Tools for incorporating a D-wave contribution in Skyrme energy density functionals

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The aim of this report is to introduce the D-wave, part of an effective force that describe a Skyrme type nucleon-nucleon interaction including next-to-next to leading order. One will particulary show that the D-wave can reproduce the equation of state in symmetric nuclear matter of each (S,T) channels. Moreover, to be able to include this D-wave in next fitting procedures, we will give the mean field equation in case of spherical symmetry.

1.1 A short introduction to the Skyrme model and the D-wave extension

The general context of the Skyrme force is low energy nuclear physics, more particularly the nuclear structure, where the many-body problem appears. Phenomenological effective forces, such as Skyrme[1] interaction, are used within a mean-field approach to solve it. The development is done using energy density functional method.

1.1.1 Skyrme pseudo-potential

The Skyrme interaction has been developped in the last 50's in an attempt to reproduce phenomenologically the nucleon-nucleon interaction in nuclear medium. The version presented below is the *standard* central part version, adapted from Skyrme's original interaction for practical and computational reasons by Vautherin and Brink [2].

$$
\begin{aligned}
v(\vec{r_1},\vec{r_2})_{Sk} = \quad & \mathbf{t_0}\ (1+\mathbf{x_0}\ P_\sigma)\ \delta(\vec{r}) && (1.1)\\
+ \quad & \frac{1}{6}\ \mathbf{t_3}\ (1+\mathbf{x_3} P_\sigma)\rho^{\boldsymbol{\alpha}}\delta(\vec{r}) && (1.2)\\
+ \quad & \frac{1}{2}\ \mathbf{t_1}\ (1+\mathbf{x_1}\ P_\sigma)\left[\vec{k}'^2\delta(\vec{r})+\delta(\vec{r})\vec{k}^2\right] && \\
+ \quad & \mathbf{t_2}\ (1+\mathbf{x_2}\ P_\sigma)\ \vec{k}'\cdot\delta(\vec{r})\vec{k} && (1.3)\\
+ \quad & i\mathbf{W_0}\ \vec{\sigma}\cdot\left[\vec{k}'\times\delta(\vec{r})\vec{k}\right], && (1.4)
\end{aligned}
$$

where $\vec{r}$ is the relative position of the two nucleons, $\vec{k}$ is the relative momentum (and $\vec{k}'$ its complex conjugate) and $\vec{\sigma}$ the sum of nucleon's spins. The 10 parameters are represented in bold.
The goal of such an interaction is to mimic the nucleon-nucleon interaction. This is consequently, as can be seen, a two-body interaction and the short range of nuclear forces is implemented by a zero-range approximation (given by the $\delta(\vec{r})$). Let's now investigate each of the terms.
The terms 1.1 and 1.2 are purely local since they don't have momentum dependence. The first is an attractive term and the second is short-range repulsive, these two properties being used to balance and reproduce the nuclear saturation density. One can notice the density dependence in 1.2. This interaction depending on the medium, this is not a "true" potential but a pseudo-potential.
Like nucleon-nucleon interaction is not sctricly zero-range, finite range effects are simulated with momentum dependences in 1.3.
Finally, the last term, 1.4, is the spin-orbit term.

This interaction has been mainly use in nuclear physics for several reasons : the zero-range allow analytic expressions and it can describe properties of magic or semi-magic nuclei such as ground-state energies or charge radii. However, improvements must be made for exotic nuclei or spectroscopic properties. Recently, the UNEDF collaboration [3] has concluded, after testing many parametrisations, that extensions for the standard Skyrme interaction are necessary to describe correctly the nuclear matter. The D-wave is a proposition of such an extension.

1.1.2 D-wave extension

Before getting straight to the D-wave equation, let's just recall that this name comes from the spectroscopic notation, where S means a contribution of a spherical harmonics of angular momentum ℓ equal to 0, where P-wave means ℓ =1 and D-wave is induced by a ℓ =2 contribution.[1]
The presence of non-negligeable D-wave contributions in nuclei has been confirmed by nucleon-nucleon scattering, as explained by Skyrme in his paper [1]. He tried to introduce a purely phenomenologic D-wave, but the latter had some pathologies and was abandonned by the time. Our D-wave, presented in Eq. (1.5), corrects some of its flaws.

