Derivation of the Central Term of the Skyrme Energy Functional

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We show how to derive the energy density from the central part of the Skyrme force. Its antisymmetrized form is

$$\hat{\bar{v}}(x_1, x_2) = t_0(1 + x_0\hat{P}_\sigma)\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)(1 - \hat{P}_x\hat{P}_\sigma\hat{P}_\tau), \tag{1}$$

and this operator acts on a two-body state $|ab\rangle$ (or alternatively $\psi_a(\boldsymbol{r}\sigma_a)\psi_b(\boldsymbol{r}\sigma_b)$).

1 Preliminaries

We do not consider proton neutron mixing, i.e., the density matrix reads, in configuration space

$$\rho_{ac} = \delta_{\tau_a\tau_c}\rho_{ac} = \delta_{\tau_a\tau_c}\rho_{ac}^{(\tau_a)} \tag{2}$$

Recall that the mean-field potential Γ reads

$$\Gamma_{ac} = \sum_{bd} \bar{v}_{abcd}\rho_{db} = \sum_{\tau_b\tau_d}\sum_{bd} \bar{v}_{abcd}\rho_{db}^{(\tau_d\tau_b)} = \sum_{\tau_b}\sum_{bd} \bar{v}_{abcd}\rho_{db}^{(\tau_b)}, \tag{3}$$

and the potential energy will be

$$E_{\text{int}} = \sum_{ac} \Gamma_{ac}\rho_{ca} = \sum_{\tau_a\tau_c}\sum_{ac} \Gamma_{ac}\rho_{ca}^{(\tau_c\tau_a)} = \sum_{\tau_a}\sum_{ac} \Gamma_{ac}\rho_{ca}^{(\tau_a)}, \tag{4}$$

Let's have a look at the action of $\hat{P}_\tau$ on the state $|cd\rangle$. The contribution of this term to the HF potential will be

$$\Gamma \propto \sum_{\tau_b\tau_d}\sum_{bd} \langle ab|\hat{v}\hat{P}_\tau|cd\rangle\rho_{db}^{(\tau_d\tau_b)} \propto \sum_{\tau_b\tau_d}\sum_{bd} \langle ab|\hat{v}|c^{\tau_d}d^{\tau_c}\rangle\rho_{db}^{(\tau_d\tau_b)} \tag{5}$$

The last equality implies $\tau_d = \tau_b = \tau_c$. Hence the action of isospin exchange operator reduces to a $\delta_{\tau_c \tau_d}$. Also, the space-exchange operator commutes with the Dirac delta function, and can be replaced by 1.

2 Coordinate Space Representation

Introducing the resolution of the identity, we find in general

$$v_{abcd} = (ab|\hat{v}|cd) = (ab|x_1 x_2)(x_1 x_2|\hat{v}|x_1' x_2')(x_1' x_2'|cd) \tag{6}$$

with $x \equiv (\boldsymbol{r}, \sigma)$. For our spatially-local Skyrme potential, this gives

$$v_{abcd} = \int d^3\boldsymbol{r}_1 \int d^3\boldsymbol{r}_2 \sum_{\sigma_a \sigma_b \sigma_c \sigma_d} \psi_a^*(\boldsymbol{r}_1 \sigma_a) \psi_b^*(\boldsymbol{r}_2 \sigma_b) (\sigma_a \sigma_b|\hat{v}(x_1, x_2)|\sigma_c \sigma_d) \psi_c(\boldsymbol{r}_1 \sigma_c) \psi_d(\boldsymbol{r}_2 \sigma_d) \tag{7}$$

Hence, the HF potential becomes

$$\Gamma_{ac}^{(\tau_a)} = \sum_{\tau_b} \int d^3\boldsymbol{r}_1 \int d^3\boldsymbol{r}_2 \, \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) \sum_{bd} \rho_{db}^{(\tau_b)} \sum_{\sigma_a \sigma_b \sigma_c \sigma_d} \psi_a^*(\boldsymbol{r}_1 \sigma_a) \psi_b^*(\boldsymbol{r}_2 \sigma_b) \langle \sigma_a \sigma_b | t_0 (1 + x_0 \hat{P}_\sigma)(1 - \hat{P}_\sigma \delta_{\tau_b \tau_d}) | \sigma_c \sigma_d \rangle \psi_c(\boldsymbol{r}_1 \sigma_c) \psi_d(\boldsymbol{r}_2 \sigma_d). \tag{8}$$

Let us replace the spin-exchange operator by its expression

$$\hat{P}_\sigma = \frac{1}{2} (1 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2). \tag{9}$$

We find

$$\Gamma_{ac}^{(\tau_a)} = \sum_{\sigma_a \sigma_c} \sum_{\tau_b} \int d^3\boldsymbol{r}_1 \int d^3\boldsymbol{r}_2 \, \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2) \sum_{\sigma_b \sigma_d} \sum_{bd} \rho_{db}^{(\tau_b)} \psi_a^*(\boldsymbol{r}_1 \sigma_a) \psi_b^*(\boldsymbol{r}_2 \sigma_b) \langle \sigma_a \sigma_b | t_0 \left[\left(1 + \frac{1}{2} x_0\right) - \left(x_0 + \frac{1}{2}\right) \delta_{\tau_c \tau_d} \right] + \left(\frac{1}{2} x_0 - \delta_{\tau_c \tau_d}\right) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 | \sigma_c \sigma_d \rangle \times \psi_c(\boldsymbol{r}_1 \sigma_c) \psi_d(\boldsymbol{r}_2 \sigma_d). \tag{10}$$

