Compressibility, effective mass and density dependence in Skyrme forces

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Generalized density dependence in Skyrme effective interactions is investigated to get forces valid beyond the mean field approximation. Preliminary results are presented for infinite symmetric and asymmetric nuclear matter up to pure neutron matter.

1. INTRODUCTION

It is commonly accepted that it does exist a relation between compressibility, effective mass and the density dependence of a given effective force. Studies with Skyrme forces [1] have shown that the incompressibility $K_\infty$ and the effective mass cannot be chosen independently once the analytical form of the (single) density-dependent term has been chosen. This has led to the $\rho^{1/6}$ density dependence in Skyrme forces like SkM* which allows a value of $K_\infty$ around 220 MeV close to that extracted from the experimental breathing mode analyses [2, 3] and an effective mass $m^*$ around 0.7$m$ simultaneously. The present status about compressibility has been summarized by G. Colò during this conference [4].

Recently, the density dependence of phenomenological effective interactions, such as Skyrme or Gogny forces, has been revisited in the context of beyond mean field calculations [5, 6]. Indeed, while a dependence of the interaction on the density is well established for calculations at the mean field level [7], no strongly motivated prescription exists when several mean fields are mixed as in the Generator Coordinate Method (GCM) and the Projected Mean Field Method (PMFM). First, an extension of the Goldstone-Brueckner theory has motivated the GCM and the PMFM from a perturbative point of view for the first time [8]. In this extended context, a generalized Brueckner $G$ matrix summing particle-particle ladders has been defined and may be used as a reference from which phenomenological interactions in GCM or PMFM calculations should be approximated. It is possible to simplify this in-medium interaction to extend the validity of the Skyrme force [8, 9] and to identify approximately the density dependence originating from Brueckner correlations in the context of mixed nonorthogonal vacua [6]. The renormalization of three-body forces has also been advocated as an important source of density dependence...
dependence in phenomenological interactions. Indeed, their renormalization through a
density-dependent two-body interaction has been proved to be justified at the mean field
level in some particular cases [7,9]. As for the resummation of Brueckner correlations,
the corresponding density turns out to be the one of the mean field which is calculated.
Consequently, a single density-dependent term has often been used in phenomenological
forces, e.g. Gogny [10] and Skyrme [9] effective interactions. On the other hand, the
density dependence renormalizing three-body force effects has been shown to be different
from the one taking care of Brueckner correlations when going beyond the mean field
approximation [6]. In fact, the use of two different, and theoretically motivated, density-
dependent terms happens to have non negligible effects on collective spectra [11]. Based
on this analysis, it is legitimate to redefine the Skyrme interaction at the mean field level.
Including two density-dependent terms, each related to a given physical origin, will allow
a proper extrapolation of the interaction to GCM and PMFM calculations.

A first attempt is presented in this paper, where we concentrate on the practical advan-
tages of having two different density-dependent terms. Relating them to the resummation
of Brueckner correlations and to the renormalization of three-body forces is the aim of
our on-going work. In this way, this paper is concerned by a systematic investigation
of infinite matter, symmetric and asymmetric up to pure neutron matter, using multi
density-dependent terms in Skyrme forces. Our analysis is focuse d on $\rho^{1/3}$ terms which
are connected with a $k_F$ expansion of the Brueckner $G$ matrix.

2. STANDARD SKYRME EFFECTIVE INTERACTIONS

When using Skyrme effective forces with a standard density dependence $\rho^\alpha$, where $\rho$ is
the total density, the adjustable parameter $\alpha$ is strongly correlated to the incompressibility
and the effective mass in nuclear matter. This is illustrated on Figure 1 for different
standard Skyrme forces with various powers $\alpha$. In all cases, the different parameters of
the force have been adjusted in order to obtain the saturation density $\rho_0 = 0.16$ fm$^{-3}$
and the energy per particle $E/A = -16$ MeV in infinite symmetric nuclear matter. Once
these two properties are fixed, the relation between $m^*/m$ and $K_\infty$ is entirely determined
by $\alpha$. This well-known feature, discussed in [1], yields to the conclusion that a value of
$\alpha$ around 1, like in SIII, does not allow to reach a correct compression modulus [2,12].
Only values of $\alpha$ ranging from 1/6 to 1/3 allow for an acceptable set \{m$^*/m$, $K_\infty$\}.

