Nonrelativistic approaches derived from point-coupling relativistic models

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We construct nonrelativistic versions of relativistic nonlinear hadronic point-coupling models, based on new normalized spinor wave functions after small component reduction. These expansions give us energy density functionals that can be compared to their relativistic counterparts. We show that the agreement between the nonrelativistic limit approach and the Skyrme parametrizations becomes strongly dependent on the incompressibility of each model. We also show that the particular case $A = B = 0$ (Walecka model) leads to the same energy density functional of the Skyrme parametrizations SV and ZR2, while the truncation scheme, up to order $\rho^4$, leads to parametrizations for which $\sigma = 1$.

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In nonrelativistic many-nucleon systems, point-coupling interactions have been successfully used for decades through Skyrme models to obtain finite-nuclei spectra and nuclear matter bulk properties [1–5]. Curiously, the Skyrme-Hartree-Fock (SHF) treatment shows similarities to the Kohn-Sham density functional theory [6,7], as pointed out by Brack [8]. A study along this line, raising many interesting and still unanswered questions regarding density functional theory and its application to many-nucleon systems, based on effective field theory, was done by Furnstahl [9]. The issues of whether the SHF model includes the driven physical contributions for nuclear matter and whether the nucleon-nucleon correlations may be considered small in this context are still under discussion.

Nonlinear relativistic point-coupling (NLPC) models have been applied by Nikolaus et al. [10] to extract nuclear ground-state observables, with results comparable in quality to those obtained by the usual nonlinear Walecka model [3,11]. In particular, the nonrelativistic limit of Boguta-Bodmer models has been investigated [12].

The construction of relativistic NLPC models from the usual relativistic nonlinear models, after choosing the heavy-meson mass limit properly, has already been addressed [13,14].

In common, the SHF and NLPC models have density functionals that are parameterized directly by fitting the unknown constants to nuclear ground-state data. With this strategy, the microscopic role of the nucleon-nucleon ($NN$) interaction that underlies the density functional is obscured. The success of these functionals leads to the investigation of the nonlinear density dependence of the nonlinear Walecka and NLPC models [13]. Following the nonrelativistic limit prescription proposed in Ref. [15], the authors also obtain the nonrelativistic limit of the NLPC model and suggest a modification of the SHF model with a density-dependent spin-orbit potential. A better understanding of point-coupling models becomes of interest when one addresses the important theoretical challenge of constructing a universal nuclear effective density functional [16].

Infinite nuclear matter, as well as finite-nucleus properties, can be described reasonably well within the scope of point-coupling models. We have studied NLPC models described by the following Lagrangian density:

$$
\mathcal{L}_{NLPC} = \bar{\psi} (i \gamma^\mu \partial_\mu - M) \psi - \frac{1}{2} G_0^s (\bar{\psi} \gamma^\mu \psi)^2
$$

$$
+ \frac{1}{2} G_2^s (\bar{\psi} \gamma^\mu \psi)^2 + \frac{A}{3} \bar{\psi} \psi \bar{\psi} + \frac{B}{4} (\bar{\psi} \psi)^4,
$$

where only the isovector-scalar and isovector-vector interactions are present. In a mean-field approach, the energy density functional at zero temperature for infinite nuclear matter is given by

$$
\mathcal{E} = \frac{1}{2} G_0^s \rho^2 + \frac{1}{2} G_2^s \rho^4 + \frac{2}{3} A \rho_3 + \frac{3}{4} B \rho_4^4
$$

$$
+ \frac{2}{\pi^2} \int_0^{k_F} k^2 (k^2 + M^2)^{1/2} dk
$$

with

$$
M^* \equiv M - G_0^s \rho_3 - A \rho_2^3 - B \rho_4^3.
$$

The vector and scalar densities are

$$
\rho = \frac{2}{\pi^2} \int_0^{k_F} k^2 dk,
$$

$$
\rho_3 = \frac{2}{\pi^2} \int_0^{k_F} \frac{M^*}{(k^2 + M^2)^{1/2}} k^2 dk,
$$

where $k_F$ is the Fermi momentum. The set of Eqs. (2)–(4) has to be solved self-consistently. The scalar and vector potentials are given by

$$
S = -G_0^s \rho_3 - A \rho_2^3 - B \rho_4^3 \text{ and } V = G_0^s \rho.
$$

Equation (3), $M^* = M + S$, defines the effective mass of the model—or Dirac mass, in the language of Ref. [17]. This definition is purely relativistic: the scalar field $S$ shifts the bare nucleon mass $M$ and the vector field $V$ shifts the energy of the Dirac equation in such a way that the energy dispersion relation reads $E - V = \sqrt{k^2 + M^2}$. This definition is, however, not unique and this point is addressed in Ref. [17], where a very rich discussion about the multiple possibilities of the effective mass concept is presented. Some discussion of this issue is in

