# Finite-range separable pairing interaction within the new N$^3$LO DFT approach

**Veselý P.**[1], **Dobaczewski J.**[1,2], **Michel N.**[1], **and Toivanen J.**[1]

[1] Department of Physics, P.O. Box 35 (YFL), University of Jyväskylä, FI-40014, Finland
[2] Institute of Theoretical Physics, University of Warsaw, ul. Hoża 69, 00-681 Warsaw, Poland

E-mail: vesely@ipnp.troja.mff.cuni.cz

**Abstract.** For over four decades, the Skyrme functional within various parametrizations has been used to calculate nuclear properties. In the last few years there was a number of attempts to improve its performance and introduce generalized forms. In particular, the most general phenomenological quasi-local energy density functional, which contains all combinations of density, spin-density, and their derivatives up to the sixth order (N$^3$LO), was proposed in [1]. Since in the phenomenological-functional approaches, the particle-particle (pp) channel is treated independently of the particle-hole (ph) channel, there remains a question of what pairing interaction is suitable to use within the N$^3$LO energy functional. In the present study, we use the separable, finite-range, translationally invariant interaction given in [2] and we present the first test-case application of this pairing interaction within the code HOSPHE that is able to treat the N$^3$LO energy density functional.

## 1. Construction of the N$^3$LO functional

Following [1], the construction of the N$^3$LO functional can be outlined in three steps. First we define basic building blocks: (i) the general non-local densities, which include both the scalar and vector (spin) terms,

$$\rho(\vec{r}\sigma,\vec{r}'\sigma') = \frac{1}{2}\rho_{00}(\vec{r},\vec{r}')\delta_{\sigma,\sigma'} + \frac{1}{2}\sum_{\mu=-1,0,1}\langle\sigma|\sigma_\mu|\sigma'\rangle\rho_{1\mu}(\vec{r},\vec{r}'), \tag{1}$$

(ii) the derivative operator,

$$\nabla_{1,\mu=\{-1,0,1\}} = -i\left\{\frac{1}{\sqrt{2}}(\nabla_x - i\nabla_y), \nabla_z, -\frac{1}{\sqrt{2}}(\nabla_x + i\nabla_y)\right\}, \tag{2}$$

and (iii) the relative momentum operator,

$$k_{1\mu} = \frac{1}{2i}(\nabla_{1\mu} - \nabla'_{1\mu}). \tag{3}$$

In the second step, we construct more general building blocks: (iv) the tensor derivative operator of order $m$ and rank $I$,

$$D_{mI} = \underbrace{[\nabla...[\nabla[\nabla\nabla]_{I_2}]_{I_3}...]}_{m}{}_I\ , \tag{4}$$

