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New density-independent interactions for nuclear structure calculations

K. Bennaceur[1], J. Dobaczewski[2,3], and F. Raimondi[4]

[1] *Université de Lyon, F-69003 Lyon, France; Institut de Physique Nucléaire de Lyon, CNRS/IN2P3, Université Lyon 1, F-69622 Villeurbanne Cedex, France*
[2] *Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Hoża 69, PL-00681 Warsaw, Poland*
[3] *Department of Physics, PO Box 35 (YFL), FI-40014 University of Jyväskylä, Finland*
[4] *TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T2A3, Canada*

Abstract. We present a new two-body finite-range and momentum-dependent but density-independent effective interaction, which can be interpreted as a regularized zero-range force. We show that no three-body or density-dependent terms are needed for a correct description of saturation properties in infinite matter, that is, on the level of low-energy density functional, the physical three-body effects can be efficiently absorbed in effective two-body terms. The new interaction gives a satisfying equation of state of nuclear matter and opens up extremely interesting perspectives for the mean-field and beyond-mean-field descriptions of atomic nuclei.

The two most widely used effective forces for nonrelativistic energy-density-functional calculations, the Gogny [1, 2] and the Skyrme interaction [3], have in common a two-body density dependent term. For the case of the Skyrme force, the original three-body contact force of the form $t_3\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_3)$ [3] was in fact replaced by an isoscalar density-dependent two-body contact force, $\frac{1}{6}\, t_3 \left(1 + x_3 \hat{P}^{\sigma}\right) \rho_0^{\alpha} \left(\frac{\mathbf{r}_1+\mathbf{r}_2}{2}\right) \delta(\mathbf{r}_1 - \mathbf{r}_2)$, due to the appearance of spin instabilities [4–6]. Later, it was employed as a convenient way of simulating the density dependence of the effective interaction rather than a three-body force [7].

For Skyrme and Gogny effective interactions, the density dependent term appears to play a determinant role, especially in generating the mechanism of saturation. The non-integer powers of the density seem to be mandatory if one wants to obtain acceptable values for incompressibility and isoscalar effective mass. These considerations concern only the description of nuclei at the mean-field level. However, several years ago it was identified that effective interactions that depend on non-integer powers of density do not allow for beyond-mean-field calculations that use standard techniques of symmetry restoration or Generator Coordinate Method [8, 9].

This observation triggered efforts to define a new generation of effective interactions without density dependence. A promising way is to consider two- and three-body momentum dependent zero-range terms along with a four-body momentum independent one [10]. Another way, discussed in this study, consists in using a form very similar to the two-body part of the Skyrme interaction and replacing the δ Dirac functions by finite-range form factors. This corresponds to the next-to-leading-order expansion of the effective interaction introduced in Ref. [11].

Below we show that the use of a finite-range momentum-dependent, but density-independent, two-body interaction allows us to describe most of the medium effects in a realistic way.

We use the notation $x \equiv (\mathbf{r}, \sigma, q)$ where σ and q are the spin and isospin projections. For a general nonlocal two-body effective interaction v, the mean-field average value of the potential energy can be written as $\langle V\rangle = \frac{1}{2}\int \mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3\,\mathrm{d}x_4\, v(x_1, x_2; x_3, x_4)\left[\rho(x_3, x_1)\rho(x_4, x_2) - \rho(x_4, x_1)\rho(x_3, x_2)\right]$, where ρ is the nonlocal one-body density. Following Ref. [11], we choose the interaction as:

$$v = \sum_{k=0}^{2}\left[T_k^{(1)}\hat{\delta}^{\sigma q} + T_k^{(2)}\hat{\delta}^{q}\hat{P}^{\sigma} - T_k^{(3)}\hat{\delta}^{\sigma}\hat{P}^{q} - T_k^{(4)}\hat{P}^{\sigma}\hat{P}^{q}\right]\hat{O}_k(\mathbf{k}_{12}^*, \mathbf{k}_{34})\delta(\mathbf{r}_1 - \mathbf{r}_3)\delta(\mathbf{r}_2 - \mathbf{r}_4)g_a(\mathbf{r}_2 - \mathbf{r}_1), \quad (1)$$

