

Phenomenological Effective Potentials

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July 21, 2014

Introduction

The Quantum Many-body Problem

The Hamiltonian for a quantum many-body system of A fermions in interaction read

$$\hat{H} = \hat{T} + \hat{V}_1 + \hat{V}_2 + \cdots + \hat{V}_A, \quad (1)$$

with \hat{V}_n a n -body *potential*, e.g., an operator that depend on n spatial coordinates, spins and isospins ($2n$ if non-local),

$$\hat{V}_n \equiv \hat{V}_n(x_1, \dots, x_n, x'_1, \dots, x'_n), \quad (2)$$

with $x_i \equiv (\mathbf{r}_i, \sigma_i, \tau_i)$. The kinetic energy operator reads

$$\hat{T} = \sum_{i=1}^A \frac{\hbar^2}{2m_i} \nabla_i^2. \quad (3)$$

The goal of many-body quantum theory is to find the exact eigenstates $|\Psi_\alpha(x_1, \dots, x_A)\rangle$ of \hat{H} .

Electronic Structure Theory

For an isolated A -electron atomic or molecular system in the Born-Oppenheimer, non-relativistic approximation, the Hamiltonian reads [1]

$$\hat{H} = \hat{T} + \sum_{i=1}^A \hat{v}_{ext}(x_i) + \sum_{ij} \frac{e^2}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (4)$$

where

- Here $x_i \equiv \mathbf{r}_i$ (usually no spin, always no isospin);
- $\hat{V}_1 \equiv \hat{v}_{ext}(x_i)$ is the one-body potential representing the nucleus-electron Coulomb attraction;
- $\hat{V}_2 \equiv \frac{e^2}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$ is the two-body potential representing the electron-electron repulsion.

In other words, the full A -body Hamiltonian is *completely known*, and only involves two-body potentials. Eigenstates of the two-body Hamiltonian, however, are still A -body wave functions!

Nuclear Structure Theory

For an isolated A -nucleon system in the non-relativistic approximation, the Hamiltonian reads

$$\hat{H} = \hat{T} + \hat{V}_2 + \cdots + \hat{V}_A, \quad (5)$$

where

- There are no one-body terms = no external potential to confine the nucleus, the system is *self-bound*;
- The two-body term \hat{V}_2 contains the Coulomb potential seen before;
- The nuclear part of the two-body potential can be probed by scattering experiments: it has a hard-core and a finite-range;
- There is evidence that three-body terms are necessary, at least in light nuclei.

Everything else comes from other theoretical models: QCD, lattice QCD, effective field theory, etc.

Introducing Effective Forces

The nuclear mean-body problem combines two difficulties:

- As in a electronic structure theory, we must find methods to obtain the A -body eigenstates of the Hamiltonian but...
- ...contrary to electronic structure theory, the actual Hamiltonian is unknown.

How to turn a weakness (ignorance of \hat{H}) into a strength?

- *Fix the form* of the many-body ground state wave function $|\Psi\rangle$, e.g., a single Slater determinant, or a HFB vacuum, or a RPA form, etc. We will note $|\Phi\rangle$ such a *reference state*;
- Invent a good potential \hat{V}_0 ($\hat{H}_0 = \hat{T} + \hat{V}_0$), which we will call *pseudopotential*, such that $\langle\Phi|\hat{H}_0|\Phi\rangle$ is really close, e.g. to the observed ground-state energy, $\langle\Phi|\hat{H}_0|\Phi\rangle \approx \langle\Psi|\hat{H}|\Psi\rangle = E^{\text{exp}}$

This is the exact opposite of *ab initio* methods which, based on a given Hamiltonian (assumed to be the true one), try and find the exact wave functions $|\Psi_\alpha\rangle$ (with all its complications).