3 The Spin-independent Component

We start by working out the part that does not depend on the Pauli matrices. It gives the following contribution to the mean-field,

$$\Gamma_{ac}^{(\tau_a)} = \sum_{\sigma_a\sigma_c}\sum_{\tau_b}\int d^3\boldsymbol{r}_1\int d^3\boldsymbol{r}_2\ \delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\sum_{\sigma_b\sigma_d}\sum_{bd}\rho_{db}^{(\tau_b)}\psi_a^*(\boldsymbol{r}_1\sigma_a)\psi_b^*(\boldsymbol{r}_2\sigma_b)$$
$$\times\ \langle\sigma_a\sigma_b|t_0\left[\left(1+\frac{1}{2}x_0\right)-\left(x_0+\frac{1}{2}\right)\delta_{\tau_c\tau_d}\right]|\sigma_c\sigma_d\rangle\psi_c(\boldsymbol{r}_1\sigma_c)\psi_d(\boldsymbol{r}_2\sigma_d). \quad (11)$$

The δ function allows us to simplify the double integral by eliminating one of the spatial dimensions. Moreover, since the spin-functions are orthonormal, we must have: $\sigma_a = \sigma_c$ (particle 1) and: $\sigma_b = \sigma_d$ (particle 2). We therefore obtain

$$\Gamma_{ac}^{(\tau_a)} = \delta_{\sigma_a\sigma_c}\sum_{\sigma_a\sigma_c}\sum_{\tau_b}\int d^3\boldsymbol{r}\ \psi_a^*(\boldsymbol{r}\sigma_a)\psi_c(\boldsymbol{r}\sigma_c)\sum_{\sigma_b}\delta_{\sigma_b\sigma_d}\sum_{bd}\rho_{db}^{(\tau_b)}\psi_b^*(\boldsymbol{r}\sigma_b)\psi_d(\boldsymbol{r}\sigma_d)$$
$$\times\ t_0\left[\left(1+\frac{1}{2}x_0\right)-\left(x_0+\frac{1}{2}\right)\delta_{\tau_c\tau_d}\right], \quad (12)$$

In the summations over indices b and d, we recognize the local density

$$\sum_{\sigma_b}\delta_{\sigma_b\sigma_d}\sum_{bd}\rho_{db}^{(\tau_b)}\psi_b^*(\boldsymbol{r}\sigma_b)\psi_d(\boldsymbol{r}\sigma_d) = \sum_{\sigma_b}\delta_{\sigma_b\sigma_d}\rho^{(\tau_b)}(\boldsymbol{r}\sigma_b,\boldsymbol{r}\sigma_d) = \rho^{(\tau_b)}(\boldsymbol{r}). \quad (13)$$

Therefore,

$$\Gamma_{ac}^{(\tau_a)} = \delta_{\sigma_a\sigma_c}\sum_{\sigma_a\sigma_c}\sum_{\tau_b}\int d^3\boldsymbol{r}\ \psi_a^*(\boldsymbol{r}\sigma_a)\psi_c(\boldsymbol{r}\sigma_c)\rho^{(\tau_b)}(\boldsymbol{r})$$
$$\times\ t_0\left[\left(1+\frac{1}{2}x_0\right)-\left(x_0+\frac{1}{2}\right)\delta_{\tau_c\tau_d}\right] \quad (14)$$

The total energy is given by

$$E_0^{(1)} = \frac{1}{2}\sum_{\tau_a}\sum_{ac}\Gamma_{ac}^{(\tau_a)}\rho_{ca}^{(\tau_a)}. \quad (15)$$

Following the exact same reasoning, it is straightforward to find that it reads

$$E = \frac{1}{2}\sum_{\tau_a\tau_b}\int d^3\boldsymbol{r}\ \rho^{(\tau_a)}(\boldsymbol{r})\rho^{(\tau_b)}(\boldsymbol{r})t_0\left[\left(1+\frac{1}{2}x_0\right)-\left(x_0+\frac{1}{2}\right)\delta_{\tau_a\tau_b}\right]. \quad (16)$$

We then work out explicitely the summations over the isospins τ_a and τ_b. Each of these indices run from $-1/2$ to $+1/2$, with $\tau = -1/2$ corresponding to protons, and $\tau = +1/2$ to neutrons. We find immediately

$$E = \int d^3\boldsymbol{r}\mathcal{H}(\boldsymbol{r}) \tag{17}$$

with

$$\boxed{\mathcal{H}(\boldsymbol{r}) = \frac{1}{2}t_0\left(1 + \frac{1}{2}x_0\right)\rho^2(\boldsymbol{r}) - \frac{1}{2}t_0\left(x_0 + \frac{1}{2}\right)[\rho_n^2(\boldsymbol{r}) + \rho_p^2(\boldsymbol{r})].} \tag{18}$$