It is enlightening to study a bit further the relation between $m^*/m$ and $K_\infty$ in the case
of the standard parameterizations of Skyrme forces. Introducing as in [1] the notation
$\Theta_s = 3t_1 + (5 + 4x_2)t_2$, one has

$$
\frac{m^*}{m} = \left(1 + \frac{1}{8} \frac{m}{\hbar^2 \rho_0 \Theta_s} \right)^{-1},
$$

and

$$
K_\infty = -\frac{3\hbar^2}{5m} \left(\frac{3\pi^2}{2} \rho_0^{2/3} + \frac{3}{8} \Theta_s \frac{3\pi^2}{2} \rho_0^{5/3} + \frac{9}{16} \alpha (\alpha + 1) t_3 \rho_0^{\alpha + 1} \right).
$$

The energy per particle in infinite nuclear matter at saturation density is given by:

$$
\frac{E}{A} = \frac{3\hbar^2}{10m} \left(\frac{3\pi^2}{2} \rho_0^{2/3} + \frac{3}{8} t_0 \rho_0 + \frac{3}{80} \Theta_s \frac{3\pi^2}{2} \rho_0^{5/3} + \frac{1}{16} t_3 \rho_0^{\alpha + 1} \right).
$$
Figure 1. Correlation between incompressibility, effective mass and density dependence of standard parameterizations of Skyrme effective interactions.

The saturation density being determined by the condition on the pressure \( P(\rho_0) = 0 \) which gives (if \( \rho_0 \neq 0 \))

\[
\frac{\hbar^2}{5m} \left( \frac{3\pi^2}{2} \right)^{2/3} \rho_0^{2/3} + \frac{3}{8} t_0 \rho_0 + \frac{1}{16} \Theta_s \left( \frac{3\pi^2}{2} \right)^{2/3} \rho_0^{5/3} + \frac{1}{16} t_3 (\alpha + 1) \rho_0^{\alpha + 1} = 0 .
\]  

(4)

The three equations (2), (3) and (4) form a system with three unknown quantities \( t_0, t_3 \) and \( \Theta_s \). Solving this system for a given set \( (\rho_0, E/A, K_\infty) \) provides the coefficients \( t_0, t_3 \) and \( \Theta_s \), this latter determining uniquely the effective mass \( m^*/m \) through Eq. (1).

Actually, the previous conclusion is incorrect in one special case. To see that, let us set

\[
F(\Theta_s, t_3) = \frac{1}{16} \left[ \Theta_s \left( \frac{3\pi^2}{2} \right)^{2/3} + \frac{5}{3} t_3 \right].
\]  

(5)

It is trivial to check that if and only if \( \alpha = 2/3 \) we have

\[
\begin{align*}
- \frac{3\hbar^2}{5m} \left( \frac{3\pi^2}{2} \right)^{2/3} \rho_0^{2/3} + 6 F(\Theta_s, t_3) \rho_0^{5/3} &= K_\infty , \\
\frac{3\hbar^2}{10m} \left( \frac{3\pi^2}{2} \right)^{2/3} \rho_0^{2/3} + \frac{3}{8} t_0 \rho_0 + \frac{3}{5} F(\Theta_s, t_3) \rho_0^{5/3} &= \frac{E}{A} , \\
\frac{\hbar^2}{5m} \left( \frac{3\pi^2}{2} \right)^{2/3} \rho_0^{2/3} + \frac{3}{8} t_0 \rho_0 + F(\Theta_s, t_3) \rho_0^{5/3} &= 0 .
\end{align*}
\]  

(6)

In this particular case, there are three equations and two unknown quantities, \( t_0 \) and \( F(\Theta_s, t_3) \), and, in general, this system has no solution. However, we can use the last two
equations to determine \( t_0 \) and \( F(\Theta_s, t_3) \) and then calculate the corresponding value of \( K_\infty \). Because of the definition (5), \( \Theta_s \) can be freely chosen. This situation is illustrated on Figure 1 by the vertical dashed line, when \( \alpha = 2/3 \), the value of \( K_\infty \) is fixed and the effective mass can be freely chosen. However, this case is not interesting since it does not correspond to a realistic value of \( K_\infty \).