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order, as the nonrelativistic definition is different and makes sense only after the nonrelativistic limit is chosen. Still at the relativistic level, the procedure of finding the effective mass from the definition of a real optical potential as the difference between the total \( E \) and the kinetic energies of a nucleon traveling in nuclear matter with momentum \( \mathbf{k} \), \( U_{\text{opt}} = E - \sqrt{k^2 + M^2} \), is well accepted. By using this definition [18,19], \( U_{\text{opt}} = E - [(E - V)^2 - S(2M + S)]^2 \). The nonrelativistic limit, up to order \((k/M)^2\), is \( U_{\text{opt}} = (M^*/M)(S + V) + [1 - (M^*/M)](E - M) \). So, the nonrelativistic slope of \( U_{\text{opt}} \) versus \( E - M \) gives the nucleon effective mass. But this nonrelativistic limit still has some "relativistic" content, as the small component of the Dirac equation was not completely removed; this is done next. Moreover, the definition of the effective mass \( M^* \) is obtained from the single-particle energy \( \epsilon(k) \), through \( M^* = k[\partial \epsilon(k)/\partial k]^{-1} \).

Following Ref. [15], we perform the nonrelativistic limit of the NLPC models by rewriting the small component \( \chi \) of the fermion field \( \psi \) in terms of the large one \( \phi \) in the Dirac equation:

\[
(\mathbf{\sigma} \cdot k B \mathbf{\sigma} \cdot k + M + S + V)\phi = E\phi, \tag{6}
\]

with

\[
B = B_0 \left[ 1 + (\epsilon - S - V)B_0 \right] \approx B_0 + B_0(S + V - \epsilon), \tag{7}
\]

\[
B_0 = \frac{1}{2(M + S)}. \tag{8}
\]

In the equation above, the expansion parameter is \( x = (\epsilon - S - V)B_0 = (E - M - S - V)B_0 \). However, if we use the dispersion relation for the model, \( E - V = \sqrt{k^2 + (M + S)^2} \), we have \( x = \left[ \sqrt{1 + \frac{M^2}{2}} \right]/2 \), where \( z^2 = k^2/(M + S)^2 \). For the relativistic models we consider in this paper, \( x \approx 0.1 \) up to about 1.5 times the nuclear matter saturation density \( \rho_0 \), in the worst-case scenario.

This procedure reduces Eq. (6) to the Schrödinger equation:

\[
\hat{H}^{\text{class}} \psi^{\text{class}} = \epsilon \psi^{\text{class}}, \tag{9}
\]

where \( \psi^{\text{class}} = \hat{I}^{1/2} \phi \).

\[
\hat{H}^{\text{class}} = \hat{I}^{-1/2} \left[ \mathbf{\sigma} \cdot k B_0 \mathbf{\sigma} \cdot k + S + V \right. \\
+ \left. \mathbf{\sigma} \cdot k B_0^2(S + V)\mathbf{\sigma} \cdot k \right] \hat{I}^{-1/2}. \tag{10}
\]

and

\[
\hat{I} = 1 + \mathbf{\sigma} \cdot k B_0^2 \mathbf{\sigma} \cdot k \\
= 1 + \frac{z^2}{4} = 1 + x(x + 1). \tag{11}
\]

To write \( \hat{H}^{\text{class}} \) as an explicit sum of a kinetic and potential energy, we proceed by expanding the operators \( \hat{I}^{-1/2} \) and \( \hat{I}^{-1} \), up to order \( v^4 \), or equivalently \((k/M)^2\), using \( z^2/4 \) as the expansion parameter, which should therefore be small for the expansion to be reliable. If we require, for instance, \( z^2/4 < 0.1 \), then \( x < 0.09 \), which restricts the density range to \( \rho/\rho_0 \ll 1.4 \).

