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Separable approximation to two-body matrix elements

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Two-body matrix elements of arbitrary local interactions are written as the sum of separable terms in a way that is well suited for the exchange and pairing channels present in mean-field calculations. The expansion relies on the transformation to center of mass and relative coordinate (in the spirit of Talmi's method) and therefore it is only useful (finite number of expansion terms) for harmonic oscillator single particle states. The converge of the expansion with the number of terms retained is studied for a Gaussian two body interaction. The limit of a contact (delta) force is also considered. Ways to handle the general case are also discussed.

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I. INTRODUCTION

The evaluation of the pairing field in mean field theories like Hartree-Fock plus Bardeen-Cooper-Schrieffer (HF + BCS) or Hartree-Fock-Bogolubov (HFB) is a computationally intensive task due to the non-local character of the pairing tensor and the effort is comparable to the one devoted to the evaluation of the exchange field in the HF method. Therefore, zero range pairing interactions are thoroughly used in standard mean field calculations in order to reduce the computational burden (see Ref. [1] for a recent review). The price to pay for the use of zero range pairing forces is the introduction of an "active space" around the Fermi level to cut away the ultraviolet divergences inherent to any contact interaction (the pairing matrix elements are independent of the momentum transfer in nuclear matter). Thus, it is customary to take into account in the gap equation only those single particle levels lying inside a so called "active window" around the Fermi level and whose (sharp or soft) boundaries are defined using reasonable (but arbitrary) assumptions. The boundaries of the window as well as the pairing interaction strength are usually fixed locally but they are usually not allowed to vary as a function of other relevant degrees of freedom like the quadrupole deformation of the nucleus. As a consequence, the impact of the rigid definition of the "pairing active window" in some observable magnitudes can be relevant (see, for instance, [2] for a discussion on the impact of the window's size on fission barriers). From this perspective, the use of finite range pairing forces seems to be quite unavoidable and this is a common argument to praise the use of Gogny type interactions [3] in HFB or HF + BCS like mean field calculations [1,4]. It has to be mentioned that a renormalization scheme for the phenomenological contact pairing interactions has been proposed in Refs. [5,6] to cure the "active window" problem. Recently, proposals to use as pairing interaction in finite nuclei a realistic finite range two body bare interaction [7] or a low momentum evolved version of it [7–9] have been discussed in the literature: the essence of the proposals is to introduce a separable interaction in momentum representation [7] that is used to fit the realistic interaction (or a low momentum evolved version of it) by resorting to fitting protocols involving nucleon-nucleon phase shifts or pairing gaps in nuclear matter. As a consequence of the separable character in momentum space the force is nonlocal in real space but in a way that simplifies the evaluation of the matrix elements needed for finite nuclei calculations [8,9]. Separable interactions were also used as a way to tackle the solution of the Lippman-Schwinger equation for the T operator with realistic nucleon-nucleon potentials [10]. Recently, a separable form in momentum space of the pairing interaction of a Gaussian two-body force (as in the Gogny force) has been proposed [11–13] as an alternative to more standard approaches based on zero range contact pairing interactions. As the approximation relies on the same ideas of Refs. [8,9] a nonlocal form of the approximate interaction in real space is obtained. The non locality of the interaction suggests the introduction of the Talmi-Brody-Moshinsky transformation [14–16] to center of mass and relative coordinate to simplify the evaluation of the pairing matrix elements in the harmonic oscillator basis. Explicit expression for the matrix elements are given in [11] for an harmonic oscillator basis with spherical quantum numbers and a Gaussian interaction. Next, it has been shown that this new form is consistent with the RPA framework [12]. Finally, the scheme has been extended [13] to the case of a harmonic oscillator basis with axial quantum numbers. The extension to the case of a harmonic oscillator basis with triaxial quantum numbers is straightforward. In the present paper I show that the transformation to center of mass and relative coordinates can be used for general two body interactions to obtain a kind of separable expression for the pairing two-body matrix elements which involves the one-body matrix elements of the interaction for the relative coordinate wave functions. The use of the spectral representation of this interaction matrix leads to a more explicit separable form of the kind considered in [7–9,11–13]. By using two specific examples in one dimension it is shown that the number of separable terms in the expansion can be severely cut down for short range interactions. The validity of the expansion concerning ultraviolet divergences is also discussed. Finally, computational schemes to deal with the Yukawa (and Coulomb) potential are discussed. It has to be stressed that the present approach is not limited to pairing matrix elements and can easily be extended to deal with the exchange matrix elements required for the evaluation of the Fock potential and therefore it could be used as an

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approximation scheme to shorten the numerical burden of HFB calculations with finite range forces like Gogny [3], other recent proposals based on the Yukawa potential [17], and even the Coulomb potential.

II. SEPARABLE APPROXIMATION TO TWO-BODY MATRIX ELEMENTS

A. General procedure

Let us consider the (not antisymmetrized) two-body matrix element $v_{n_1,n_2,n_3,n_4} = \int d\vec{r}_1 \int d\vec{r}_2 \phi^*_{n_1}(\vec{r}_1)\phi^*_{n_2}(\vec{r}_2)v(\vec{r}_1 - \vec{r}_2)\phi_{n_3}(\vec{r}_1)\phi_{n_4}(\vec{r}_2)$ for harmonic oscillator (HO) wave functions $\phi_n(\vec{r})$ (this is not a fundamental restriction as more general single particle wave functions can always be expanded in a HO basis). Taking into account that at the end we will be folding this matrix elements with a matrix (either the pairing tensor or the density for the exchange potential) with indexes n_3 and n_4 the best approach for the evaluation of this matrix element is that of Talmi [14] and Brody-Moshinsky [15,16] (see also [18,19] for a general discussion). Within this method, the product of HO single particle wave functions with different arguments $\phi_{n_3}(\vec{r}_1)\phi_{n_4}(\vec{r}_2)$ is expanded in terms of suitable center of mass $\vec{R} = \frac{1}{\sqrt{2}}(\vec{r}_1 + \vec{r}_2)$ and relative coordinate $\vec{r} = \frac{1}{\sqrt{2}}(\vec{r}_1 - \vec{r}_2)$ wave functions (this unusual definition of the center of mass and relative coordinate renders some of the expressions simpler than with the usual definition)

$$\phi_{n_3}(\vec{r}_1)\phi_{n_4}(\vec{r}_2) = \sum_{Nn} M^{Nn}_{n_3n_4}\phi_N(\vec{R})\phi_n(\vec{r}). \tag{1}$$