where $\hat{P}^{\sigma}$ and $\hat{P}^{q}$ denote the standard spin and isospin exchange operators, respectively, $\hat{\delta}^{\sigma}$, $\hat{\delta}^{q}$, and $\hat{\delta}^{\sigma q}$ are the identity operators in the spin and/or isospin spaces, and $\hat{O}_0 = 1$,$\hat{O}_1 = \frac{1}{2}\left[\mathbf{k}_{12}^{*2} + \mathbf{k}_{34}^{2}\right]$,$\hat{O}_2 = \mathbf{k}_{12}^{*}\cdot\mathbf{k}_{34}$, and $g_a(\mathbf{r}) = e^{-\mathbf{r}^2/a^2}/(a\sqrt{\pi})^3$. Here, $\mathbf{k}_{ij}$ represents the relative momentum operator between particles i and j and the regularized δ function $g_a(\mathbf{r})$ defines the profile of the interaction, with a representing the regularization scale and range of the interaction. This effective interaction depends on 13 parameters, that is, on 12 parameters $T_k^{(i)}$, for $k = 0, 1, 2$ and $i = 1, 2, 3, 4$, which control the strengths in each channel, and on the range a. As usual, integration by parts of matrix elements transforms the nonlocal interaction (1) into a local finite-range momentum-dependent pseudopotential. Although a construction of the analogous finite-range spin-orbit force poses no difficulty, in the present implementation we use the standard zero-range form of it, with one strength parameter W_0.

By using methods of symbolic programming, one can derive the nuclear-matter characteristics of interaction (1). For that, we introduce the following auxiliary functions:

$$F_0(\xi) = \frac{12}{\xi^3}\left[\frac{1 - e^{-\xi^2}}{\xi^3} - \frac{3 - e^{-\xi^2}}{2\xi} + \frac{\sqrt{\pi}}{2}\,\mathrm{Erf}\,\xi\right], \quad (2)$$

$$F_1(\xi) = \frac{48}{\xi^8}\left(1 - e^{-\xi^2}\right) + \left(\frac{12}{\xi^6} + \frac{6}{\xi^4}\right)\left(e^{-\xi^2} - 5\right) + \left(1 + \frac{5}{\xi^2}\right)\frac{6\sqrt{\pi}}{\xi^3}\,\mathrm{Erf}\,\xi, \quad (3)$$

$$F_2(\xi) = \frac{720}{\xi^{10}}\left(e^{-\xi^2} - 1\right) + \frac{120}{\xi^8}\left(e^{-\xi^2} + 5\right) + \frac{60}{\xi^6}\left(e^{-\xi^2} - 5\right) + \frac{60\sqrt{\pi}}{\xi^5}\,\mathrm{Erf}\,\xi, \quad (4)$$

$$G_0(\xi) = \frac{12}{\xi^6}\left(e^{-\xi^2} - 1\right) + \frac{6}{\xi^4}\left(e^{-\xi^2} + 1\right), \quad (5)$$

$$G_1(\xi) = \frac{12}{\xi^6}\left(1 - e^{-\xi^2}\right) - \frac{12}{\xi^4} - \frac{3}{\xi^2}\left(1 + e^{-\xi^2}\right) + \frac{6\sqrt{\pi}}{\xi^3}\,\mathrm{Erf}\,\xi, \quad (6)$$

$$G_2(\xi) = \frac{60}{\xi^8}\left(e^{-\xi^2} - 1\right) + \frac{30}{\xi^6}\left(3e^{-\xi^2} - 1\right) + \frac{15}{\xi^4}\left(e^{-\xi^2} - 1\right) + \frac{30\sqrt{\pi}}{\xi^5}\,\mathrm{Erf}\,\xi, \quad (7)$$