Hierarchy of Reference States

Acronym	Reference State
Spherical HF	$ \Phi\rangle = \text{HF}\rangle$
Deformed HF	$ \Phi\rangle = \text{HF}(\mathbf{q})\rangle, \hat{J}^2$ broken
Deformed HFB	$ \Phi\rangle = \text{HFB}(\mathbf{q})\rangle, \hat{J}^2, \hat{N}$ broken
Deformed QRPA	$ \Phi\rangle \propto \sum_{\mu\nu} \beta_{\mu}^{\dagger} \beta_{\nu}^{\dagger} \text{HFB}(\mathbf{q})\rangle, \hat{J}^2, \hat{N}$ broken; Small amplitude collective motion (involving only a few s.p. or q.p.)
Projected HFB	$ \Phi\rangle = \hat{P}_N \hat{P}_{JM} \text{HFB}(\mathbf{q})\rangle, \hat{J}^2, \hat{N}$ restored
Projected GCM	$ \Phi\rangle \propto \int d^N \mathbf{q} f(\mathbf{q}) \hat{P}_N \hat{P}_{JM} \text{HFB}(\mathbf{q})\rangle;$ Large amplitude collective motion (involving all s.p. or q.p.)

Handling Two-Body Potentials

Single-Particle Bases

We note $x \equiv (\mathbf{r}, \sigma, \tau)$ the generalized coordinates of a nucleon, and $|a\rangle$ a basis of s.p. states with $\langle x|a\rangle = \varphi_a(\mathbf{r}, \sigma, \tau) = \varphi(\mathbf{r}) \otimes \chi_\sigma \otimes \chi_\tau$.

The spin and isospin operators are Pauli matrices; We will denote them by $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$ for the spin, $\hat{\tau} = (\hat{\tau}_1, \hat{\tau}_2, \hat{\tau}_3)$ for the isospin.

We have: $\hat{\sigma}_z|\sigma\rangle = \sigma|\sigma\rangle$ and $\hat{\tau}_3|\tau\rangle = \tau|\tau\rangle$, with $\sigma, \tau = \pm 1/2$ and $\tau = 1/2$ (neutrons) and $\tau = -1/2$ (protons).

We use the generic notation

$$\int dx \equiv \int d^3\mathbf{r} \sum_{\sigma=\pm 1/2} \sum_{\tau=\pm 1/2} \quad (6)$$

Resolution of the identity

$$1 = \sum_a |a\rangle\langle a| = \int dx |x\rangle\langle x| = \int d^3\mathbf{r} \sum_{\sigma,\tau} |\mathbf{r}\sigma\tau\rangle\langle \mathbf{r}\sigma\tau| \quad (7)$$

Matrix Elements of a Two-Body Operator

We consider two-body matrix elements of a generic, non-local, operator $\hat{V}(x_1, x_2, x'_1, x'_2)$, in the basis of states $|a\rangle$, i.e., quantities of the type

$$v_{abcd} = (ab|\hat{V}|cd). \quad (8)$$

For multi-fermion systems, the matrix elements of the potential (or the potential itself) must be antisymmetrized

$$\bar{v}_{abcd} = v_{abcd} - v_{abdc} \quad \text{or} \quad \bar{v}_{abcd} = \langle ab|\hat{V}|cd\rangle = (ab|\hat{\mathcal{V}}|cd), \quad (9)$$

with

$$\hat{\mathcal{V}}(x_1, x_2, x'_1, x'_2) = \hat{V}(x_1, x_2, x'_1, x'_2)(1 - \hat{P}_r\hat{P}_\sigma\hat{P}_\tau). \quad (10)$$

In coordinate space, the matrix elements are

$$(x_1x_2|\hat{V}|x'_1, x'_2) = (\sigma_1, \tau_1, \sigma_2, \tau_2|\hat{V}(x_1, x_2, x'_1, x'_2)|\sigma'_1, \tau'_1, \sigma'_2, \tau'_2). \quad (11)$$

Common Types of Two-Body Operators

- Local potentials,

$$\hat{V}(x_1, x_2) = \hat{V}(x_1, x_2, x'_1, x'_2)\delta(x_1 - x'_1)\delta(x_2 - x'_2). \quad (12)$$