The center of mass and relative coordinate wave functions have the same structural form as the original wave functions and the expansion is finite (the range of values of N and n is finite). This is a direct consequence of the special structure of the HO wave functions (the product of a Gaussian times a polynomial). Apart from the HO, this peculiarity is only preserved in the case of plane waves and the developments considered below can be extended easily to this case too. The expansion coefficients $M^{Nn}_{n_1n_2}$ are referred to as Talmi-Brody-Moshinsky [14–16] coefficients (TBMC). The TBMC have a selection rule that will help to reduce the number of final separable terms, it is $n_1 + n_2 = N + n$ (see Appendix A for the general expression and selection rules in the one-dimensional case) which implies that only one of the two sums in Eq. (9) is relevant. Explicit forms of the TBMC coefficients have been discussed several times in the literature both in the 3D spherical form of the HO wave functions [14–16] as in the one-dimensional case [20]. Introducing the expansion of Eq. (9) into the definition of the matrix element we obtain the result

$$v_{n_1,n_2,n_3,n_4} = \sum_N \sum_{nn'} M^{*Nn}_{n_1n_2} v_{nn'} M^{Nn'}_{n_3n_4}, \tag{2}$$

where we have made use of the orthogonality of the center of mass wave functions $\phi_N(\vec{R})$ and introduced the matrix elements

$$v_{nn'} = \int d\vec{r}\,\phi^*_n(\vec{r})v(\sqrt{2}\vec{r})\phi_{n'}(\vec{r}). \tag{3}$$

Please note the $\sqrt{2}$ factor in the argument of the interaction that is a direct consequence of the definition of the relative coordinate. This result can be easily generalized to nonlocal interactions of the form

$$\langle \vec{r}_1\vec{r}_2|\hat{v}|\vec{r}_1\,'\vec{r}_2\,'\rangle = \delta(\vec{R} - \vec{R}\,')v(\vec{r},\vec{r}\,'), \tag{4}$$

where $\vec{R}\,'$ and $\vec{r}\,'$ are the center of mass and relative coordinates associated to $\vec{r}_1\,'$ and $\vec{r}_2\,'$. Applying the transformation of Eq. (1) we obtain for the HO matrix elements the same expression as in Eq. (2) but replacing $v_{nn'}$ of Eq. (3) by

$$v_{nn'} = \int d\vec{r} \int d\vec{r}\,'\phi^*_n(\vec{r})v(\vec{r},\vec{r}\,')\phi_{n'}(\vec{r}\,'). \tag{5}$$

The $v_{nn'}$ are matrix elements of a hermitian matrix and therefore can be written, by resorting to the spectral decomposition of the matrix, as

$$v_{nn'} = \sum_L D^*_{nL} v_L D_{n'L}, \tag{6}$$

where the coefficients v_L (the eigenvalues of $v_{nn'}$) are real quantities. By introducing the coefficients

$$\tilde{M}^{NL}_{n_1n_2} = \sum_n M^{Nn}_{n_1n_2} D_{nL} \tag{7}$$

we can finally cast Eq. (2) in a form that corresponds clearly to a separable expansion for pairing and exchange matrix elements as

$$v_{n_1,n_2,n_3,n_4} = \sum_N \sum_L \tilde{M}^{*NL}_{n_1n_2} v_L \tilde{M}^{NL}_{n_3n_4}. \tag{8}$$

This separable expansion is still exact and can be used to express the pairing field also as a sum of separable terms

$$\Delta_{n_1n_2} = \sum_{n_3n_4} v_{n_1,n_2,n_3,n_4}\kappa_{n_3n_4} = \sum_{NL} \tilde{M}^{*NL}_{n_1n_2} v_L \Lambda_{NL}$$

with $\Lambda_{NL} = \sum_{n_3n_4} \tilde{M}^{NL}_{n_3n_4}\kappa_{n_3n_4}$. At this point it is worth mentioning that this procedure can be straightforwardly extended to the evaluation of the exchange field by introducing the new TBMC as

$$\phi^*_{n_1}(\vec{r}_1)\phi_{n_4}(\vec{r}_2) = \sum_{Nn} \bar{M}^{Nn}_{n_1n_4}\phi_N(\vec{R})\phi_n(\vec{r}) \tag{9}$$

to obtain

$$v_{n_1,n_2,n_3,n_4} = \sum_N \sum_{nn'} \bar{M}^{Nn}_{n_1n_4} v_{nn'} \bar{M}^{*Nn'}_{n_2n_3}$$

which can be used for the evaluation of the exchange field. This possibility has not been considered in Refs. [11,13].