and $H_0(\xi) = \left(1 - e^{-\xi^2}\right)/\xi^2$, $H_1(\xi) = G_0(\xi)$. In the following, we use these functions at $\xi = k_F a$, which fixes their dependence on the Fermi momentum k_F and range a. With definitions $A_i^{\rho_0} = \frac{1}{2}T_1^{(i)} + \frac{1}{4}T_2^{(i)} - \frac{1}{4}T_3^{(i)} - \frac{1}{8}T_4^{(i)}$, $B_i^{\rho_0} = -\frac{1}{8}T_1^{(i)} - \frac{1}{4}T_2^{(i)} + \frac{1}{4}T_3^{(i)} + \frac{1}{2}T_4^{(i)}$, $A_i^{\rho_1} = -\frac{1}{4}T_3^{(i)} - \frac{1}{8}T_4^{(i)}$, and $B_i^{\rho_1} = -\frac{1}{8}T_1^{(i)} - \frac{1}{4}T_2^{(i)}$ we then have the energy per particle, $\frac{E}{A}$, incompressibility, K_∞, effective mass, m^*, symmetry energy, J, slope of the symmetry energy, L, and curvature of the symmetry energy, K_{sym}, given as:

$$\frac{E}{A} = \frac{\hbar^2}{2m}\frac{\tau_0}{\rho_0} + \left[A_0^{\rho_0} + B_0^{\rho_0}F_0(\xi)\right]\rho_0 + \frac{1}{2}\left(A_1^{\rho_0} + A_2^{\rho_0}\right)\tau_0 + \frac{1}{2}\left(B_1^{\rho_0} - B_2^{\rho_0}\right)\left[F_1(\xi) - \frac{\xi^2}{10}F_2(\xi)\right]\tau_0, \quad (8)$$

$$\begin{aligned} K_\infty = &-2\frac{\hbar^2}{2m}\frac{\tau_0}{\rho_0} + B_0^{\rho_0}\left[4\xi F_0'(\xi) + \xi^2 F_0''(\xi)\right]\rho_0 + 5\left(A_1^{\rho_0} + A_2^{\rho_0}\right)\tau_0 \\ &+\frac{1}{2}\left(B_1^{\rho_0} - B_2^{\rho_0}\right)\left[10F_1(\xi) + 8\xi F_1'(\xi) + \xi^2 F_1''(\xi) - \frac{14\xi^2}{5}F_2(\xi) - \frac{6\xi^3}{5}F_2'(\xi) - \frac{\xi^4}{10}F_2''(\xi)\right]\tau_0, \end{aligned} \quad (9)$$

$$\frac{\hbar^2}{2m^*} = \frac{\hbar^2}{2m} - \frac{1}{2}B_0^{\rho_0}a^2\rho_0 G_0(\xi) + \frac{1}{2}\left(A_1^{\rho_0} + A_2^{\rho_0}\right)\rho_0 + \frac{1}{2}\left(B_1^{\rho_0} - B_2^{\rho_0}\right)\rho_0\left[G_1(\xi) - \frac{\xi^2}{5}G_2(\xi)\right], \quad (10)$$

$$
\begin{aligned}
J =& \frac{5}{9}\frac{\hbar^2}{2m}\frac{\tau_0}{\rho_0} - B_0^{\rho_0}\frac{\xi^2}{6}G_0(\xi)\rho_0 + \frac{5}{18}\left(A_1^{\rho_0} + A_2^{\rho_0}\right)\tau_0 + \frac{5}{18}\left(B_1^{\rho_0} - B_2^{\rho_0}\right)\left[G_1(\xi) - \frac{\xi^2}{5}G_2(\xi)\right]\tau_0 \\
&+ \left[A_0^{\rho_1} + B_0^{\rho_1}H_0(\xi)\right]\rho_0 + \frac{5}{6}\left(A_1^{\rho_1} + A_2^{\rho_1}\right)\tau_0 + \frac{5}{6}\left(B_1^{\rho_1} - B_2^{\rho_1}\right)\left[H_0(\xi) - \frac{\xi^2}{6}H_1(\xi)\right]\tau_0\,, \qquad (11)
\end{aligned}
$$