3. MODIFIED DENSITY DEPENDENCE IN SKYRME FORCES

Following several previous attempts \[13, 14\] and adding a density dependence on each term of the force, one can investigate the properties of generalized Skyrme effective interactions written as:

\[
V(\mathbf{r}_1, \mathbf{r}_2) = \sum_i t_{0i} \rho^{i/3} (1 + x_{0i} P_\sigma) \delta(\mathbf{r}) + \frac{1}{2} \sum_j t_{1j} \rho^{j/3} (1 + x_{1j} P_\sigma) \left[ \delta(\mathbf{r}) \mathbf{P}^2 + \mathbf{P}^2 \delta(\mathbf{r}) \right] + \sum_j t_{2j} \rho^{j/3} (1 + x_{2j} P_\sigma) \mathbf{P} \cdot \delta(\mathbf{r}) \mathbf{P} + i \sum_k W_{0k} \rho^{k/3} \mathbf{\sigma} \cdot \left[ \mathbf{P} \times \delta(\mathbf{r}) \mathbf{P} \right]
\]  \tag{7}

where \( \rho \equiv \rho(\mathbf{R}) \) is the total density and see ref. [1] for the other notations. Standard parameterizations discussed in Section 2 correspond to \( j = k = 0 \) and \( i = 0, 3 \) in SIII and \( i = 0, 1/2 \) in SkM* and SLy4 for instance.

This generalized parameterization increases the number of parameters in the force, making it more phenomenological and reducing its predictive power. Besides, the fitting procedure may become intractable if most of the parameters are free. In this first exploratory work, we limit our study to the case with \( t_{1j} = t_{2j} = 0 \) except for \( j = 0 \) (hereafter we omit the second index) and three non zero values for \( t_{0i} \), namely \( i_1, i_2 \) and \( i_3 \) out of the set \( \{0, 1, 2, 3\} \). The corresponding forces will be labeled by \([i_1, i_2, i_3]\). The spin-orbit term will not be discussed here since it has no contribution in infinite nuclear matter.

The problems faced with the Skyrme forces with one density-dependent term are cured with this family of parameterizations. Following the same procedure to adjust the coefficients, we can fix the saturation properties of infinite symmetric nuclear matter \( \rho_0, E/A, K_\infty \) and \( m^*/m \) independently and determine the coefficients \( t_{0i} \) of the force.

However this procedure only guarantees to have realistic properties of nuclear matter in the vicinity of the saturation point. If we want a force which gives an equation of state in agreement with \textit{ab initio} calculations at low density as well as high density (up to \( \sim 3\rho_0 \)) one should adopt a different fitting procedure. First, one can fit a set of points \([\rho_i, E/A(\rho_i)]_{i=1,\ldots,N}\) which samples a realistic equation of state of nuclear matter. Then, the parameters of the force will provide the characteristic properties of nuclear matter \( (\rho_0, E/A, K_\infty \) and \( m^*/m) \) using equations (1) to (4). In this kind of approach,
the presence of a density-dependent term with the power 2/3 in the force is particularly interesting. Indeed, the coefficient $\Theta_s$ is only constrained by the function $F(\Theta_s, t_{02})$ whose value comes out of the fit. So, by choosing correctly the parameter $t_{02}$ one can obtain any desired value of the effective mass.