The drawback of the (still exact) separable expansion being considered is that the number of terms involved is enormous unless some property of the interaction is invoked to restrict it. To do so, we can use the general ideas of linear algebra on how to approximate an arbitrary matrix in terms of low rank Kronecker tensor products (see [21,22] for an introduction to the subject) to justify the rank one approximation

$$v_{nn'} \approx d^*_n d_{n'}, \tag{10}$$

where $d_n = \sqrt{v_0}D_{n0}$ and we are assuming that the $L = 0$ term in Eq. (6) corresponds to the largest eigenvalue v_0 of

the interaction matrix $v_{nn'}$. In this way we have reduced the number of separable terms by a factor that corresponds to the dimension of the matrix $v_{nn'}$. For better accuracy, we can pursue further this idea to suggest the approximation

$$v_{nn'} \approx \sum_{L=0}^{L_C} D^*_{nL} v_L D_{n'L} \tag{11}$$

(where v_L with $L = 0, \ldots, L_C$ stand for the $L_C + 1$ largest eigenvalues of the matrix $v_{nn'}$). Obviously, low rank Kronecker tensor products do not necessarily have to be based on the eigenvectors of the interaction matrix v and other alternatives inspired in the physics to be described could be incorporated easily [a possibility that comes up immediately is to use for d_n in Eq. (10) a linear combination of the eigenvectors of v with weights physically inspired by the problem to be treated and to be fitted for the optimal reproduction of some quantity].

B. Zero range interaction

In the following we will consider some typical interactions to asses the validity of the preceding approximation scheme and we will start by considering a zero range contact interaction $v(\vec{r}) = G\delta(\vec{r})$. In this case, the matrix $v_{nn'}$ is simply given by

$$v_{nn'} = \frac{G}{2^{3/2}} \phi^*_n(0)\phi_{n'}(0) \tag{12}$$

which implies, in the language of Eq. (6), that all the eigenvalues v_L are zero except the $L = 0$ one. For this interaction, the rank one approximation of Eq. (10) is exact and the reduction in the number of separable term is quite significant. Introducing the quantity

$$\tilde{M}^N_{n_1 n_2} = \sum_n M^{Nn}_{n_1 n_2} \phi_n(0)$$

we finally obtain

$$v_{n_1,n_2,n_3,n_4} = \frac{G}{2^{3/2}} \sum_N \tilde{M}^{*N}_{n_1 n_2} \tilde{M}^N_{n_3 n_4}. \tag{13}$$

Apart from the analytical result, this formula is telling us that for short range interactions the expansion of Eq. (11) is expected to be accurate enough by considering only a limited number of terms.

In order to get a deeper insight into the number of separable terms in the preceding expansion for the zero range force we will focus on the one-dimensional case. Our basis will be the one-dimensional harmonic oscillator basis $\phi_n(x)$ with $n = 0, \ldots, M$ and containing $M + 1$ elements. The TBM expansion of the 1-D HO wave functions is an expansion of the product of two polynomials in the variables x_1 and x_2 in terms of the product of polynomials in the variables $X = \frac{1}{\sqrt{2}}(x_1 + x_2)$ and $x = \frac{1}{\sqrt{2}}(x_1 - x_2)$. Although its explicit expression is known since a long time [20], we present in Appendix A a brief derivation based on the generating function of the Hermite polynomials. As a consequence of the explicit form of the TBM coefficients, both quantum numbers N (center of mass) and n (relative) should range from 0 up to $2M$ (i.e., $2M + 1$ possible values) if none of the selection rules of the TBM coefficients is taken into account. The parity selection rule $(-1)^{n_1+n_2} = (-1)^{N+n}$ of the TBM coefficients can be used to reduce the number of terms in the N sum. As $\phi_n(0)$ is only different from zero for even values of n, the parity of N has to be the one of $n_1 + n_2$ and therefore the number of terms in the N sum of Eq. (13) gets reduced to half the initial value ($M + 1$ to be more precise).

C. Gaussian interaction

In order to analyze in more detail the consequences of the proposed expansion, we will study the example of a Gaussian interaction of range μ in one dimension. The more realistic three-dimensional case can be elucidated from the results obtained here as, in that case, the matrix elements are the product of the one-dimensional ones along each of the three spatial dimensions. In addition, the zero-range interaction results can be recovered in the limit $\mu \to 0$ providing further insight into the number of terms to be retained as well as potential problems with ultraviolet divergences. The one-dimensional HO wave functions will be denoted as $\varphi_n(z; b) = \exp(-\frac{1}{2}\frac{z^2}{b^2})\tilde{\varphi}_n(z/b)$ where $\tilde{\varphi}(z/b)$ is the polynomial part of the HO wave function given by the product of the Hermite polynomial of degree n times the normalization constant of the 1D HO wave function. The quantity to evaluate is

$$\begin{aligned} v_{nn'} &= \int dz\, \varphi^*_n(z; b) \exp\left(-\frac{2z^2}{\mu^2}\right) \varphi_{n'}(z; b) \\ &= \int dz\, \tilde{\varphi}^*_n(z/b) \exp\left[-\left(\frac{2}{\mu^2} + \frac{1}{b^2}\right) z^2\right] \tilde{\varphi}_{n'}(z/b). \end{aligned}$$

This integral can be carried out in many different ways but for our purposes it is better to use the transformation matrix $D(b'/b)$ connecting $\tilde{\varphi}_n(z/b)$ with $\tilde{\varphi}_n(z/b')$

$$\tilde{\varphi}_n(z/b) = \sum_{n'=0}^{n} D_{nn'}(b'/b)\tilde{\varphi}_{n'}(z/b'),$$

defined in Appendix B, to write

$$v_{nn'} = \sum_L D^*_{nL}(B/b) D_{n'L}(B/b)$$

with $B/b = \mu/\sqrt{\mu^2 + 2b^2} = \eta$. It is better to write the preceding result as

$$v_{nn'} = \sum_L \tilde{D}^*_{nL}(\eta)\eta^{2L+1}\tilde{D}_{n'L}(\eta) \tag{14}$$

to make explicit the dependence in the range of the Gaussian μ. Although this expression is not an explicit power expansion in η due to the dependence of $\tilde{D}$ on this parameter, it is close to be so because the ratio between the $L + 2$ term of the sum and the L one is given by $\eta^4[1 + \mu^2/(2b^2)]^2(n - L)(n' - L)/[(L + 2)(L + 1)]$ that shows a dominant η^4 behavior. As η typically goes as μ/b we can conclude that Eq. (14) is a kind of expansion on the range of the interaction μ. For small ranges $\mu \to 0$ the parameter η tends to $\mu/(\sqrt{2}b)$ and therefore the most significant term in the sum is $L = 0$. The remaining

