vec{r}\vec{r}\,'}\Big|_{\vec{r}=\vec{r}\,'} &= \triangle\rho(\vec{r}) - 2\,\tau(\vec{r})\ , && (17)\\
\vec{\nabla}\,\rho_{\vec{r}\vec{r}\,'}\Big|_{\vec{r}=\vec{r}\,'} &= \frac{1}{2}\,\vec{\nabla}\rho(\vec{r}) + i\,\vec{j}(\vec{r})\ , && (18)\\
\vec{\nabla}'\,\rho_{\vec{r}\vec{r}\,'}\Big|_{\vec{r}=\vec{r}\,'} &= \frac{1}{2}\,\vec{\nabla}\rho(\vec{r}) - i\,\vec{j}(\vec{r})\ , && (19)
\end{aligned}$$

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

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[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.

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 $v^{\rm sk}$ 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

Prove that

$$\mathcal{E}^{\rho}_{\rm kin} = \frac{\hbar^2}{2m}\int d\vec{r}\,\tau(\vec{r}) \ . \tag{20}$$

B. Potential energy

1. *General expression*

Express the potential energy $\mathcal{E}^{\rho\rho}_{\rm sk}$ in terms of single-particle wave-functions and matrix elements $\langle 1:\vec{r}_{1'};2:\vec{r}_{2'}|\,v^{\rm sk}\,|1:\vec{r}_1;2:\vec{r}_2\rangle$ to prove that it can be written under the general form

$$\mathcal{E}^{\rho\rho}_{\rm sk} = \frac{1}{2}\int d\vec{r}\, f(\overrightarrow{\nabla}_1,\overrightarrow{\nabla}_2,\overrightarrow{\nabla}'_1,\overrightarrow{\nabla}'_2)\,\rho_{\vec{r}_{1'}\vec{r}_1}\,\rho_{\vec{r}_{2'}\vec{r}_2}\Big|_{\vec{r}} \ , \tag{21}$$

where f denotes the set of derivative operators coming from $v^{\rm sk}$, 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.

2. *t_0 term*

Demonstrate that the direct contribution of the t_0 term gives

$$\mathcal{E}^{\rho\rho}_{t_0\,,\,\rm direct} = \int d\vec{r}\,\frac{t_0}{2}\,\rho(\vec{r})\,\rho(\vec{r}) \ , \tag{22}$$

and that the exchange term gives the exact opposite contribution. Given that we omit spin and isospin degrees of freedom, explain in simple terms the reason why the t_0 term does not contribute to the potential energy.

3. *t_2 term*

Putting the direct contribution from the t_2 term under the form of Eq. 21 and using Eqs. 18-19, demonstrate that

$$\mathcal{E}^{\rho\rho}_{t_2\,,\,\rm direct} = \int d\vec{r}\,\frac{t_2}{4}\Big(\rho(\vec{r})\tau(\vec{r}) - \vec{j}(\vec{r})\cdot\vec{j}(\vec{r}) + \frac{1}{4}\rho(\vec{r})\Delta\rho(\vec{r})\Big) \ , \tag{23}$$

and that the exchange term provides the exact same contribution.

III. ONE-BODY FIELDS

Using a chain rule, calculate the matrix elements of the field h

$$h_{ji} \;\equiv\; \frac{\delta \mathcal{E}[\rho]}{\delta \rho_{ij}} \;\; . \tag{24}$$

Prove that such matrix elements can be put under the form

$$h_{ji} \equiv \int d\vec{r}\, \varphi_j^*(\vec{r})\, h(\vec{r})\, \varphi_i(\vec{r}) \;\; , \tag{25}$$

where

$$h(\vec{r}) \;=\; -\vec{\nabla}\cdot B(\vec{r})\vec{\nabla} + U(\vec{r}) - \frac{i}{2}\Big[\vec{A}(\vec{r})\cdot\vec{\nabla} + \vec{\nabla}\cdot\vec{A}(\vec{r})\Big] \;\; , \tag{26}$$

and compute the explicit form of $B(\vec{r}) \equiv \delta\mathcal{E}/\delta\tau(\vec{r})$, $U(\vec{r}) \equiv \delta\mathcal{E}/\delta\rho(\vec{r})$ and $A_\mu(\vec{r}) \equiv \delta\mathcal{E}/\delta j_\mu(\vec{r})$.