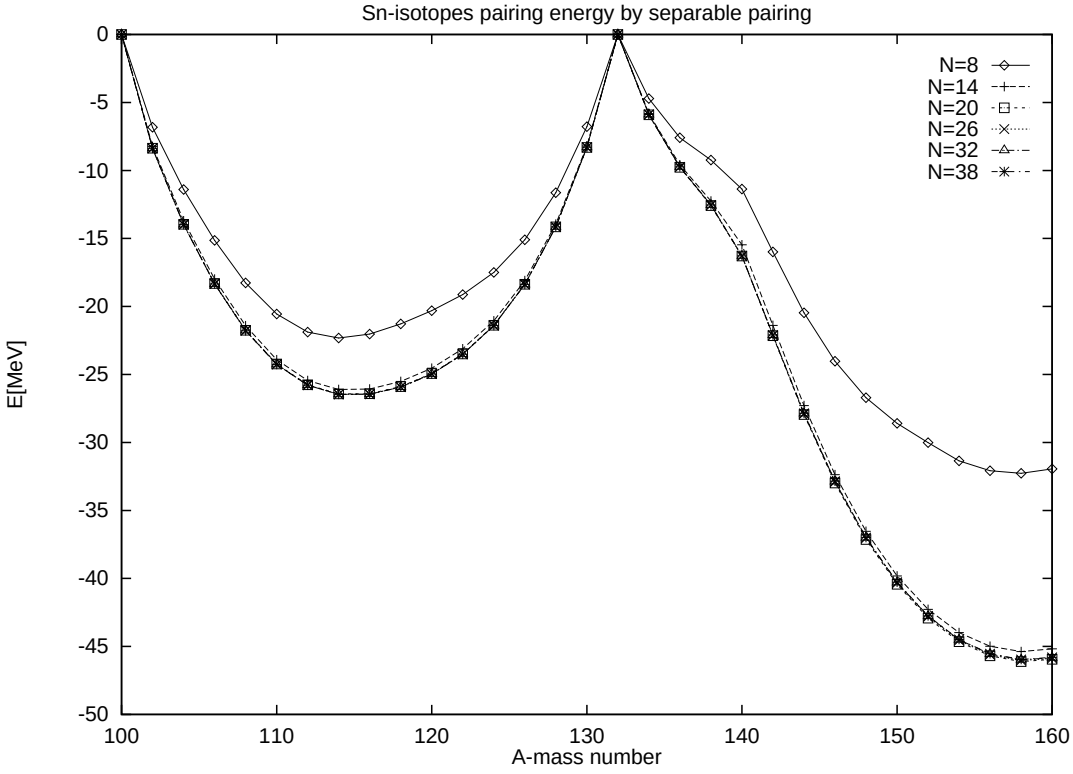


**Figure 1.** Pairing energies for the chain of even-even tin isotopes, obtained in the HO bases of N=8, 14, 20, 26, 32, and 38 shells.

and in analogous way (v) the tensor operator of relative momentum,

$$K_{mI} = \underbrace{[k...[k[kk]_{I_2}]_{I_3}...]_I}_{m} \ , \tag{5}$$

and finally (vi) the generalized local (primary) density,

$$\rho_{nLvJ}(\vec{r}) = \left\{ \left[ K_{nL} \otimes \rho_v(\vec{r},\vec{r}') \right]_J \right\}_{\vec{r}=\vec{r}'} \ . \tag{6}$$

In the third step, we use the building blocks to construct the energy density,

$$\mathcal{H}(\vec{r}) = \sum_{mI,nLvJ} \sum_{n'L'v'J'} C^{n'L'v'J'}_{mI,nLvJ} \left[ \rho_{n'L'v'J'}(\vec{r}) [D_{mI} \rho_{nLvJ}(\vec{r})]_{J'} \right]_0 \ , \tag{7}$$

and the energy density functional (EDF) is defined as the integral of $\mathcal{H}(\vec{r})$. Each term in the summation in Eq. (7) can be characterized by its order, which is defined as:

$$\text{order} = m + n + n' \ . \tag{8}$$

This general EDF contains a large number of coupling constants $C^{n'L'v'J'}_{mI,nLvJ}$; however, there are several symmetries (spherical, Galilean, gauge) that significantly reduce the number of terms in the energy density (7) (see [1] for details).