$$
\begin{aligned}
L =& \frac{10}{9}\frac{\hbar^2}{2m}\frac{\tau_0}{\rho_0} - B_0^{\rho_0}\left[\frac{5\xi^2}{6}G_0(\xi) + \frac{\xi^3}{6}G_0'(\xi)\right]\rho_0 + \frac{25}{18}\left(A_1^{\rho_0} + A_2^{\rho_0}\right)\tau_0 + 3A_0^{\rho_1}\rho_0 \\
&+\frac{1}{18}\left(B_1^{\rho_0} - B_2^{\rho_0}\right)\left[25G_1(\xi) - 7\xi^2G_2(\xi) + 5\xi G_1'(\xi) - \xi^3G_2'(\xi)\right]\tau_0 + 3B_0^{\rho_1}\left[H_0(\xi) + \frac{\xi}{3}H_0'(\xi)\right]\rho_0 \\
&+\frac{25}{6}\left(A_1^{\rho_1} + A_2^{\rho_1}\right)\tau_0 + \frac{25}{6}\left(B_1^{\rho_1} - B_2^{\rho_1}\right)\left[H_0(\xi) + \frac{\xi}{5}H_0'(\xi) - \frac{7\xi^2}{30}H_1(\xi) - \frac{\xi^3}{30}H_1'(\xi)\right]\tau_0\,, \qquad (12)
\end{aligned}
$$

$$
\begin{aligned}
K_{\rm sym} =& -\frac{10}{9}\frac{\hbar^2}{2m}\frac{\tau_0}{\rho_0} - B_0^{\rho_0}\left[\frac{5\xi^2}{3}G_0(\xi) + \frac{4\xi^3}{3}G_0'(\xi) + \frac{\xi^4}{6}G_0''(\xi)\right]\rho_0 + \frac{25}{9}\left(A_1^{\rho_0} + A_2^{\rho_0}\right)\tau_0 \\
&+ \frac{1}{9}\left(B_1^{\rho_0} - B_2^{\rho_0}\right)\left[25G_1(\xi) - 14\xi^2G_2(\xi) + 20\xi G_1'(\xi) - 6\xi^3G_2'(\xi) + \frac{5\xi^2}{2}G_1''(\xi) - \frac{\xi^4}{2}G_2''(\xi)\right]\tau_0 \\
&+ \frac{25}{3}\left(B_1^{\rho_1} - B_2^{\rho_1}\right)\left[H_0(\xi) + \frac{4\xi}{5}H_0'(\xi) + \frac{\xi^2}{10}H_0''(\xi) - \frac{7\xi^2}{15}H_1(\xi) - \frac{\xi^3}{5}H_1'(\xi) - \frac{\xi^4}{60}H_1''(\xi)\right]\tau_0 \\
&+ B_0^{\rho_1}\left[4\xi H_0'(\xi) + \xi^2H_0''(\xi)\right]\rho_0 + \frac{25}{3}\left(A_1^{\rho_1} + A_2^{\rho_1}\right)\tau_0\,. \qquad (13)
\end{aligned}
$$

In the present study, we present results for two preliminary sets of $a = 0.8$ fm parameters. First, by using conditions $T_2^{(i)} = -T_1^{(i)}$, we obtained parameters REG2a.130531 that correspond to a local finite-range momentum-independent potential [11]. Second, by releasing these constraints, we obtained parameters REG2b.130531. On the one hand, both sets correspond to the same values of $\rho_{\rm sat} = 0.16$ fm, $E/A = -16$, $K_\infty = 230$, and $J = 32$. On the other hand, they correspond to different values of $L = 100.2$ and 58, $K_{\rm sym} = 83.26$ and -175, and $m^*/m = 0.38$ and 0.41, respectively (all energies are in MeV). Values of parameters are listed in Table 1. In both cases, saturation in symmetric matter is obtained through the interplay between the $T_0^{(i)}$ attractive and $T_1^{(i)}$ and $T_2^{(i)}$ repulsive terms.