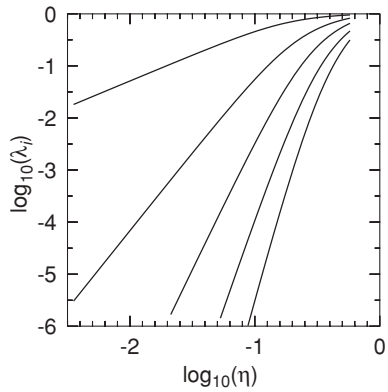

FIG. 1. Largest eigenvalues λ_i of the interaction matrix in the case of a one-dimensional Gaussian interaction of range μ. The eigenvalues shown are plotted as a function of the parameter η defined in the text. Notice the log-log character of the plot.

terms decrease as μ^{2L} and justify to cut the expansion of Eq. (14) at some small L_C

$$v_{nn'}^{\text{App}} = \sum_{L=0}^{L_C} \tilde{D}_{nL}^{*}(\eta)\eta^{2L+1}\tilde{D}_{n'L}(\eta). \tag{15}$$

Using the connection between a Gaussian of vanishing range and the δ function

$$\delta(x_1 - x_2) = \lim_{\mu\to 0} \frac{1}{\sqrt{\pi}} \frac{e^{-(x_1-x_2)^2/\mu^2}}{\mu}$$

it is possible to obtain Eq. (12) from Eq. (14) by appropriately taking the $\mu \to 0$ limit. As can be shown easily, the $\mu \to 0$ limit of $\tilde{D}_{n0}(\eta)$ (the only remaining term is $L = 0$) is given by $\pi^{1/4}b^{1/2}\varphi_n(0)$ as required.

At this point it is worth noticing that neither the eigenvalues nor the eigenvectors of the $v_{nn'}$ matrix in the Gaussian case are given by η^{2L+1} or by the coefficients $\tilde{D}_{n'L}(\eta)$ above [see Eq. (14)]. In order to understand the differences, the largest eigenvalues obtained by numerical diagonalization in the case $N = 40$ and for $b = 2$ fm are plotted in Fig. 1 as a function of η. We observe in the log-log plot that for small values of η the eigenvalues have a linear behavior that corresponds to η^{2L+1} for $L = 0, \ldots,$ recovering in this case the result of Eq. (14). However, for larger values of η this is not the case indicating that the eigenvalues of $v_{nn'}$ depart from the quantities in Eq. (14). An interesting observation regarding the behavior of the eigenvalues is that they are a decreasing function as μ decreases, justifying the idea that keeping only the largest eigenvalues is a kind of short-range expansion of the matrix elements. Obviously, if all the terms are considered, both the expansion of Eq. (14) and the general one of the spectral decomposition of the matrix $v_{nn'}$ give the exact answer. The differences will show up in the approximate case when only a finite number of terms is retained. We have checked that the spectral decomposition always gives the best results if quantified in terms of the mean square deviation $\sigma_v = \sqrt{\sum_{nn'}(v_{nn'} - v_{nn'}^{\text{App}})^2/(N+1)}$, but none of the approximate matrix elements $v_{nn'}^{\text{App}}$ reproduce the exact ones, as it may happen when using Eq. (15). As a consequence of the selection rules of the D coefficients involved, the exact values of $v_{nn'}$ for low values of n and n' can be obtained from Eq. (15) even for small values of L_C. This is not in contradiction with what it was said about σ_v, as the approximation based on Eq. (15) provides, for large values of n and n', worse matrix elements than the ones obtained using the spectral decomposition of $v_{nn'}$. The analysis below of the two-body matrix elements has been carried out in parallel using both possibilities and it has been found that, although the spectral decomposition provides again a better overall approximation for the two-body matrix elements, those with small quantum numbers (the most relevant for the physics of the system to be described) are slightly better reproduced by the approximations based in Eq. (15). For the above reasons we will only show results based on Eq. (15).

The result obtained in Eq. (15) for short ranges μ suggests to approximate $v_{nn'}$ by keeping only the $L = 0$ term. However, taking into account that the transformation coefficients $D(\eta)$ preserve parity, we realize that the $L = 0$ approximation will make automatically zero the $v_{nn'}$ matrix elements with odd n. Therefore, we have to include both $L = 0$ and $L = 1$ as the leading order. The next-to-leading order will correspond to take $L = 2$ and 3 and so on. In order to test the convergence rate of such an approximation we have performed calculations comparing the exact matrix elements of the one-dimensional Gaussian interaction with those obtained using Eq. (8) and restricting the sum in L from 0 up to a parameter denoted L_C as well as the sum in N from 0 up to N_C. The size of the one-dimensional HO basis considered is of 21 shells ($n = 0, \ldots, 20$) and there are 97 241 nonzero matrix elements. The results for a Gaussian of range $\mu = 0.7$ fm are depicted in Fig. 2. In the left-hand side panels all the matrix elements are plotted (y axis, approximate values, x axis exact ones) for different values of N_C and L_C. On the right-hand side panels, the same plot is presented but this time only the matrix elements with n_1, n_2, n_3, and n_4 smaller than 7 are shown. There are two reasons: first that the realistic single particle orbitals are usually close to the HO wave functions with the same quantum number n and therefore its expansion on the HO basis usually requires the $n - 2$, n and $n + 2$ states for a reasonable representation. The second reason is that only a limited number of orbitals around the Fermi level usually play a role in the pairing properties and therefore only the quantum numbers n required to accommodate A particles are required. Usually seven major shells (the corresponding quantity in the three-dimensional case) are required to well accommodate of the order of 200 particles. Therefore, in the left-hand side panels there are many matrix elements that will contribute little to the pairing field and can be safely disregarded for the discussion of the quality of the approximation. That is, the matrix elements depicted in the right-hand side panels are supposed to be the most relevant for the pairing properties of the nucleus. Obviously these are tentative arguments that can only be validated by performing numerical test in specific cases. For instance, the results obtained in Refs. [11,13] clearly validate the above arguments in the cases considered. By looking at the plot we observe how the bigger the values of N_C and L_C are the better the approximation is (the points gather around the $y = x$ line). We even observe how the $N_c = 10$