Recall that this means (for momentum space, replace r with p),

$$\begin{aligned} \hat{V}(x_1, x_2) = & \hat{V}(x_1, x_2, x'_1, x'_2) \\ & \times \delta(\mathbf{r}_1 - \mathbf{r}'_1)\delta_{\sigma_1\sigma'_1}\delta_{\tau_1\tau'_1}\delta(\mathbf{r}_2 - \mathbf{r}'_2)\delta_{\sigma_2\sigma'_2}\delta_{\tau_2\tau'_2}. \end{aligned} \quad (13)$$

The term $\delta_{\sigma_1\sigma'_1}$ means that, in a quantity such as v_{abcd} , we would have $\sigma_a = \sigma_c$ and $\sigma_b = \sigma_d$ (same for isospin projection, i.e. neutron or proton nature of the s.p. states).

- Zero-range, local potentials (here in coordinate space),

$$\hat{V}(x_1, x_2) = \hat{V}(x_1, x_2)\delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (14)$$

Spin-isospin Expansion of One-Body Operators

An arbitrary, possibly non-local, one-body operator \hat{U} acting in space, spin- and isospin-space can be written

$$\hat{U}(x, x') = \sum_{\mu=0,x,y,z} \sum_{k=0,1,2,3} \hat{U}_{\mu k}(\mathbf{r}, \mathbf{r}') \hat{\sigma}_{\mu} \hat{\tau}_k \quad (15)$$

with

- $\hat{\sigma}_{\mu}$ ($\mu = x, y, z$) is the μ -component of the spin 1/2 operator (=Pauli matrix) and lives in $SU(2)$ space;
- $\hat{\tau}_k$ ($k = 1, 2, 3$) is the k -component of the isospin operator. It is also a Pauli matrix, also lives in $SU(2)$, but not the same $SU(2)$ as the spin operator;
- $\hat{U}_{\mu k}(\mathbf{r}, \mathbf{r}')$ is a purely spatial *operator*: it can depend on gradients, etc., but does not contain any spin or isospin dependence anymore;
- $\hat{\sigma}_0$ and $\hat{\tau}_0$ are the unit 2×2 matrices.

Spin-isospin Expansion of Two-Body Operators

The spin-isospin expansion can be generalized to arbitrary, non-local, two-body operators,

$$\hat{V}(x_1, x_2, x'_1, x'_2) = \sum_{\mu k} \hat{V}_{\mu k}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}'_1, \mathbf{r}'_2) \hat{\sigma}_{\mu}^{(1)} \hat{\sigma}_{\mu}^{(2)} \hat{\tau}_k^{(1)} \hat{\tau}_k^{(2)}. \quad (16)$$

The spin and isospin operators appear in a *tensor* product in the space $(SU(2) \otimes SU(2))_1 \otimes (SU(2) \otimes SU(2))_2$ representing the spin and isospin of each of the two nucleons.

For n -body operators

$$\begin{aligned} \hat{V}(x_1, \dots, x_n, x'_1, \dots, x'_n) \\ = \sum_{\mu k} \hat{V}_{\mu k}(\mathbf{r}_1, \dots, \mathbf{r}_n, \mathbf{r}'_1, \dots, \mathbf{r}'_n) \prod_{\alpha=1}^n \hat{\sigma}_{\mu}^{(\alpha)} \prod_{\beta=1}^n \hat{\tau}_k^{(\beta)}, \end{aligned} \quad (17)$$

Hartree-Fock Interaction Energy (1/2)

In configuration space (in a basis), the HF energy for a potential \hat{V} is given by

$$E_{\text{int}} = \frac{1}{2} \sum_{abcd} \bar{v}_{abcd} \rho_{db} \rho_{ca}. \quad (18)$$

This expression does not say anything about the locality (or lack thereof) of the potential.

