Now we solve the many-body Hamiltonian with two-body forces only, that is, with the Hamiltonian of (5.35). The expectation value with the wavefunction (5.121) is

$$\begin{aligned}\langle\phi|H|\phi\rangle = &-\frac{\hbar^2}{2m}\sum_i^A \int \psi_i^*(\mathbf{r})\nabla^2\psi_i(\mathbf{r})d^3r \\ &+\frac{1}{2}\sum_{ij}^A \iint \psi_i^*(\mathbf{r})\psi_j^*(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\psi_i(\mathbf{r})\psi_j(\mathbf{r}')d^3rd^3r' \\ &-\frac{1}{2}\sum_{ij}^A \iint \psi_i^*(\mathbf{r})\psi_j^*(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\psi_i(\mathbf{r}')\psi_j(\mathbf{r})d^3rd^3r'. \end{aligned} \tag{5.124}$$

The last term is a consequence of antisymmetrization. Applying the variation on $\psi_i(r)$ we obtain

$$\begin{aligned}-\frac{\hbar^2}{2m}\nabla^2\psi_i(\mathbf{r}) + &\sum_j^A \int d^3r'\psi_j^*(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\psi_j(\mathbf{r}')\psi_i(\mathbf{r}) \\ &-\sum_j^A \int d^3r'\psi_j^*(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\psi_j(\mathbf{r})\psi_i(\mathbf{r}') = \epsilon_i\psi_i(\mathbf{r}) \end{aligned} \tag{5.125}$$

where ϵ_i is seen as a Lagrange multiplier that enforces the constraint (5.123). It has the significance of a single particle energy.

We can rewrite (5.125) as

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(\mathbf{r}) + \int d^3r'U(\mathbf{r},\mathbf{r}')\psi_i(\mathbf{r}') = \epsilon_i\psi_i(\mathbf{r}), \tag{5.126}$$

where $U(r,r')$ is the self-consistent field

$$U(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\sum_j^A \int d^3r'\,v(\mathbf{r},\mathbf{r}')\psi_j(\mathbf{r}')\psi_j^*(\mathbf{r}') - \sum_j^A v(\mathbf{r},\mathbf{r}')\psi_j(\mathbf{r})\psi_j^*(\mathbf{r}'). \tag{5.127}$$

The first term is the direct term (*Hartree field*). The second is called the exchange interaction and is nonlocal. This nonlocality is closely related to the range of the two-body interaction. If we use a δ-force, then the Fock (or exchange) term is also local.

In constructing the HF (Hartree-Fock) determinant one naturally selects the A lowest energy wavefunctions. Thus the HF state corresponds to a Fermi sea of particles with a sharp Fermi surface.

As in the Hartree method, one guesses an initial $U^{(0)}$, solves (5.126), finds ψ_i, calculates (5.127), finds new $\psi_i's$, and so on, until the desired accuracy is achieved.

5.10.2 The Skyrme interaction

The most popular effective interaction used in Hartree-Fock calculations is the *Skyrme interaction*. It is based on the fact that a finite range interaction can be simulated by a momentum dependence. This can be shown by transforming an interaction $V(r)$, where

$r = r_1 - r_2$, into momentum space,

$$\langle \mathbf{p}\,|v|\mathbf{p}'\rangle = \frac{1}{(2\pi\hbar)^3}\int e^{-i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar}\,v(\mathbf{r})d^3r. \tag{5.128}$$

This integral gives a constant if $v(r) = \delta(r)$. A finite range $v(r)$ will represent a p-dependence in momentum space.

The simplest form that one may find for $\langle p\,|v|p'\rangle$ which is rotationally invariant is

$$(2\pi\hbar)^3\langle \mathbf{p}\,|v|\mathbf{p}'\rangle = v_0 + v_1\,\mathbf{p}'^2 + v_1\,\mathbf{p}^2 + v_2\mathbf{p}\cdot\mathbf{p}', \tag{5.129}$$

which in coordinate space is related to the momentum-dependent operator

$$v(\mathbf{r}) = v_0\delta(\mathbf{r}) + v_1\left[\hat{\mathbf{p}}^2\delta(\mathbf{r}) + \delta(\mathbf{r})\,\hat{\mathbf{p}}^2\right] + v_2\,\hat{\mathbf{p}}\cdot\delta(\mathbf{r})\hat{\mathbf{p}}. \tag{5.130}$$