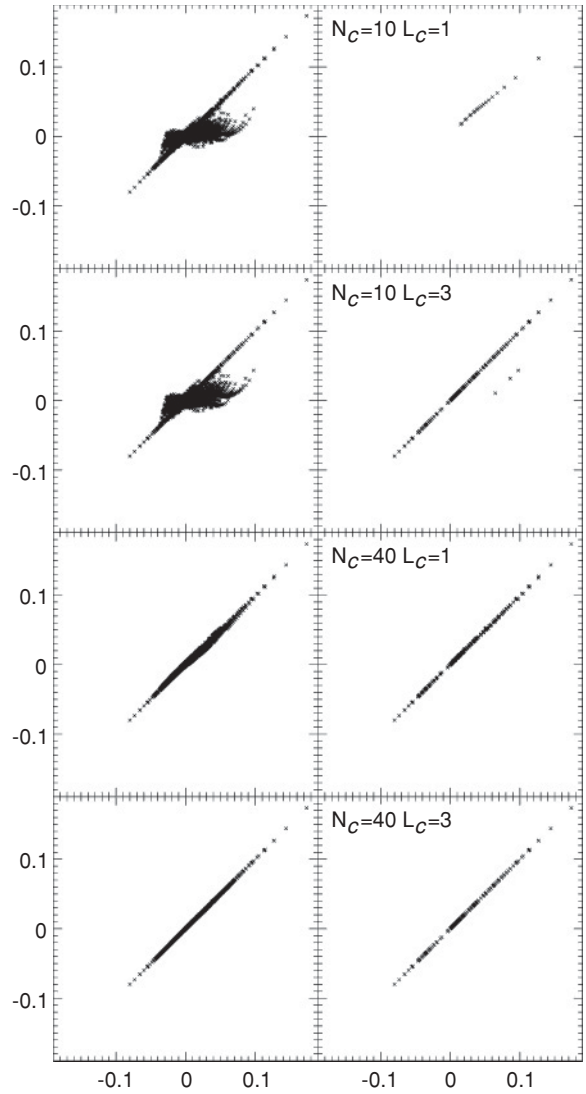

FIG. 2. Approximate matrix elements (y axis) for different values of L_C and N_C are plotted versus the exact values (x axis) for the one-dimensional Gaussian interaction with range $\mu = 0.7$ fm and harmonic oscillator length $b_z = 2.0$ fm. In the left-hand side panels, all matrix elements with n_1, n_2, n_3, and n_4 ranging from 0 up to 20 (i.e., a total of 21^4 matrix elements) are depicted. On the right-hand side panels only those matrix elements with n_1, n_2, n_3, and n_4 smaller than 7 are depicted (see text for details).

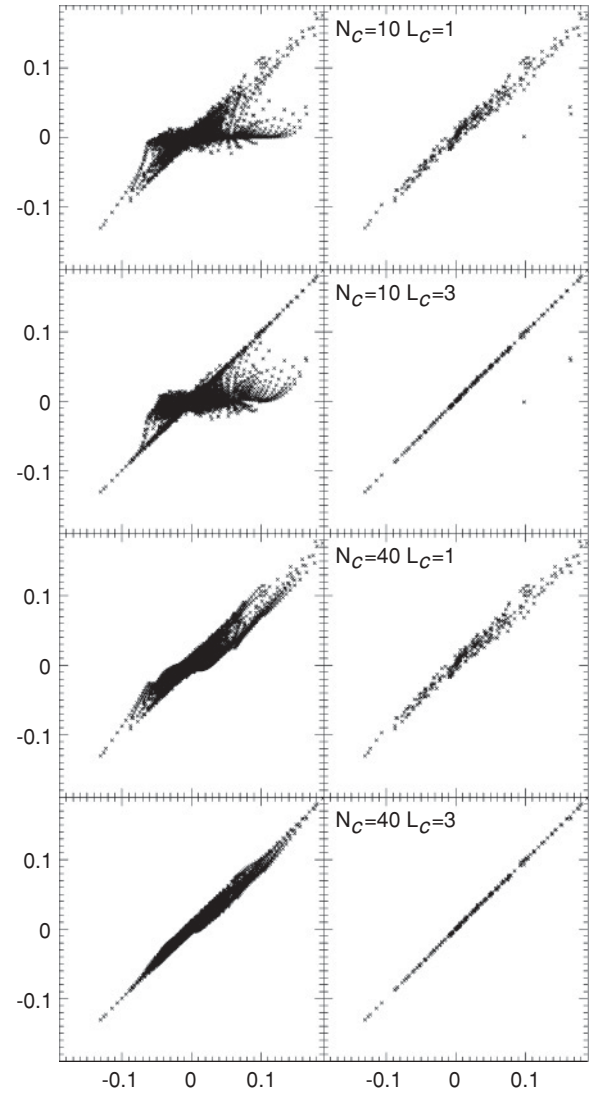

FIG. 3. Same as Fig. 2 but for a range $\mu = 1.4$ fm of the Gaussian interaction.

and $L_C = 1$ approximation, including 11 separable terms, is already quite reasonable for the reduced set of relevant matrix elements (right hand side panels). In Fig. 3 the same kind of plots as the ones of Fig. 2 are presented but this time for a Gaussian twice the previous range, i.e., $\mu = 1.4$ fm. We immediately realize the worsening of the approximation, what is consistent with the previous findings that this is a kind of "short-range" expansion. In this figure we observe that the convergence with N_c is much faster than the one with L_C because already the $N_C = 10$ numbers compare quantitatively well with the ones of $N_C = 40$ whereas for L_C the results with $L_C = 3$ are much better than the ones for $L_C = 1$.