In coordinate space, introduce the decomposition of the antisymmetrized potential

$$\hat{\mathcal{V}} = \hat{V}(1 - \hat{P}_r \hat{P}_\sigma \hat{P}_\tau) = \hat{V}^D - \hat{V}^E \hat{P}_r, \quad (19)$$

- \hat{V}^D is the *direct* potential (or Hartree term);
- \hat{V}^E is the *exchange* potential (or Fock term).

Next, consider the HF interaction energy for a *local* pseudopotential in coordinate space.

Hartree-Fock Interaction Energy (2/2)

$$\begin{aligned}
 E_{\text{int}} = & \frac{1}{2} \int d^3 \mathbf{r}_1 \int d^3 \mathbf{r}_2 \sum_{\sigma\sigma', \tau\tau'} (\sigma_1\tau_1, \sigma_2\tau_2 | \hat{V}^D(\mathbf{r}_1, \mathbf{r}_2) | \sigma'_1\tau'_1, \sigma'_2\tau'_2) \\
 & \rho(\mathbf{r}_1\sigma'_1\tau'_1, \mathbf{r}_1\sigma_1\tau_1) \rho(\mathbf{r}_2\sigma'_2\tau'_2, \mathbf{r}_2\sigma_2\tau_2) \\
 - & \frac{1}{2} \int d^3 \mathbf{r}_1 \int d^3 \mathbf{r}_2 \sum_{\sigma\sigma', \tau\tau'} (\sigma_1\tau_1, \sigma_2\tau_2 | \hat{V}^E(\mathbf{r}_1, \mathbf{r}_2) | \sigma'_1\tau'_1, \sigma'_2\tau'_2) \\
 & \rho(\mathbf{r}_2\sigma'_1\tau'_1, \mathbf{r}_1\sigma_1\tau_1) \rho(\mathbf{r}_1\sigma'_2\tau'_2, \mathbf{r}_2\sigma_2\tau_2). \quad (20)
 \end{aligned}$$

Using the spin-isospin expansion

$$\begin{aligned}
 E_{\text{int}} = & \frac{1}{2} \int d^3 \mathbf{r}_1 \int d^3 \mathbf{r}_2 \sum_{\mu k} \hat{V}_{\mu k}^D(\mathbf{r}_1, \mathbf{r}_2) \rho_{\mu k}(\mathbf{r}_1) \rho_{\mu k}(\mathbf{r}_2) \\
 - & \frac{1}{2} \int d^3 \mathbf{r}_1 \int d^3 \mathbf{r}_2 \sum_{\mu k} \hat{V}_{\mu k}^E(\mathbf{r}_1, \mathbf{r}_2) \rho_{\mu k}(\mathbf{r}_2, \mathbf{r}_1) \rho_{\mu k}(\mathbf{r}_1, \mathbf{r}_2). \quad (21)
 \end{aligned}$$

On Locality

The direct contribution to the energy only depends on *local densities*, while the exchange term involves *non-local densities*. Locality has, therefore, two different meanings:

- In the theory of effective pseudopotentials, “local” refers to potentials and means $\hat{V}(x_1, x_2, x'_1, x'_2)$ does not depend on x'_1 and x'_2 ; a looser interpretation is that \hat{V} does not depend on r'_1 and r'_2 but possibly on $\sigma'_1, \tau'_1, \sigma'_2$ and τ'_2 ;
- In density functional theory (DFT) (and its variant the energy density functional (EDF) approach), “local” refers to the densities involved.

As should be visible from the previous slide, the exchange term for zero-range potentials is formally identical to the direct term as it involves only local densities (although the latter may be constructed from non-local densities, see later); only for finite-range potentials do the exchange term require explicitly non-local densities.

Non-relativistic Effective Pseudopotentials

Essential Ingredients

Nucleons are considered as pointlike particles characterized by their position r (or momentum p), their intrinsic spin projection $\sigma = \pm 1/2$ and their isotopic spin projection $\tau = \pm 1/2$.

Until very recently, all effective pseudopotentials were two-body only; no three-body forces were considered since the 50^{ies}.