In Fig. 1 we show equations of state (EOS) for symmetric, neutron, polarized symmetric and polarized neutron matter for the effective interactions Skyrme SV [7] (zero-range density-independent), Gogny D1N [12] (finite-range density-dependent) and the two regularized δ interactions. The Skyrme SV interaction is the only two-body density-independant interaction commonly used nowadays while D1N is a succesful finite-range density-dependent interaction. The regularized δ interactions have effective masses that are too low at saturation density but a more realistic incompressibility, similar to that obtained with D1N. Different dependences on momenta and densities of the four EOS make their behavior in neutron, polarized symmetric, and polarized neutron matter very different, although symmetric matter remains the ground state upto very high densities.

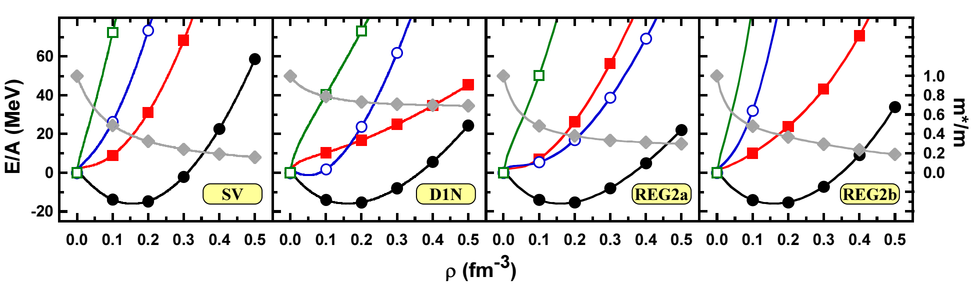

Figure 1. Equation of state of the symmetric (full circles), neutron (full squares), polarized symmetric (open circles), and polarized neutron (open squares) infinite matter (left scale). The effective mass (right scale) is shown with diamonds.

Table 1. Values of coupling constants $T_k^{(i)}$ that define the a = 0.8 fm parametrizations REG2a.130531 (top, $T_2^{(i)} = -T_1^{(i)}$) and REG2b.130531 (bottom) of the regularized δ interaction (1), in units of MeV fm^3 ($k = 0$) and MeV fm^5 ($k = 1, 2$). Standard zero-range spin-orbit forces with W_0 = 209.30 and 168.35 MeV fm^5, respectively, were used.

$T_k^{(i)}$	$i = 1$	$i = 2$	$i = 3$	$i = 4$
$k = 0$	−968.645	1645.515	−1400.680	−451.892
$k = 1$	−653.038	1349.673	−2011.063	1692.524
$k = 0$	−12250.143	7277.075	−6952.679	10744.723
$k = 1$	−1149.333	1594.666	−2342.666	2413.333
$k = 2$	3184.584	−513.696	4681.530	−5127.553

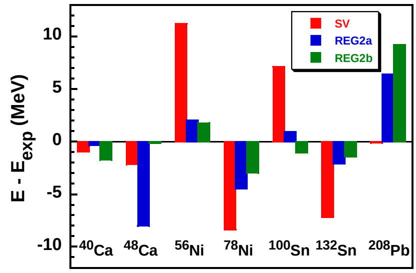

Figure 2. Deviations of ground-state energies of doubly magic nuclei from experimental data.

To calculate finite nuclei, in the HFODD (v2.64p) solver [13] we implemented self-consistent solutions for the regularized δ interaction (1). Masses of doubly magic nuclei are shown in Fig. 2. We see that REG2a.130531 and, even more, REG2b.130531 represent an improvement compared to the Skyrme SV interaction.

The new effective interaction presented in this work seems to be promising. Although it does not contain any density-dependent term, it reproduces all empirical properties of the saturation point but the isoscalar effective mass, which is rather low. To our knowledge, this has never been achieved with any other density independent two-body interaction. Since this interaction has a finite range, it can be used in any calculation at the mean field level or beyond, without the need to introduce any additional momentum cut-off.

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