Finally, in Fig. 4 we present a more detailed study of the convergence with N_C in the case of $\mu = 1.4$ fm keeping fixed L_C to the reasonable value of 3. We observe how decreasing the value of N_C from 10 to 8 to 6 degrades the quality of the approximation for the relevant matrix elements (right-hand side panels) but this is not significant and it is quite likely that even $N_C = 6$ (12 separable terms) will provide already reasonable values of the pairing tensor in calculations with real nuclei. This point can only be tested in realistic calculations and work along this direction is in progress.

It is also interesting to compare the approach of Refs. [7–9,11–13] with the present one. In those references the two-body Gaussian interaction is replaced by

$$\langle \vec{r}_1 \vec{r}_2 | v | \vec{r}_1\,', \vec{r}_2\,' \rangle = G\delta(\vec{R} - \vec{R}\,') \sum_\alpha \lambda_\alpha P_\alpha(r) P_\alpha(r'), \qquad (16)$$

where $\vec{R}$ and $\vec{r}$ are the center of mass and relative coordinate of $\vec{r}_1$ and $\vec{r}_2$. The functions $P_\alpha(r)$ are taken as Gaussian with widths adjusted to reproduce nucleon-nucleon phase

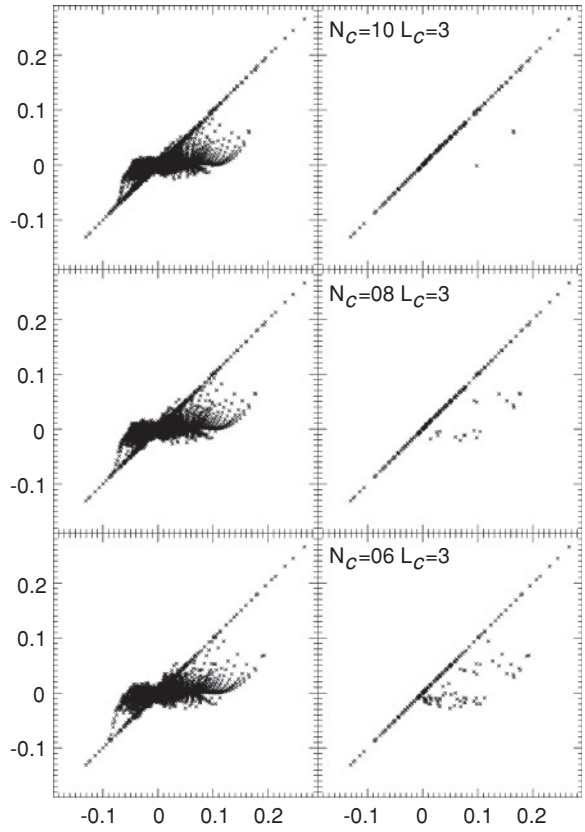

FIG. 4. Comparison between exact (x axis) and approximate (y axis) pairing matrix elements of an one-dimensional Gaussian interaction with range $\mu = 1.4$ fm as a function of N_C (see text for details as well as Fig. 2 for the meaning of the left-hand side and right-hand side panels).

shifts [7,9] or the nuclear matter pairing gap [11–13]. More involved expressions and fitting strategies were used in [8]. This form of the interaction corresponds to the class introduced in Eq. (4) and therefore we can use Eq. (5) to obtain $v_{nn'} = \sum_\alpha \lambda_\alpha (P_\alpha)^*_n (P_\alpha)_{n'}$, where $(P_\alpha)_n = \int d\vec{r} \phi_n(\vec{r}) P_\alpha(r)$. For each of the $P_\alpha(r)$ factors, the corresponding term is nothing but a rank one Kronecker approximation to the exact $v_{nn'}$ matrix of the interaction. The vectors $(P_\alpha)_n$ considered in Refs. [7–9,11–13] are inspired by physical requirements and the free parameters entering their definitions can be used (as it is the case) to find an optimal (in physical terms) approximation to $v_{nn'}$ by the requirements of reproducing as well as possible some nuclear properties. From our previous numerical study we can conclude that our "blind" approximation is also well suited to deal with the problem.

D. Ultraviolet divergence

From the previous results one could conclude that, because the low rank separable expansion is a kind of "short-range" expansion, it should show some sort of ultraviolet divergence like the pairing matrix elements of a zero-range contact interaction. In this section I will show that this is not the case. First of all, I will remind the reader about the origin of the ultraviolet divergence. It is a direct consequence of the fact that the nuclear matter pairing matrix elements

$$-G\langle \vec{k}_1, \vec{k}_2 | \delta(\vec{r}_1 - \vec{r}_1) | \vec{k}'_1, \vec{k}'_2 \rangle = -\frac{G}{(2\pi)^3 2^{3/2}} \delta(\vec{K} - \vec{K}') \tag{17}$$