Some of the components of effective forces are the same as can be obtained from symmetry considerations: (i) a central potential, (ii) a spin-orbit force needed to reproduce the structure of doubly-magic nuclei, (iii) a tensor force.

In addition, many popular pseudopotentials include density-dependent terms (more later).

Since nucleons are fermions, they obey the Pauli principle; either the potential or the matrix elements must always be antisymmetrized.

The Skyrme Pseudopotential

Historic references are [2, 3]

$$\begin{aligned}\hat{v}_{\text{Skyrme}}(x_1, x_2) &= t_0(1 + x_0\hat{P}_\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2) \\ &+ \frac{1}{2}t_1(1 + x_1\hat{P}_\sigma)[\hat{\mathbf{k}}'^2\delta(\mathbf{r}_1 - \mathbf{r}_2) + \delta(\mathbf{r}_1 - \mathbf{r}_2)\hat{\mathbf{k}}^2] \\ &+ t_2(1 + x_2\hat{P}_\sigma)\hat{\mathbf{k}}'\delta(\mathbf{r}_1 - \mathbf{r}_2) \cdot \hat{\mathbf{k}} \\ &+ \frac{1}{6}t_3(1 + x_3\hat{P}_\sigma)\rho^\alpha(\mathbf{R}) \\ &+ iW_0(\hat{\sigma}_1 + \hat{\sigma}_2) \cdot \left[\hat{\mathbf{k}}' \wedge \delta(\mathbf{r}_1 - \mathbf{r}_2)\hat{\mathbf{k}} \right],\end{aligned}$$

where

$$\begin{cases} \mathbf{R} = \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \right), \\ \hat{\mathbf{k}} = -\frac{i}{2}(\vec{\nabla}_1 - \vec{\nabla}_2), \quad \hat{\mathbf{k}}' = -\frac{i}{2}(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2). \end{cases} \quad (22)$$

By convention, $\hat{\mathbf{k}}'$ acts on the left.

Skyrme Energy Density

The Skyrme HF interaction energy can be recast into

$$E_{\text{int}} = \int d^3\mathbf{r} \sum_{t=0,1} \chi_t(\mathbf{r}), \quad (23)$$

with $\chi(\mathbf{r})$ the *energy density functional* (EDF).

The time-even Hamiltonian density is

$$\chi_t^{(\text{even})}(\mathbf{r}) = C_t^{\rho\rho} \rho_t^2 + C_t^{\rho\Delta\rho} \rho_t \Delta\rho_t + C_t^{\rho\tau} \rho_t \tau_t + C_t^{\rho J} \mathbb{J}_t^2 + C_t^{\rho\nabla J} \rho_t \nabla \cdot \mathbf{J}_t. \quad (24)$$

The time-odd Hamiltonian density is

$$\chi_t^{(\text{odd})}(\mathbf{r}) = C_t^{ss} \mathbf{s}_t^2 + C_t^{s\Delta s} \mathbf{s}_t \cdot \Delta \mathbf{s}_t + C_t^{sT} \mathbf{s}_t \cdot \mathbf{T}_t + C_t^{sj} \mathbf{j}_t^2 + C_t^{s\nabla j} \mathbf{s}_t \cdot (\nabla \wedge \mathbf{j}_t). \quad (25)$$

The components of the energy density are functionals of a bunch of *local densities* all derived from the density matrix ρ .

Local Densities

Noting $\tau = n, p$ the type of nucleon, the densities relevant to the Skyrme EDF are

- Particle Density: $\rho_\tau(\mathbf{r}) = \sum_{\sigma} \rho_\tau(\mathbf{r}\sigma, \mathbf{r}\sigma);$

- Spin Density: $\mathbf{s}_\tau(\mathbf{r}) = \sum_{\sigma\sigma'} \rho_\tau(\mathbf{r}\sigma, \mathbf{r}\sigma') \langle \sigma' | \boldsymbol{\sigma} | \sigma \rangle;$