IV. INFINITE NUCLEAR MATTER

A. Introduction

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 $\rho_{\text{sat}} = 0.16$ fm^{-3}
   - The energy per nucleon $e_{\text{sat}} = -16$ MeV
   - The compressibility $K_\infty \approx 230$ MeV
   - The symmetry energy $a_{\text{sym}} \approx 32$ MeV

The energy per nucleon as a function of the density defines the so-called equation of state (EOS)

$$\frac{\mathcal{E}}{N}[\rho] \;=\; \frac{V}{N}\epsilon[\rho] \;=\; \frac{\epsilon[\rho]}{\rho} \;\; , \tag{27}$$

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

$$\frac{\partial \epsilon[\rho]/\rho}{\partial \rho}\Big|_{\rho=\rho_{\text{sat}}} = 0 \;\; , \tag{28}$$

such that the pressure of the system

$$P \equiv -\frac{\partial \mathcal{E}}{\partial V}\Big|_N = \frac{N}{V^2}\frac{\partial \mathcal{E}}{\partial \rho}\Big|_N = \rho^2\,\frac{\partial \epsilon[\rho]/\rho}{\partial \rho}\Big|_N \;\; , \tag{29}$$

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

$$K_\infty \equiv 9\rho_{\text{sat}}^2\,\frac{\partial^2 \epsilon[\rho]/\rho}{\partial \rho^2}\Big|_{\rho=\rho_{\text{sat}}} \;\; . \tag{30}$$

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

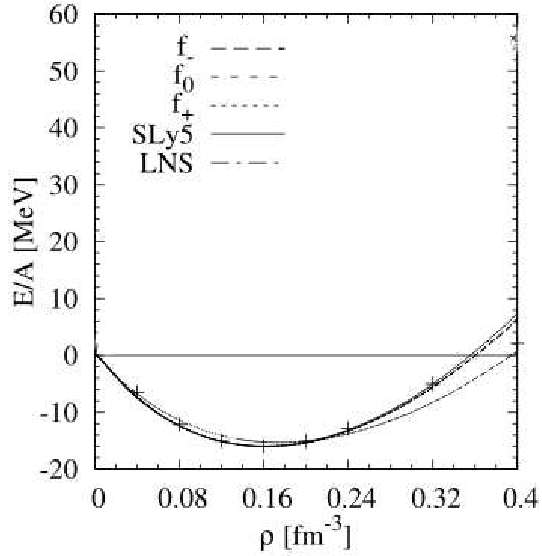

FIG. 1: Equation of state of symmetric nuclear matter calculated with a selection of realistic Skyrme energy density functionals [3].

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. **Prove that such single-particle states are necessarily plane-waves of the form**

$$\psi_{\vec{k}}(\vec{r}) \equiv \frac{1}{(2\pi)^{3/2}} \, e^{i\vec{k}\cdot\vec{r}} \quad , \tag{31}$$

orthonormalized in the Dirac sense. Given the basis $\{\psi_{\vec{k}}\}$, the Slater determinant (Eq. 2) is obtained by filling all states with $|\vec{k}|$ smaller or equal to the Fermi momentum k_F. Realizing that in the present case a sum over single particle states $\sum_i$ is in fact an integral $\int d\vec{k}$, **prove that**

$$\rho(\vec{r}) \; = \; \frac{k_F^3}{6\pi^2} \quad , \tag{32}$$

$$\tau(\vec{r}) \; = \; \frac{k_F^5}{10\pi^2} \quad , \tag{33}$$

$$\vec{j}(\vec{r}) \; = \; \vec{0} \quad . \tag{34}$$

C. Equation of state

Prove that the equation of state provided by the simplified Skyrme EDF is

$$\frac{\epsilon[\rho]}{\rho} \; = \; \frac{\hbar^2}{2m}\,\frac{\tau}{\rho} + A^{\rho\tau}\,\tau = \frac{3}{10}\frac{\hbar^2}{m}\left(6\pi^2\right)^{2/3}\rho^{2/3} + \frac{3}{5}A^{\rho\tau}\left(6\pi^2\right)^{2/3}\rho^{5/3} \quad , \tag{35}$$

that the pressure is

$$P[\rho] \; = \; \rho\left\{\frac{1}{5}\frac{\hbar^2}{m}\left(6\pi^2\right)^{2/3}\rho^{2/3} + A^{\rho\tau}\left(6\pi^2\right)^{2/3}\rho^{5/3}\right\} \quad . \tag{36}$$

and that the incompressibility is

$$K_\infty \; = \; -\frac{3}{5}\frac{\hbar^2}{m}\left(6\pi^2\right)^{2/3}\rho_{\text{sat}}^{2/3} + 6A^{\rho\tau}\left(6\pi^2\right)^{2/3}\rho_{\text{sat}}^{5/3} \quad . \tag{37}$$

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.

[1] G. C. Wick, Phys. Rev. **80**, 268 (1950).
[2] J. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (MIT Press, Cambridge, Massachusetts, 1986).
[3] T. Lesinski, K. Bennaceur, T. Duguet, and J. Meyer, Phys. Rev. **C74**, 044315 (2006).