of a contact interaction do not depend on the momentum transfer vector $\vec{q} = \vec{k} - \vec{k}'$ (we have introduced the vectors $\vec{K} = \frac{1}{\sqrt{2}}(\vec{k}_1 + \vec{k}_2)$ and $\vec{k} = \frac{1}{\sqrt{2}}(\vec{k}_1 - \vec{k}_2)$) favoring infinitely high momentum transfers unless some cut off is introduced. In the one-dimensional HO case, the structure of the general matrix elements is more difficult to visualize, but for the sake of discussion, we can restrict to the specific matrix elements $-G\langle n, 0 | \delta(x_1 - x_2) | n, 0 \rangle$ which, as can be shown easily using the preceding formulas, are independent of n and given by $-G/\sqrt{2}$. The constant value favors, as in the nuclear matter case, the scattering of the $n = 0$ state into high n states. For an one-dimensional Gaussian of range μ the expression of the previous matrix element is not as simple as in the case of the zero range force, and therefore it is preferable to plot it as a function of n in order to discuss its properties. In Fig. 5 we have plotted the matrix elements $\langle n, 0 | \exp[-(x_1 - x_2)^2/\mu^2] | n, 0 \rangle$ as a function of n as well as three of the low rank approximations corresponding to $N_C = 60$ and $L_C = 1$ and 3 and $N_C = 10$ and $L_C = 3$ (see caption for details). The conclusions from this plot are that the matrix element is a decreasing function of n quenching the promotion to high n states and therefore the ultraviolet divergence. Also, the similarities between the exact matrix elements and the two typical low rank approximations with $N_C = 60$ for all values of n are remarkable. In the case $N_C = 10$ and $L_C = 3$ the approximation is reasonable up to $n = 15$ and from there on the matrix elements are too small as compared to the exact ones. In any case, we conclude that the low rank approximations maintain the characteristic decreasing with n of the matrix elements that is needed to prevent the ultraviolet divergence.

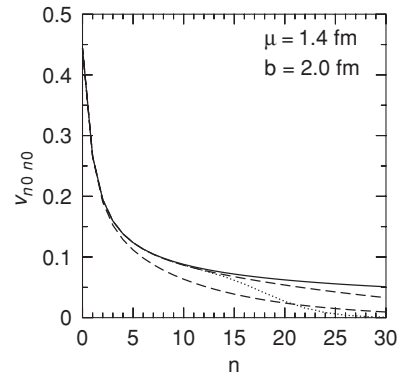

FIG. 5. Matrix element $v_{n,0,n,0}$ for the one-dimensional Gaussian interaction of range $\mu = 1.4$ fm and oscillator length parameter b =2.0 fm plotted as a function of n. Full curve corresponds to the exact result, dashed ones to the approximation with $N_C = 60$ and $L_C = 1$ and $L_C = 3$ (the one closer to the exact result). The dotted curve corresponds to the $N_C = 10$ and $L_C = 3$ approximation.

E. General interactions

As discussed previously the case of a general interaction involves the evaluation of the matrix $v_{nn'}$ and its diagonalization. The evaluation of $v_{nn'}$ can be carried out numerically using, for instance, Gauss-Hermite integration thanks to the presence of the HO wave functions in the matrix elements. The resulting formula is also in the form of Eq. (6) as can be inferred by using an one-dimensional example

$$\begin{aligned} v_{nn'} &= \int_{-\infty}^{\infty} dz\, \varphi_n^*(z;b) v(\sqrt{2}z) \varphi_{n'}(z;b) \\ &\approx \sum_{i=-N_H}^{N_H} w_i \tilde{\varphi}_n^*(z_i) v(\sqrt{2}b_i z_i) \tilde{\varphi}_{n'}(z_i) \\ &= \sum_{i=-N_H}^{N_H} D_{ni}^* [w_i v(\sqrt{2}b_i z_i)] D_{n'i}, \end{aligned} \tag{18}$$

where z_i and w_i are the nodes and weights of the Gauss-Hermite integration, $\tilde{\varphi}_{n'}(z)$ is the reduced HO wave function defined above and the coefficients $D_{ni} = \tilde{\varphi}_n(z_i)$. Also in this case, if $v(r)$ is short range, the quantity $w_i v(\sqrt{2}b_i z_i)$ will decrease as z_i increases. In the case of a Gaussian interaction this procedure will reproduce the exact answer and will provide an alternative (but equivalent) description of the previous results for the Gaussian. Another alternative to this procedure, that lends more analytical results, is to represent the interaction to be treated by means of its Gauss transform. The Gauss transform is a derivative of the more popular Laplace transform, where a change of variables allows to express given functions as linear combinations of Gaussian with different widths. The best known example of this treatment is that of the Yukawa potential [23]

$$\frac{e^{-\mu r}}{r} = \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-r^2 t^2 - \mu_2/(4t^2)} dt \tag{19}$$

that can straightforwardly be used to deal with the Coulomb interaction by taking the $\mu \to 0$ limit (see Ref. [24] for an early application in nuclear physics). The advantages of this method are first that the separable expansion for the Gaussian is known analytically and can be used straight ahead and second that the Gaussian interaction is separable along the three spatial directions allowing to treat the problem as three uncorrelated one-dimensional problems one for each spatial direction. The latter advantage is specially helpful to deal with the Coulomb interaction. Given the long range of the Coulomb force the number of terms required for an accurate separable expansion of a general matrix element is expected to be larger than for a gaussian. However, the relevant Coulomb matrix elements for the nuclear case involve single particle wave functions which are located inside the nucleus and therefore explore the Coulomb potential in the interior of the nucleus. For those matrix elements, the Coulomb force can be considered as a short-range interaction with a range of the order of the size of the nucleus and therefore the number of separable terms required for an accurate representation are expected to be much smaller than the ones required for a general matrix element of the Coulomb interaction.

F. Density dependent forces

In the applications of the HFB method it is common to find terms in the interaction/energy functional that are referred to as "density dependent" (DD) terms and are given by the general expression

$$v(\vec{r}_1, \vec{r}_2) = f(\vec{r}) G(\vec{R}). \tag{20}$$

Usually, $f(\vec{r}) = \delta(\sqrt{2}\vec{r})$ and $G = \rho^{\alpha}$, that is, the density raised to some (usually noninteger) power α. Applying the ideas developed in this article it is easy to obtain in this case

$$v_{n_1,n_2,n_3,n_4} = \sum_K \sum_L \tilde{M}^{*\,KL}_{n_1 n_2} f_L g_K \tilde{M}^{KL}_{n_3 n_4}, \tag{21}$$

where we have introduced the coefficients

$$\tilde{M}^{KL}_{n_1 n_2} = \sum_{Nn} M^{Nn}_{n_1 n_2} D_{nL} E_{NK} \tag{22}$$

given in terms of the spectral decomposition of the matrices f and G with eigenvalues f_L and g_K, respectively. In the common situation where $f(\vec{r}) = \delta(\sqrt{2}\vec{r})$ the f_L are constant and equal to $1/2^{3/2}$ and $D_{nL} = \phi_n(0)$ independent of L.