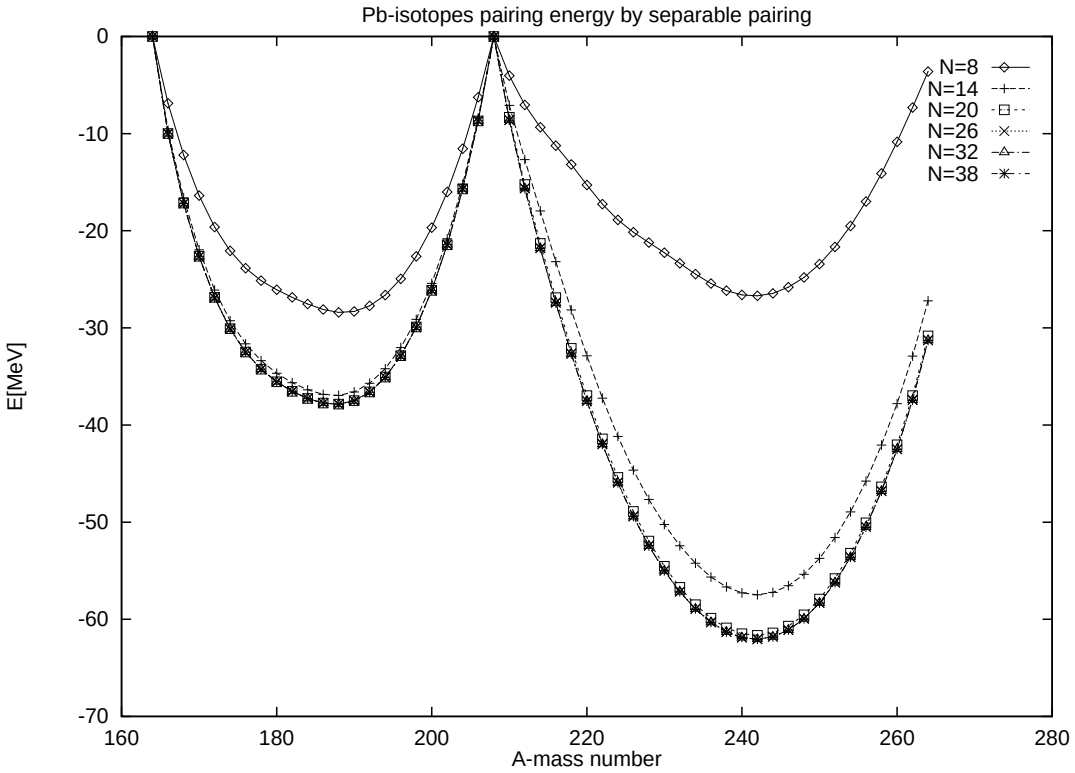


**Figure 2.** Same as in Fig. 1 but for the lead isotopes.

## 2. Finite-Range Separable Pairing Interaction

In the phenomenological-functional approaches, the particle-particle (pp) channel is treated independently of the particle-hole (ph) channel. Traditionally, for the Skyrme functional, the delta pairing interaction,

$$\hat{V}^{pp} = V_0 \delta(\vec{r} - \vec{r}'), \tag{9}$$

or its density-dependent variant have been used. The main disadvantage of this pairing interaction is, however, its cut-off dependence, as discussed, e.g., in [3]. This requires using renormalization or regularization procedures (see [4] and references cited therein), which may depend on the order of derivatives appearing in the mean-field Hamiltonian. Because of this reason, we decided to apply in the pp channel of our phenomenological functional the finite-range separable pairing interaction, as it was introduced in [2], which does not lead to any cut-off dependence.

The finite-range separable pairing interaction is defined in the momentum representation as:

$$\langle \vec{k}_1 \vec{k}_2 | V^{pp} | \vec{k}_1' \vec{k}_2' \rangle = (2\pi)^3 \delta(\vec{K} - \vec{K}') \langle \vec{k} | V^{pp} | \vec{k}' \rangle \ . \tag{10}$$

From the beginning, the total momentum, $\vec{K} = \vec{k}_1 + \vec{k}_2$, is separated from the relative momentum, $\vec{k} = \frac{1}{2}(\vec{k}_1 - \vec{k}_2)$. The term $\delta(\vec{K} - \vec{K}')$ in Eq. (10) ensures the conservation of the total momentum of the interacting pair. In terms of relative momenta, the pairing interaction for neutrons ($\nu = n$) and protons ($\nu = p$) is then defined by

$$\langle \vec{k} | V_\nu^{pp} | \vec{k}' \rangle = -G_\nu p(k) p(k') \tag{11}$$

where functions $p(k)$ have the form of sum of $m$ Gaussian terms

$$p(k) = \frac{1}{m}\sum_{i=1}^{m} \mathrm{e}^{-a_i^2 k^2} \ . \tag{12}$$

After the Fourier transform to the coordinate representation, one obtains

$$\langle \vec{r}|V_\nu^{pp}|\vec{r}'\rangle = -G_\nu P(r)P(r') \tag{13}$$

with

$$P(r) = \frac{1}{m}\sum_{i=1}^{m} \frac{1}{(4\pi a_i^2)^{3/2}} \mathrm{e}^{-\frac{r^2}{4a_i^2}} \ . \tag{14}$$

One can now express this pairing interaction by using its matrix elements in the standard harmonic oscillator (HO) basis. To this end, one can use two more transformations – the Talmi-Moshinsky transformation to separate the total and relative coordinates and coupling of angular momenta of the interacting pair [5]. The final, fully separable, form of the pairing energy reads:

$$\begin{aligned} E^{pp} = &-\frac{1}{4}G_+ \sum_J \sum_N \sum_{\mu\nu\mu'\nu'} V_{\mu\nu}^{J,NJ} V_{\mu'\nu'}^{J,NJ} \Big( \langle \Psi_{\alpha_\mu j_\mu} || \kappa_0'^{+J} || \Psi_{\alpha_\nu j_\nu} \rangle \langle \Psi_{\alpha'_\mu j'_\mu} || \kappa_0^J || \Psi_{\alpha'_\nu j'_\nu} \rangle + \\ &\qquad + \langle \Psi_{\alpha_\mu j_\mu} || \kappa_1'^{+J} || \Psi_{\alpha_\nu j_\nu} \rangle \langle \Psi_{\alpha'_\mu j'_\mu} || \kappa_1^J || \Psi_{\alpha'_\nu j'_\nu} \rangle \Big) \\ &-\frac{1}{4}G_- \sum_J \sum_N \sum_{\mu\nu\mu'\nu'} V_{\mu\nu}^{J,NJ} V_{\mu'\nu'}^{J,NJ} \Big( \langle \Psi_{\alpha_\mu j_\mu} || \kappa_0'^{+J} || \Psi_{\alpha_\nu j_\nu} \rangle \langle \Psi_{\alpha'_\mu j'_\mu} || \kappa_1^J || \Psi_{\alpha'_\nu j'_\nu} \rangle + \\ &\qquad + \langle \Psi_{\alpha_\mu j_\mu} || \kappa_1'^{+J} || \Psi_{\alpha_\nu j_\nu} \rangle \langle \Psi_{\alpha'_\mu j'_\mu} || \kappa_0^J || \Psi_{\alpha'_\nu j'_\nu} \rangle \Big), \end{aligned} \tag{15}$$