4. RESULTS USING THE GENERALIZED SKYRME FORCES

In this section, we present some results using the generalized forces $[0,1,2]$, $[0,1,3]$ and $[0,2,3]$ for symmetric nuclear matter as well as pure neutron matter. For this purpose, we need to determine the coefficients $t_{0i}$, $x_{0i}$ and the two combinations of coefficients $\Theta_s$ and $\Theta_v = t_1(2 + x_1) + t_2(2 + x_2)$, this latter expression is related to the isovector enhanced factor $\kappa$ [1] occurring in the Thomas-Reiche-Kuhn sum rule of the isovector giant dipole resonance. The quantities $E/A = -16$ MeV, $\rho_0 = 0.16$ fm$^{-3}$, $K_\infty = 230$ MeV, $m^*/m = 0.8$ and $\kappa = 0.5$ allow the determination of the parameters $t_{0i}$, $\Theta_s$ and $\Theta_v$. The coefficient $x_{0i}$ are determined by fitting the neutron matter equation of state provided by Akmal et al. [15]. The coefficients obtained accordingly are summarized in Table 1.

Table 1
Coefficients $t_{0i}$ and $x_{0i}$ of the forces used in this section. See the text for the remaining parameters.

| Force   | $t_{00}$   | $x_{00}$ | $t_{01}$   | $x_{01}$ | $t_{02}$   | $x_{02}$ | $t_{03}$   | $x_{03}$ |
|---------|------------|----------|------------|----------|------------|----------|------------|----------|
| [0,1,2] | -1855.38   | 0.4006   | 2343.12    | 0.7589   | -488.28    | 3.6176   | -          | -        |
| [0,1,3] | -1807.41   | 0.3291   | 2078.04    | 0.4094   | -          | -        | -299.81    | 3.4464   |
| [0,2,3] | -1431.36   | 0.2828   | -          | -        | 3827.79    | 0.3814   | -2650.09   | 0.7640   |

Figure 2 shows the two EOS (energy per particle as a function of equilibrium density) for symmetric nuclear matter and pure neutron matter compared with the EOS of Akmal et al. [15]. The results are quite reasonable and rather similar for densities from 0 to $\sim 3\rho_0$. The most salient feature of the parameterizations is that the coefficient of the term with the highest density dependence is always negative, leading to the pathological property for high density $E/A \to -\infty$. Nevertheless, as can be expected from the figure or check numerically, this problem shows up only at extremely large and unphysical densities and, thus, is not relevant for the applications to atomic nuclei and neutron stars.

Another important property which can be extracted from this study is the symmetry energy $a_I$. Its expression, obtained by a straightforward calculation [1], depends upon the coefficients $t_{0i}$ and $x_{0i}$. On Figure 3 the symmetry energy is plotted as a function of the density and compared with the variational results of Lagaris et al. [17] and the schematic parameterizations of Bao-An Li [16]. The three forces $[0,1,2]$, $[0,1,3]$ and $[0,2,3]$ give results in good agreement with the variational approach, especially for $\rho \lesssim 0.3$ fm$^{-3}$, even though this quantity has not been directly fitted. For $\rho = \rho_0$, the three forces give exactly the same symmetry energy, $a_I \approx 32.5$ MeV, which is close to the commonly accepted value. This result is very encouraging and reinforce the idea that the two density-dependent terms in the Skyrme force open pertinent degrees of freedom.
5. CONCLUSION

We have shown that the choice of a standard Skyrme effective force with a modified density dependence based on two terms enables to choose independently the incompressibility and the isoscalar effective mass. The gross properties of nuclear matter investigated here are quite reasonable: incompressibility ($\sim 230$ MeV), isoscalar effective mass ($\sim 0.8 m$) and symmetry energy ($\sim 32.5$ MeV). With this generalized density dependence we have been able to construct new Skyrme like parameterizations without collapse at relevant densities and which exhibit reasonable equation of state (EOS) for symmetric nuclear matter as well as for pure neutron matter compared to the recent realistic variational EOS of Akmal et al. [15].

Other choices can be explored for the density dependence provided they are physically well grounded. The choice $\rho^{2/3}$ for one of the density-dependent term lets total freedom for the effective mass. This feature is extremely interesting from the perspective of developing accurate and predictive force since it gives a control on the density of state around the Fermi energy where the correlations beyond the Hartree-Fock approximation can develop. Furthermore it implies only two additional parameters so that their total number remains quite small.

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