III. CONCLUSIONS

By means of the transformation properties of the HO basis to the center of mass and relative coordinate a separable expansion of the pairing and exchange matrix elements of a general two-body interaction is obtained. The study of two specific examples: the contact delta force and the one-dimensional Gaussian interaction show that the number of terms of the separable expansion to be considered can be substantially reduced without affecting too much the accuracy of the approximate formula. The separable expansion turns out to be a kind of "short-range" expansion. The issue of ultraviolet divergences inherent to any short range expansion is analyzed. The proposed separable expansion opens up a new avenue to deal with finite range interactions both in the pairing and exchange channel. In the former case, the cumbersome definition of the "cut-off window" is avoided by the implicit finite range. The possibility to extend these considerations to other finite-range interactions like the Coulomb potential is also discussed.

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APPENDIX A: TALMI-BRODY-MOSHINSKY COEFFICIENTS IN ONE DIMENSION

The Talmi-Brody-Moshinsky coefficients in one dimension are defined as

$$\varphi_{n_1}(x_1)\varphi_{n_2}(x_2) = \sum_{Nn} M^{Nn}_{n_1 n_2} \varphi_N(X)\varphi_n(x),$$

where $X = \frac{1}{\sqrt{2}}(x_1 + x_2)$ and $x = \frac{1}{\sqrt{2}}(x_1 - x_2)$ are the center of mass and relative coordinate, respectively, and $\varphi_n(x) = (\sqrt{\pi}2^n n!b)^{-1/2} H_n(x/b)\exp(-\frac{1}{2}\frac{x^2}{b^2})$ is the one-dimensional HO wave function written in terms of the Hermite polynomials. Explicit expression of $M^{Nn}_{n_1 n_2}$ have already being obtained in the literature [20] but we will introduce here another derivation which is simple and straightforward. We will take advantage of the generating function of the one-dimensional HO wave functions

$$G(x/b,t) = \exp\left(-\frac{1}{2}\frac{x^2}{b^2} + 2\frac{x}{b}t - t^2\right) = \sum_n \chi_n(t)\varphi_n(x)$$

with $\chi_n(t) = (\sqrt{\pi}b2^n n!)^{1/2} t^n/n!$. Given the Gaussian form of the generating function we have $G(x_1/b,t_1)G(x_2/b,t_2) = G(X/b,T)G(x/b,t)$, where $T = \frac{1}{\sqrt{2}}(t_1 + t_2)$ and $t = \frac{1}{\sqrt{2}}(t_1 - t_2)$. Expanding in the right-hand side of the last identity $\chi_N(T)$ and $\chi_n(t)$ in powers of t_1 and t_2 and comparing with the same powers in the left-hand side we finally obtain

$$M^{Nn}_{n_1 n_2} = \delta_{n_1+n_2,N+n}\left(\frac{n_1!n_2!}{2^{n_1+n_2}N!n!}\right)^{1/2} \times \sum_m (-1)^m \binom{N}{n_1 - n + m}\binom{n}{m},$$

where the selection rule is made explicit.

APPENDIX B: TRANSFORMATION COEFFICIENTS

In this appendix I supply the expression for the expansion coefficients of the one-dimensional reduced HO wave function $\tilde{\varphi}_n(x/b) = \exp(\frac{1}{2}\frac{x^2}{b^2})\varphi_n(x/b) = (\sqrt{\pi}2^n n!b)^{-1/2} H_n(x/b)$ in terms of the same object but for a different length scale b'

$$\tilde{\varphi}_n(x/b) = \sum_{n'=0}^{n} D_{nn'}\left(\frac{b'}{b}\right)\tilde{\varphi}_{n'}(x/b'). \tag{B1}$$

There are many ways to obtain the D coefficients although probably the more economical one is to use the generating function of the Hermite polynomials $H_n(x/b)$ which is given by (see previous appendix)

$$\tilde{G}(x/b,t) = \exp\left(2\frac{x}{b}t - t^2\right) = \sum_n \frac{t^n}{n!}H_n(x/b). \tag{B2}$$

Using the generating function we can write $\tilde{G}(x/b,t) = \tilde{G}(x/b',t')\exp(-(1-\eta^2)t^2)$ where $\eta = b'/b$ and $t' = \eta t$. Equating equal powers in t in the previous expression and using Eq. (B2) we obtain

$$H_n(x/b) = \sum_{n'}(-1)^{\frac{n-n'}{2}}\frac{n!\eta^{n'}(1-\eta^2)^{\frac{n-n'}{2}}}{n'!\left(\frac{n-n'}{2}\right)!}\Delta_{n,n'}H_{n'}(x/b')$$

which is an identity that finally yields

$$D_{nn'}(\eta) = \Delta_{n,n'}(-1)^{\frac{n-n'}{2}}\left(\frac{n!}{n'!}\right)^{1/2}\frac{\eta^{n'+1/2}(1-\eta^2)^{\frac{n-n'}{2}}}{2^{\frac{n-n'}{2}}\left(\frac{n-n'}{2}\right)!}. \tag{B3}$$

In this expression, the function $\Delta_{n,n'} = \frac{1}{2}[1 + (-1)^{n+n'}]$ which is one if n and n' have the same parity (even or odd) and zero otherwise has been introduced. Notice also that $D_{nn'}(\eta) = 0$ if $n' > n$ in agreement with the limits of the sum in Eq. (B1).

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