1. It appears formally by expressing the cosines of the expression in terms of Legendre polynomials and then developping them on a spherical harmonic base. D-wave means here a $cos^2(\theta)$ contribution

The v_{Sk} is the potential presented in Eq.1.4 and the $\delta(\vec{r})$ are here implicit.

$$\begin{aligned} v_{tot} &= v_{Sk} + v_{D_{wave}} \\ v_{D_{wave}} &= +\frac{1}{4}\,\mathbf{t_1^{(4)}}(1+\mathbf{x_1^{(4)}}P_\sigma)\left[(\vec{k}^2+\vec{k'}^2)^2 + 4(\vec{k'}\cdot\vec{k})^2\right] \\ &\quad + \mathbf{t_2^{(4)}}(1+\mathbf{x_2^{(4)}}P_\sigma)(\vec{k'}\cdot\vec{k})(\vec{k}^2+\vec{k'}^2) \end{aligned} \tag{1.5}$$

First, it appears naturally in an expansion of gradients until 4th order, keeping all the terms that satisfies nuclear postulates. Unlike Skyrme's D-wave, it is also gauge invariant, which is necessary for a local interaction in order to assure conservation laws[4]. We chose, for convenient ways, to keep an analogy with *standard* terms, with a direct parameter and an exchange parameter in each of the terms. The new pseudo-potential including the D-wave is then composed of 14 parameters. The next section will present an application of such an interaction.

1.2 Nuclear (S,T) Channels Fit with D-wave extension

In order to test our new interaction, we have applied it on a naive and ideal model, the Infinite Symmetric Nuclear Matter, where the properties that one have to reproduce are well known ; and which is the first step toward the description of the nucleus. In this context, the objective was to fit the global equation of state and the nuclear (S,T) channels on datas obtained throught Brueckner-Hartree-Fock (BHF) calculations using a realistic nucleon-nucleon interaction.

Let's remember that the nucleon-nucleon interaction can be separate into four channels, which corresponds to the different ways 2 nucleons can interact together. To better understand how the channels can be obtained, one just have to remember that nucleons are fermions, with a 1/2 spin momentum, and that protons and neutrons can be discrimated by introducing the isospin, in an analogue way as spin, the projection +1/2 being the proton and -1/2 being the neutron, by convention. The total spin can then be S=0 or S=1 and the total isospin, which is noted T, can also be T=0 or T=1. There is consequently 4 possibles couples (S=0,T=0),(S=1,T=0),(S=0,T=1),(S=1,T=1), usually called the four nuclear (S,T) channels.

We derive the equation of state of our interaction in Infinite Nuclear Matter, and we have then be able to fit them on BHF calculations, which is presented in Fig.1.1. We also made this for the sum of the channels, the global equation of state ; where the known properties of infinite nuclear matter can be deduced. If the latter is in general reproduced by standard Skyrme interactions, it was not yet the case for the (S,T) channels. [2]

2. The fit of the global equation of state is indeed good for the three interactions, which is why it has not been incorporated here, but has been used to determine the properties in table 1.2

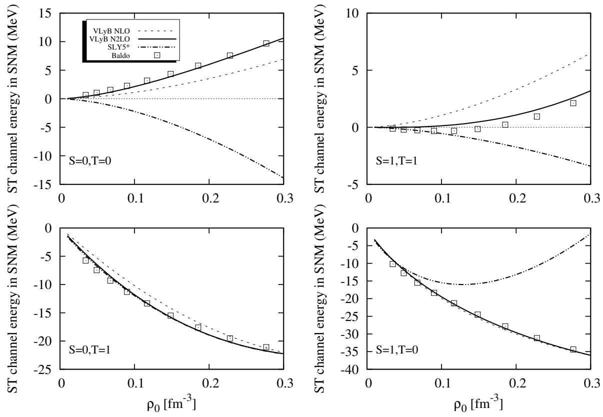

FIGURE 1.1 – Fit of nuclear (S,T) channels with our D-wave interaction (N2LO), the standard Skyrme interaction (NLO), and SLy5. Datas have been given by Baldo (points), with BHF calculations

If we examine our fit, we can see that, if the standard Skyrme interaction (NLO) can't reproduce the nuclear (S,T) channels like we told before, the interaction with the D-wave (in full lines) can properly reproduce the four of them. Compairison is made with SLy5, a well-known parametrisation of Skyrme's standard interaction which has not be fitted here, but with experimental constraints (nuclei masses, charge radii). We can see that it can't reproduce nuclear channels either. Since the D-wave interaction can reproduce them, we hope its new flexibility will manage to reproduce both (S,T) channels and experimental constraints. Moreover, concerning the properties of the infinite nuclear matter obtained with the fit, they are in agreement with theoretical values (see Table1.2).