4 The Spin-dependent Component

The spin-dependent component of the central term gives the following contribution to the mean-field,

$$\begin{aligned}\Gamma_{ac}^{(\tau_a)} = &\sum_{\sigma_a\sigma_c}\sum_{\tau_b}\int d^3\boldsymbol{r}_1\int d^3\boldsymbol{r}_2\ \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\sum_{\sigma_b\sigma_d}\sum_{bd}\rho_{db}^{(\tau_b)}\psi_a^*(\boldsymbol{r}_1\sigma_a)\psi_b^*(\boldsymbol{r}_2\sigma_b)\\ &\times\langle\sigma_a\sigma_b|t_0\left[\frac{1}{2}x_0 - \delta_{\tau_c\tau_d}\right]\left(\sum_\mu\hat{\sigma}_\mu^{(1)}\cdot\hat{\sigma}_\mu^{(2)}\right)|\sigma_c\sigma_d\rangle\psi_c(\boldsymbol{r}_1\sigma_c)\psi_d(\boldsymbol{r}_2\sigma_d).\end{aligned} \tag{19}$$

Again, the δ factor allows us to simplify integration. This leads to

$$\begin{aligned}\Gamma_{ac}^{(\tau_a)} = &\sum_{\sigma_a\sigma_c}\sum_{\tau_b}\int d^3\boldsymbol{r}\sum_\mu\left(\psi_a^*(\boldsymbol{r}\sigma_a)\psi_c(\boldsymbol{r}\sigma_c)\langle\sigma_a|\hat{\sigma}_\mu^{(1)}|\sigma_c\rangle\right)\\ &\times\left(t_0\left[\frac{1}{2}x_0 - \delta_{\tau_c\tau_d}\right]\sum_{\sigma_b\sigma_d}\sum_{bd}\rho_{db}^{(\tau_b)}\psi_b^*(\boldsymbol{r}\sigma_b)\psi_d(\boldsymbol{r}\sigma_d)\langle\sigma_b|\hat{\sigma}_\mu^{(2)}|\sigma_d\rangle\right).\end{aligned} \tag{20}$$

Introducing the spin density $\boldsymbol{s} = (s_x, s_y, s_z)$,

$$s_\mu(\boldsymbol{r}, \boldsymbol{r}') = \sum_{\sigma\sigma'}\rho(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma')\langle\sigma'|\hat{\sigma}_\mu|\sigma\rangle \tag{21}$$

we obtain, after reordering,

$$\begin{aligned}\Gamma_{ac}^{(\tau_a)} = &\sum_{\sigma_a\sigma_c}\sum_{\tau_b}\int d^3\boldsymbol{r}\sum_\mu\left(\psi_a^*(\boldsymbol{r}\sigma_a)\psi_c(\boldsymbol{r}\sigma_c)\langle\sigma_a|\hat{\sigma}_\mu^{(1)}|\sigma_c\rangle\right)\\ &\times t_0\left(\frac{1}{2}x_0 - \delta_{\tau_c\tau_d}\right)s_\mu^{(\tau_b)}(\boldsymbol{r})\end{aligned} \tag{22}$$

We then proceed similarly to compute the energy density by taking the trace of $\Gamma_{ac}^{(\tau_a)}$ times the density matrix $\rho_{ca}^{(\tau_a)}$. We find

$$\mathcal{H}(\boldsymbol{r}) = \frac{1}{2}\sum_{\mu}\sum_{\tau_a\tau_b} t_0 \left[\frac{1}{2}x_0 - \delta_{\tau_a\tau_b}\right] s_{\mu}^{(\tau_a)}(\boldsymbol{r}) s_{\mu}^{(\tau_b)}(\boldsymbol{r}). \tag{23}$$

We get rid of the isospin indices τ_a and τ_b following the exact same procedure as for the spin independent part and find

$$\boxed{\mathcal{H}(\boldsymbol{r}) = \frac{1}{4}t_0 x_0 \boldsymbol{s}^{\,2}(\boldsymbol{r}) - \frac{1}{2}t_0[\boldsymbol{s}_n^{\,2}(\boldsymbol{r}) + \boldsymbol{s}_p^{\,2}(\boldsymbol{r})].} \tag{24}$$

The total contribution to the energy density of the central term thus is

$$\boxed{\begin{aligned}\mathcal{H}(\boldsymbol{r}) = \frac{1}{2}t_0 \Bigg\{ \left(1 + \frac{1}{2}x_0\right) \rho^2(\boldsymbol{r}) - \left(x_0 + \frac{1}{2}\right) [\rho_n^2(\boldsymbol{r}) + \rho_p^2(\boldsymbol{r})] \\ + \frac{1}{2}x_0 \boldsymbol{s}^{\,2}(\boldsymbol{r}) - [\boldsymbol{s}_n^{\,2}(\boldsymbol{r}) + \boldsymbol{s}_p^{\,2}(\boldsymbol{r})] \Bigg\}. \quad (25)\end{aligned}}$$