The Skyrme interaction is based on this property and is an effective interaction with a three-body term [Sk57, Sk59]

$$v = \sum_{i<j} v(i,j) + \sum_{i<j<k} v(i,j,k). \tag{5.131}$$

For $v(i,j)$ one uses the form (5.130) with

$$\begin{aligned} v(1,2) = {} & t_0\,(1 + x_0\,P^\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2) + \frac{1}{2}\,t_1\left[\delta(\mathbf{r}_1 - \mathbf{r}_2)\hat{\mathbf{k}}^2 + \hat{\mathbf{k}}^2\,\delta(\mathbf{r}_1 - \mathbf{r}_2)\right] \\ & + t_2\,\hat{\mathbf{k}}\,\delta(\mathbf{r} - \mathbf{r}_2)\hat{\mathbf{k}} + i\,W_0\left[\boldsymbol{\sigma}^{(1)} + \boldsymbol{\sigma}^{(2)}\right]\left[\hat{\mathbf{k}}\times\delta(\mathbf{r}_1 - \mathbf{r}_2)\,\hat{\mathbf{k}}\right], \end{aligned} \tag{5.132}$$

where

$$\hat{\mathbf{k}} = \frac{1}{\hbar}\,\hat{\mathbf{p}} = \frac{1}{2i}(\nabla_1 - \nabla_2) \quad \text{and} \quad P^\sigma = \frac{1}{2}\left[1 + \boldsymbol{\sigma}^{(1)}\cdot\boldsymbol{\sigma}^{(2)}\right]. \tag{5.133}$$

with $\boldsymbol{\sigma}$ the Dirac matrices that act on the spin part of the wavefunctions. The three-body part of the Skyrme interaction is also taken as a zero range (δ-function) force,

$$v(1,2,3) = t_3\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_2 - \mathbf{r}_3). \tag{5.134}$$

The constants t_0, t_1, t_2, t_3, x_0, and W_0 are manipulated so as to adjust the experimental binding energies and radii. There are several sets of parameters, often called Skyrme I, II, etc. For example, the Skyrme III interaction uses

$$\begin{aligned} t_0 &= -1128.75\ \text{MeV fm}^3, & t_1 &= 395\ \text{MeV fm}^5, \\ t_2 &= -95\ \text{MeV fm}^5, & t_3 &= 1.4\times10^4\ \text{MeV fm}^6, \\ W_0 &= 120\ \text{MeV fm}^5, & x_0 &= 0.45. \end{aligned} \tag{5.135}$$

The parameter t_0 describes a pure δ-force with a spin-exchange; t_1 and t_2 simulate an effective range, as in (5.130). The fourth term in (5.132) represents a two-body spin-orbit interaction. It can be obtained from a normal spin-orbit term in the short range limit.

To implement numerically a Hartree-Fock calculation with the Skyrme potential a little more algebra is necessary. In a long but straightforward calculation, it can be shown [VB72]

that the HF equation in coordinate space becomes

$$\left\{-\nabla\frac{\hbar^2}{2m^*(\mathbf{r})}\nabla + U(\mathbf{r}) + \mathbf{W}\cdot\frac{1}{i}(\nabla\times\sigma)\right\}\psi_i(\mathbf{r}) = \epsilon_i\,\psi_i(\mathbf{r}), \tag{5.136}$$

where

$$m^*(\mathbf{r}) = m\left[1+\frac{2m}{\hbar^2}\frac{1}{16}(3t_1+5t_2)\rho\right]^{-1}, \tag{5.137}$$

$$\begin{aligned}U(\mathbf{r}) = {}& \frac{3}{4}\,t_0\,\rho + \frac{3}{16}\,t_3\rho^2 + \frac{1}{16}(3t_1+5t_2)\tau \\ & + \frac{1}{32}(5t_2-9t_1)\nabla^2\rho - \frac{3}{4}\,W_0\,\nabla\cdot\mathbf{J},\end{aligned} \tag{5.138}$$

and

$$\mathbf{W}(\mathbf{r}) = \frac{3}{4}\,W_0\,\nabla\rho. \tag{5.139}$$

In the equations above,

$$\rho(\mathbf{r}) = \sum_{i,s,t}|\psi_i(\mathbf{r},s,t)|^2 \tag{5.140}$$

is the nucleon density,

$$\tau(\mathbf{r}) = \sum_{i,s,t}|\nabla\,\psi_i(\mathbf{r},s,t)|^2 \tag{5.141}$$

is the kinetic energy density, and

$$\mathbf{J}(\mathbf{r}) = -i\sum_{j,t,s,s'}\psi_j^*(\mathbf{r},s,t)\left[\nabla\psi_j(\mathbf{r},s',t)\times\sigma_{ss'}\right] \tag{5.142}$$

is the "spin-orbit density." s and t denote the spin and isospin quantum numbers, respectively.

We observe that $U(r)$ is local and (5.136) is a pure differential equation. The nonlocality appears only in the r-dependence of $m^*(r)$, the effective nucleon mass. For spherical symmetry (5.136) reduces to a one-dimensional differential equation of second order in the radial coordinate r. Then the spin-orbit term in (5.138) becomes

$$\frac{3}{2}\,W_0\left(\frac{1}{r}\frac{\partial}{\partial r}\rho\right)\mathbf{l}\cdot\mathbf{s}, \tag{5.143}$$

well known in the shell model.

5.10.3 *Relativistic mean field theory*

The *relativistic mean field* theory for the nuclear dynamics is based on a Lagrangian density (see Appendix D) that ascribes to each nucleon a Dirac field (or spinor) ψ_i which interacts with meson fields, that is, the nucleon-nucleon interaction is assumed to arise from the exchange of mesons.