SNM Properties	Fit values (D_{wave})	Theoretical values
ρ_{sat} (fm^{-3})	0.18	0.16
$(E/A)_{sat}$ (Mev)	-15.9	-16
K_∞ (Mev)	242	210

TABLE 1.1 – Compairison of theoretical known values and D-wave interaction fit values for some SNM properties

1.3 Mean-field equation in Spherical Symmetry

The fact that adding the D-wave allow the fit of the nuclear (S,T) channels for the first time with a Skyrme interaction has led us to want to implement it in nucleus calculations. To do such a thing, we had to use the density functional method to obtain the functional corresponding to our interaction. More details on this point can be found in [5]. Once the functional obtained, we derive it with a variational method to find the mean-field differential equation we have to solve in order to do ajustment of our interaction and then calculate nuclei.

We were searching an equation of the form

$$\hat{h}_q(\vec{r})\,\psi_i(\vec{r}) = \varepsilon_i\,\psi_i(\vec{r}) \qquad (1.6)$$

We choose to take spherical states for the wave function, since it allows analytic calculations and because the majority of the codes used by the community in nuclear physics uses such an approximation. In spherical symmetry, the wave-function can then be decomposed in a radial part $R_{n\ell jq}(r)$ and an angular part $\Omega_{j\ell m}(\hat{r})$:

$$\psi_{n\ell jmq}(\vec{r}) = \frac{1}{r} R_{n\ell jq}(r)\;\Omega_{\ell jm}(\hat{r}) \qquad (1.7)$$

We obtained an intermediate result, Eq.(1.8), where two particular properties appear. There is a fourth derivative on the wave function represented by the two Δ and the part where appears the effective mass, $B_{q,\mu\nu}$, is a tensor contrary to the one in Skyrme *standard* functional.

$$\begin{aligned}\hat{h}_q(\vec{r}) = \quad & U_q(\vec{r}) + \Delta\Big(V_q(\vec{r})\Delta\Big) - \nabla_\mu B_{q,\mu\nu}(\vec{r})\nabla_\nu \\ + \quad & \tfrac{1}{2i}\left[W_{q,\mu\nu}(\vec{r})\,\nabla_\mu + \nabla_\mu\,W_{q,\mu\nu}(\vec{r})\right]\hat{\sigma}_\nu . \qquad (1.8)\end{aligned}$$

Finally, we obtain the final mean-field differential equation associated with the functional :

$$A_4 R^{(4)}_{n\ell j} + A_3 R^{(3)}_{n\ell j} + A_2 R^{(2)}_{n\ell j} + A_1 R^{(1)}_{n\ell j} + A_0 R_{n\ell j} = \epsilon_{n\ell j} R_{n\ell j}\,.$$

This is a fourth order diffenrential equation, instead of the second order differential equation obtained with a *standard* Skyrme interaction. The first two coefficients are purely radial, and the last three has radial and centrifugal [3]. The details of the coefficient can be find in [5].

In this article, a study has also been performed with the Linear Response Method. This study assured us that there were no pathologies in our interaction and its was stable in Symmetric Nuclear Matter.

The other promising property is the dependence in momentum brought by our interaction with the D-wave in the effective mass. This dependence can indeed means good spectrocopic properties, since the momentum is proportional with the density and the effective mass may then be peaked.[5]

The last step to include our interaction in a fit in order to obtain a new parametrisation is to solve this non-linear fourth order differential equation, with non-constant coefficients. This work is ongoing.

1.4 Conclusion

We have discussed the contribution of 4th order terms to *standard* Skyrme pseudo-potential.This extension, called the D-wave, can reproduce both equations of states in nuclear (S,T) channels and global equation of state, which is new for a Skyrme force. The functional formalism have then been worked out and specialized for the case of spherical summetry in view of a future fit.The LR formalism have also been applied to eventually detect instabilities [5]. Finally, the dependence of momentum in the effective mass may signify great spectroscopic properties. The next challenge is now to solve the mean-field fourth order differential equation, finding the appropriate numerical method to be able to fit our interaction.

3. meaning a term in $\ell(\ell+1)/r^2$

Références

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