where $G_\pm = (G_n \pm G_p)/2$ and $V_{\mu\nu}^{J,NJ}$ are the separable interaction matrix elements:

$$V_{\mu\nu}^{J,NL} = \sqrt{(2j_\mu+1)(2j_\nu+1)} \begin{Bmatrix} l_\mu & l_\nu & J \\ \frac{1}{2} & \frac{1}{2} & 0 \\ j_\mu & j_\nu & J \end{Bmatrix} \sum_{nl} M_{n_\mu l_\mu n_\nu l_\nu}^{NLnl} \sqrt{4\pi} \left( \int_0^\infty r^2 \mathrm{d}r P(r) R_{nl}(r, b_r) \right), \tag{16}$$

which include the Talmi-Moshinsky brackets $M_{n_\mu l_\mu n_\nu l_\nu}^{NLnl}$, a 9j-symbol coming from the coupling of the two nucleons to total angular momentum $J$, and a radial integral which can be calculated analytically:

$$\int_0^\infty r^2 \mathrm{d}r P(r) R_{nl}(r, b_r) = \frac{1}{b_r^{3/2}} \sqrt{\frac{(n+\frac{1}{2})!}{2n!}} \frac{1}{m} \sum_{i=1}^{m} \frac{1}{(4\pi a_i^2)^{3/2}} \left( \frac{4a_i^2 b_r^2}{1+2a_i^2 b_r^2} \right)^{3/2} \left( \frac{1-2a_i^2 b_r^2}{1+2a_i^2 b_r^2} \right)^n \delta_{l0} \ . \tag{17}$$

From relations (15)–(17), it follows that the free parameters of this pairing-interaction model are the coupling constants $G_+$ and $G_-$, and $m$ parameters $a_i$. These parameters should be fitted to the experimental data.

## 3. Calculations and preliminary results

The finite-range separable pairing interaction was implemented into the recently developed code for calculation of spherical nuclei within the N$^3$LO energy functional – HOSPHE [6].

For the first set of test calculations we chose two chains of even-even isotopes for tin ($A = 100 - 160$) and lead ($A = 164 - 264$). Since our aim here is just to check qualitative results of the method, we use the following set for $m = 1$:

$$G_+ = 738\,\mathrm{MeV\,fm^3}, \quad G_- = 0, \quad a_1 = 0.636\,\mathrm{fm}.$$

These values were fixed [2] to reproduce the gap equation of nuclear matter calculated by the Gogny force.

The obtained pairing energies are shown in figure 1 (Sn isotopes) and figure 2 (Pb isotopes). They were calculated within the Hartree-Fock-Bogolyubov method with the finite-range separable pairing force acting in the pp channel and the Skyrme SLy4 interaction acting in the ph channel. It can be seen that the pairing energies rapidly converge already for $N = 20$ HO shells. Further refinement of the nuclear pairing properties can probably be obtained by adding more Gaussian terms, and hence by fitting more parameters in the phenomenological pairing force, i.e. with $m \geq 2$.

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**References**

[1] Carlsson B G, Dobaczewski J, and Kortelainen M, 2008 *Phys. Rev.* C **78**, 044326; 2010 *Phys. Rev.* C **81**, 029904(E)
[2] Tian Y, Ma Z Y, and Ring P, 2009 *Phys. Lett.* B **676**, 44
[3] Dobaczewski J, Nazarewicz W, Werner T R, Berger J-F, Chinn C R, and Dechargé J, 1996 *Phys. Rev.* C **53**, 2809
[4] Borycki P J, Dobaczewski J, Nazarewicz W, and Stoitsov M V, 2006 *Phys. Rev.* C **73**, 044319
[5] Tian Y, Ma Z Y, and Ring P, 2009 *Phys. Rev.* C **79**, 064301
[6] Carlsson B G, Dobaczewski J, Toivanen J, and Veselý P, 2010 *Comp. Phys. Commun.* **181**, 1641