- Kinetic energy density: $\tau_\tau(\mathbf{r}) = \nabla \cdot \nabla' \rho_\tau(\mathbf{r}, \mathbf{r}') \Big|_{\mathbf{r}=\mathbf{r}'} ;$

- Spin current density:

$$\mathbb{J}_\tau(\mathbf{r}) = J_{\mu\nu,\tau}(\mathbf{r}) = \frac{1}{2i} (\nabla_\mu - \nabla'_\mu) s_{\nu,\tau}(\mathbf{r}, \mathbf{r}') \Big|_{\mathbf{r}=\mathbf{r}'} ;$$

- Current density: $\mathbf{j}_\tau(\mathbf{r}) = \frac{1}{2i} (\nabla - \nabla') \rho_\tau(\mathbf{r}, \mathbf{r}') \Big|_{\mathbf{r}=\mathbf{r}'} ;$

- Spin kinetic energy density: $\mathbf{T}_\tau(\mathbf{r}) = \nabla \cdot \nabla' \mathbf{s}_\tau(\mathbf{r}, \mathbf{r}') \Big|_{\mathbf{r}=\mathbf{r}'} ;$

Symmetries of Densities

The Skyrme EDF is a *real, scalar, time-even* and *isoscalar* quantity that depends on several *local densities* with different properties depending on symmetry operators \hat{S} [4, 5, 6, 7]

- Distinguish between isoscalar ($t = 0$) densities, $\rho_0 = \rho_n + \rho_p$ and isovector ($t = 1$) densities, $\rho_1 = \rho_n - \rho_p$;
- Densities entering the time-even (time-odd) Hamiltonian density are time-even (time-odd), e.g., $\hat{T}\rho\hat{T}^{-1} = +\rho$ (e.g., $\hat{T}s\hat{T}^{-1} = -s$);
- Usually, time-odd densities are identically zero because of the symmetries of the problem. Notable exceptions: g.s. of odd-even nuclei in the HF, HF+BCS or HFB approximation, etc.
- Attention: time-reversal symmetry here applies to the intrinsic frame of the nucleus; it is not the same as the time-reversal symmetry of, say, the *CPT* theorem;
- Symmetry operators such as point group symmetries can be used to simplify the numerical resolution of the HF equations.

Comments on the Skyrme Pseudopotential

The Skyrme *pseudopotential* is two-body only and is local in space, *but non-local in spin and isospin space*,

$$\hat{v}_{\text{Skyrme}}(x_1, x_2) = \hat{v}_{\text{Skyrme}}(x_1, x_2, x'_1, x'_2) \delta(\mathbf{r}_1 - \mathbf{r}'_1) \delta(\mathbf{r}_2 - \mathbf{r}'_2). \quad (26)$$

The pseudopotential has zero-range,

$$\hat{v}_{\text{Skyrme}}(x_1, x_2) = \hat{v}_{\text{Skyrme}}(x_1, x_2) \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (27)$$

Formally, exchange terms are not distinguishable of direct terms.

One sometimes add a *tensor force* to improve the description of shell structure [8, 9]. Below, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$,

$$\begin{aligned} \hat{v}^t(\mathbf{r}) = \frac{1}{2} t_e \left\{ [3(\boldsymbol{\sigma}_1 \cdot \mathbf{k}')(\boldsymbol{\sigma}_2 \cdot \mathbf{k}') - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \mathbf{k}'^2] \delta(\mathbf{r}) \right. \\ \left. + \delta(\mathbf{r}) [3(\boldsymbol{\sigma}_1 \cdot \mathbf{k})(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \mathbf{k}^2] \right\} \\ + t_o [3(\boldsymbol{\sigma}_1 \cdot \mathbf{k}') \delta(\mathbf{r})(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \mathbf{k}' \cdot \delta(\mathbf{r}) \mathbf{k}]. \quad (28) \end{aligned}$$

Density Dependencies

The t_3 term in the Skyrme force was introduced a long time ago to mock up three-body forces [3].

Because of this term, one can not write the Skyrme or Gogny nuclear Hamiltonian in a strict second quantization form [10].