These expansions lead to the vector and scalar densities,

\[
\rho = \phi^\dagger \phi + \chi^\dagger \chi = |\psi^{\text{class}}|^2, \tag{12}
\]

\[
\rho_s = \phi^\dagger \phi - \chi^\dagger \chi = \rho(1 - z^2/2), \tag{13}
\]

and to the single-particle energy \( \hat{H}^{\text{class}} \), which now reads

\[
\hat{H}^{\text{class}} = \frac{k^2}{2(M + S)} + S + V \tag{14}
\]

\[
= \frac{k^2}{2(M + S)} + (G_v^2 - G_s^2)\rho - A \rho^2 - B \rho^3 \\
+ 2B_0^2 k^2 \rho (G_v^2 + 2A \rho + 3B \rho^2). \tag{15}
\]

Because our aim with the nonrelativistic expansion is to compare the energy density functional with Skyrme models, we chose to use the approximation \( M + S = M \) in Eq. (13). With this procedure and using the continuous limit in \( \hat{H}^{\text{class}} \), we have

\[
E_{NR} = c_1 \rho^2 + c_2 \rho^3 + c_3 \rho^4 + c_4 \rho \frac{3}{40} \left( \frac{3 \rho^2}{2} \right)^{2/3} \rho^{8/3} \\
+ \frac{3}{10M} \left( \frac{3 \rho^2}{2} \right)^{2/3} \rho^{5/3}, \tag{16}
\]

with

\[
c_1 = G_v^2 - G_s^2, \quad c_2 = -A, \quad c_3 = -B, \quad c_4(\rho) = \frac{4}{M} \left( G_v^2 + 2A \rho + 3B \rho^2 \right). \tag{17}
\]

Note that Eq. (14) shows a \( \rho \) dependence up to, at least, order 14/3, owing to \( c_4(\rho) \).

Differently from Eq. (3), the nucleon effective mass will now be defined by its standard nonrelativistic form [4] as follows:

\[
M^* = k \left[ \frac{\partial \hat{H}^{\text{class}}}{\partial k} \right]^{-1} = M \left[ 1 + \frac{M c_4(\rho) \rho}{4} \right]^{-1}, \tag{18}
\]

where, again, we have used \( M + S = M \) in Eq. (13).

An important question here is: What results do we get from Eq. (14) if we keep the values of the coupling constants that are required by the relativistic models in order to reproduce the results for observables at the saturation point?

To answer this question we proceed to compare the ground-state observables at the saturation density, obtained through Eqs. (2) and (14), using the original coupling constants \( G_v, G_s, A, \) and \( B \), for the NL2-PC as an example. The result is disappointing, as, for the binding energy, saturation density, and incompressibility (\( K \)), we find, via Eq. (14), \(-52.94 \text{ MeV}, 0.160 \text{ fm}^{-3}, \) and 1059.35 \text{ MeV}, to be compared with the original values \(-17.03 \text{ MeV}, 0.146 \text{ fm}^{-3}, \) and 399.20 \text{ MeV}, respectively, found via Eq. (2). This disagreement is also shown for other relativistic point-coupling models. We have asked ourselves whether this poor agreement was because of the approximation \( M + S = M \); however, even if we include the \( S \) term, the approximation, albeit improving a little, remains poor. This strongly suggests that higher-order terms are needed, but as our main purpose here is to compare the nonrelativistic limit of the NLPC models, at the energy density functional level, with the well-known Skyrme parametrizations, we decided to keep only terms of order \( v^2 \) in \( \hat{H}^{\text{class}} \).

To avoid the aforementioned disagreement, and to compare nonrelativistic models that have at least the same saturation...
properties as their relativistic original counterparts, we must re-fit the parameters in Eq. (14). Now we present the energy density functional of the Skyrme models [4,21] for infinite nuclear matter,

\[ \mathcal{E}_{\text{Skyrme}} = \frac{3t_1}{8} \rho^2 + \frac{t_3}{16} \rho^3 + \frac{3}{4} \left( \frac{3\pi^2}{2} \right)^{2/3} \rho^{8/3} + \frac{3}{10M} \left( \frac{3\pi^2}{2} \right)^{2/3} \rho^{5/3}, \]

with \( t = [3t_1 + t_3 (5 + 4x_2)]/2 \).