The corresponding terms in the EDF are

$$C_t^{\rho\rho} = C_{t0}^{\rho\rho} + C_{tD}^{\rho\rho}\rho_0^\alpha \quad \text{and} \quad C_s^{ss} = C_{s0}^{ss} + C_{sD}^{ss}\rho_0^\alpha. \quad (29)$$

When computing the HF potential, this density dependency adds a *rearrangement* term

$$\Gamma_t^{\text{rearr.}} = \delta_{t0} \sum_{t'=0,1} \left(\frac{\partial C_t^{\rho\rho}}{\partial \rho_0} \rho_{t'}^2 + \frac{\partial C_s^{ss}}{\partial \rho_0} \mathbf{s}_{t'}^2 \right) \quad (30)$$

Density dependencies are also the source of formal difficulties when going beyond HF with pseudopotentials, see Week 3.

The Gogny Pseudopotential

Historic references are [11, 12]

$$\begin{aligned}\hat{v}_{\text{Gogny}}(x_1, x_2) &= \sum_{i=1,2} \left(W_i + B_i \hat{P}_\sigma - H_i \hat{P}_\tau - M_i \hat{P}_\sigma \hat{P}_\tau \right) e^{-\frac{(\mathbf{r}_1 - \mathbf{r}_2)^2}{\mu_i^2}} \\ &+ \frac{1}{6} t_3 (1 + x_3 \hat{P}_\sigma) \rho^\alpha(\mathbf{R}) \\ &+ iW_0 (\hat{\sigma}_1 + \hat{\sigma}_2) \cdot \left[\hat{\mathbf{k}}' \wedge \delta(\mathbf{r}_1 - \mathbf{r}_2) \hat{\mathbf{k}} \right].\end{aligned}$$

The interaction is also two-body only, local in space only, i.e. non-local in spin and isospin space, but it has a *finite range* (main difference with Skyrme).

In its standard form, the density dependent term and the spin-orbit term are identical (formally, actual value of parameters may be different) to the Skyrme force.

Comments on the Gogny Pseudopotential

Like the Skyrme pseudopotential, the Gogny pseudopotential is two-body and local in space only, non-local in spin and isospin space.

The finite-range of the central potential implies that the energy density $\chi_t(\mathbf{r}, \mathbf{r}')$ is non-local.

Exchange terms are clearly distinguishable of direct terms.

A Skyrme-like central potential (terms t_0, t_1, t_2) can be obtained as an expansion of the Gaussian term up to second-order in momentum space.

The finite-range of the potential makes calculations with the Gogny force substantially more expensive than with the Skyrme force. The French group (Dechargé, Berger, Hilaire, etc.) at CEA Bruyères-le-Châtel and the Spanish group (Egido, Robledo) at the Universidad Autonoma de Madrid have developed most of the DFT technology with the Gogny force.

The Coulomb Potential

Since protons carry an electric charge, the nuclear Hamiltonian also contains the two-body, local, finite-range Coulomb force

$$\hat{V}_{\text{Cou}}(\mathbf{r}_1, \mathbf{r}_2) = \frac{e^2}{4\pi\epsilon_0} \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (31)$$

The direct Coulomb HF potential is local and given by

$$\Gamma_{\text{Cou}}^{(\text{dir})}(\mathbf{r}) = \frac{e^2}{4\pi\epsilon_0} \int d^3\mathbf{r}' \frac{\rho_p(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (32)$$

while the non-local exchange contribution to the HF potential is

$$\Gamma_{\text{Cou}}^{(\text{exc})}(\mathbf{r}, \mathbf{r}') = \frac{e^2}{4\pi\epsilon_0} \frac{\rho_p(\mathbf{r}', \mathbf{r})}{|\mathbf{r} - \mathbf{r}'|}. \quad (33)$$

The Pairing Channel in the HFB Theory

The starting point of the HFB theory is the ansatz that the g.s. wave-function is a quasiparticle vacuum, with the quasi-particle transformation given by the Bogoliubov transformation.

As a consequence, contractions of the type $\langle \Psi | c_a c_b | \Psi \rangle / \langle \Psi | \Psi \rangle$ are non-zero, which defines the pairing tensor κ_{ab} .

The HFB interaction energy is given (in configuration space) by

$$E = \sum_{ab} t_{ab} \rho_{ba} + \frac{1}{2} \sum_{abcd} \bar{v}_{abcd} \rho_{db} \rho_{ca} + \frac{1}{4} \sum_{abcd} \bar{v}_{abcd} \kappa_{ab}^* \kappa_{cd}. \quad (34)$$

The third term is the pairing energy,

$$E_{\text{pair}} = \frac{1}{4} \sum_{abcd} \bar{v}_{abcd} \kappa_{ab}^* \kappa_{cd}. \quad (35)$$

Phenomenological Pairing Forces

The HFB theory suggests that pairing correlations are described by the same pseudopotential that generates the mean-field, only contracted with a different object, i.e., the pairing tensor.

However, there are “good” reasons to take a different potential in the pairing channel (leading role of the p.h. channel, difficulty to constrain effectively the p.p. channel, etc.).

Standard pairing forces are local and zero-range [13]

$$\hat{V}_{\text{pair}}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{t=n,p} V_t \left(1 - \alpha \frac{\rho(\mathbf{R})}{\rho_0} \right) \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad (36)$$

with $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, $\rho_0 = 0.16 \text{ fm}^{-3}$ is the saturation density. If $\alpha = 1$, we have a *surface* pairing force, if $\alpha = 0$ we have a *volume* pairing force; oftentimes, $\alpha = 1/2$.

Three-Body Skyrme-like Potentials

Three-body, local, zero-range pseudopotentials with similar gradient terms as the two-body Skyrme [14, 15]:

$$\hat{V}_{3N}^{\text{Skyrme}} = \sum_{i=1}^N \hat{G}_i(\hat{P}_{123}^u, \hat{\mathbf{k}}, \hat{\mathbf{k}}') \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_2 - \mathbf{r}_3), \quad (37)$$

with

- \hat{P}_{123}^u the space-, spin- or isospin-exchange operator between any two coordinate, spin projection or isospin projection of the 3 particles
- $\hat{\mathbf{k}} = \frac{1}{2i}(\nabla_p - \nabla_{p'})$, $p, p' = 1, 2, 3$ the relative momentum (acting on the right) for all combinations of any 2 of the 3 particles; similar for $\hat{\mathbf{k}}'$, only acting on the left.
- \hat{G}_i are scalar operators that are functions of $\hat{\mathbf{k}}^2$, $\hat{\mathbf{k}}'^2$ and $\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'$ and the exchange operators.

Momentum-Dependent Local Finite-Range Potentials

Energy- or momentum-dependent, local, finite-range potentials [16]

$$\hat{V}(x_1, x_2) \propto \left(W + B\hat{P}_\sigma - H\hat{P}_\tau - M\hat{P}_\sigma\hat{P}_\tau \right) \\ \times \hat{O}(\hat{\mathbf{k}}, \hat{\mathbf{k}}')\delta(\mathbf{r}'_1 - \mathbf{r}_1)\delta(\mathbf{r}'_2 - \mathbf{r}_2)g_a(\mathbf{r}_1 - \mathbf{r}_2), \quad (38)$$

with $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$ are relative momenta (both acting on the right), $\hat{O}(\hat{\mathbf{k}}, \hat{\mathbf{k}}')$ a scalar function of $\hat{\mathbf{k}}^2$, $\hat{\mathbf{k}}'^2$ and $\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'$, and $g_a(\mathbf{r})$ a normalized Gaussian function (for example). Such expressions generalize the Gogny pseudo-potential.

The goal of both $3N$ zero-range Skyrme-like and momentum-dependent finite-range local pseudopotentials is to eliminate the need for density-dependent terms and, therefore, obtain a genuine second-quantized Hamiltonian.

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