By inspecting Eqs. (14) and (17), we can see Eq. (14) as a generalized Skyme energy density and then highlight two interesting cases.

(i) \( A = B = 0 \): This particular case reduces the NLPC model to the linear point-coupling one that is fully equivalent to the Walecka model [14,22,23]. This leads the energy density functional given in Eq. (14) to the Skyme parametrizations, in \( \sigma = 0 \) or \( t_3 = 0 \) (SV model). Because both the SV parametrization and the relativistic Walecka model do not contain three-body force effects, it is consistent that in the present case, the nonrelativistic limit of the former also does not show this phenomenology. The specific ZR2 parametrization [24], for which \( \sigma = 2/3 \), is also generated in this particular case.

(ii) Truncation scheme: Truncating Eq. (14) up to order \( \rho^3 \), that is, dropping the term \( c_3 \rho^3 \) and making \( c_4 (\rho) = 4G^2 / M^2 \), one can obtain the Skyme models for which \( \sigma = 1 \) and \( t \neq 0 \). Actually, \( \sigma = 1 \) encompasses a large set of Skyme models, such as, for example, SI-SVI, which are claimed to be “natural” [25]. In that sense models in this class and with this truncation need only cubic NLPC contributions to be generated. In this way, they can be viewed as a natural consequence of the nonrelativistic expansion presented here.

The refitting of \( c_1 \) and \( c_4 \) in case (i) and \( c_1, c_2, \) and \( c_4 \) in case (ii) leads each to the corresponding Skyme model constants, \( t_0, t_3, \) and \( t \).

Now, without any truncation, and using \( A \neq 0 \) and \( B \neq 0 \) in Eq. (14), we analyze, via comparison, how the equation of state obtained from the nonrelativistic limit of the point-coupling models works. We do this in the following two steps.

1. Relativistic NLPC models and their nonrelativistic limit: Here we essentially compare Eq. (2) and Eq. (14), selecting a class of representative point-coupling versions [14] of the well-known nonlinear Boguta-Bodmer models, namely, NLB [26], NLSH [27], NL2 [15], NL1 [15], NLZ2 [13], and NL3 [28]. As previously discussed, to compare both models we re-fit the parameters in Eq. (14) in order to impose on the nonrelativistic equation of state the reproduction of the values obtained in their relativistic versions for some physical quantities (incompressibility, saturation density, binding energy, and nucleon effective mass) in the saturation regime.

2. Full generalized Skyme models and standard Skyme models: The comparison now is done between Eq. (14) and Eq. (17). We chose the following Skyme parametrizations: PRC45 [24], SIII [25], SV [25], SGI [29], SkMP [30], and SLy230a [4]. Naturally, here the parameters \( G_2^V, G_4^V, A, \) and \( B \) are also found as described previously.

The results for the binding energy as a function of \( \rho/\rho_o \) for the two cases are shown in Fig. 1. Both Fig. 1(a) and Fig. 1(b) show that the nonrelativistic limit, Eq. (14), works well up to densities \( \rho \) close to the saturation density \( \rho_o \). In Fig. 1(a) we group the models that we consider to present a good agreement between the exact models and the nonrelativistic limit, even beyond \( \rho = \rho_o \). In Fig. 1(b) we group the models in which the nonrelativistic limit does not work well for \( \rho > \rho_o \). In both panels we can see that the incompressibility seems to control the agreement between the exact models and their nonrelativistic limit. The higher the incompressibility, the better is the nonrelativistic approach to describe nuclear matter.

We have enlarged the set of point-coupling and Skyme models to verify whether the findings in Fig. 1 remain valid (not shown). Indeed, the quality of the nonrelativistic limit for
$\rho > \rho_o$ continued to be completely determined by the value of $K$ in the same way that we discussed before. Therefore, we conclude that $K$ seems to be a robust quantity with which to predict whether the nonrelativistic limit of a relativistic point-coupling model taken up to order $v^2$ will give good results as regards its comparison both with the original models and with the Skyrme parametrizations.

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