

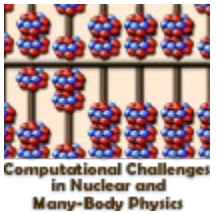

Computational challenges in (nuclear) energy density functional theory

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Nuclear EDF vs DFT

Nuclear Energy Density functional (EDF) is not the same as density functional theory (DFT)

- In **DFT** the minimum of E[n] provides the **exact** ground state energy and the exact density n. The exact ground state density has symmetry properties consequence of a ground state wave function with the proper quantum numbers.

- In the **nuclear EDF** the (mean field inspired) functional provides an approximation to the energy (to be supplemented with additional correlations) and the associated density (mean field wave function) breaks symmetries that help to understand experimental data (parity doublets, rotational bands, etc). Therefore the EDF does not provide the exact answer and going beyond mean field is essential.

  Typical EDF are those derived from the Skyrme, Gogny, etc interactions or relativistic lagrangians supplemented with extra density dependent terms which are typically of the form

$$t_3(1 + x_3 P_\sigma)\rho(\vec{r})^\alpha$$

  added to obtain saturation (binding energy proportional to A). α is a non-integer.

  The variational principle applied to the EDF leads to the solution of the Hartree- Fock-Bogoliubov (HFB) equation for the quasiparticle amplitudes U and V of the quasiparticle operators in a given basis.

Challenges of the nuclear EDF

The nuclear EDF should provide a meaningful description of nuclear properties over the whole periodic chart with the same level of accuracy for all nuclei (even-even, even-odd, odd-even, odd-odd). Observables include binding energies, radii, moments of inertia, spins and parities of odd-A ground states, etc

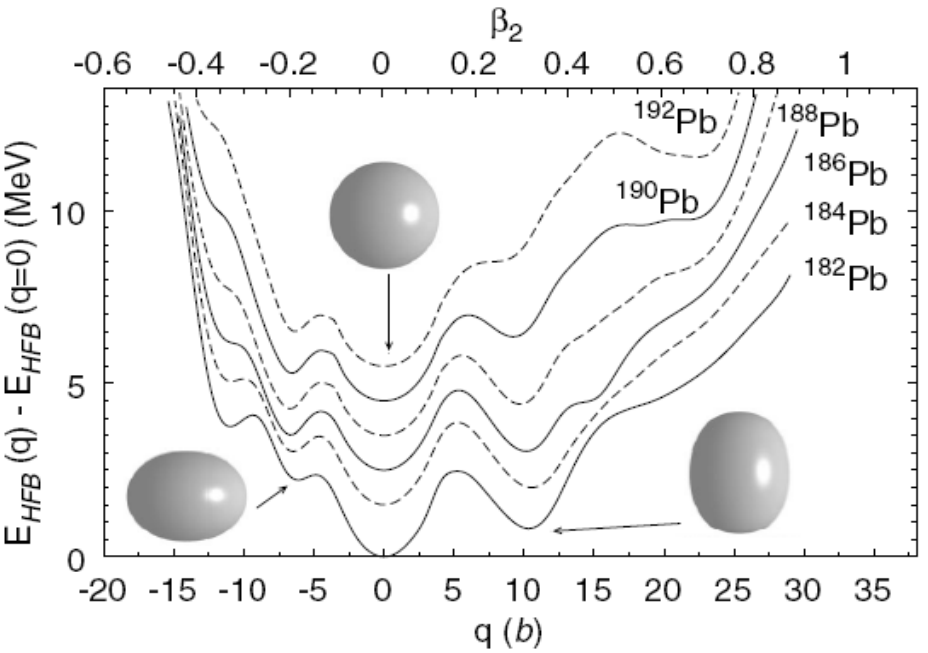
Challenges

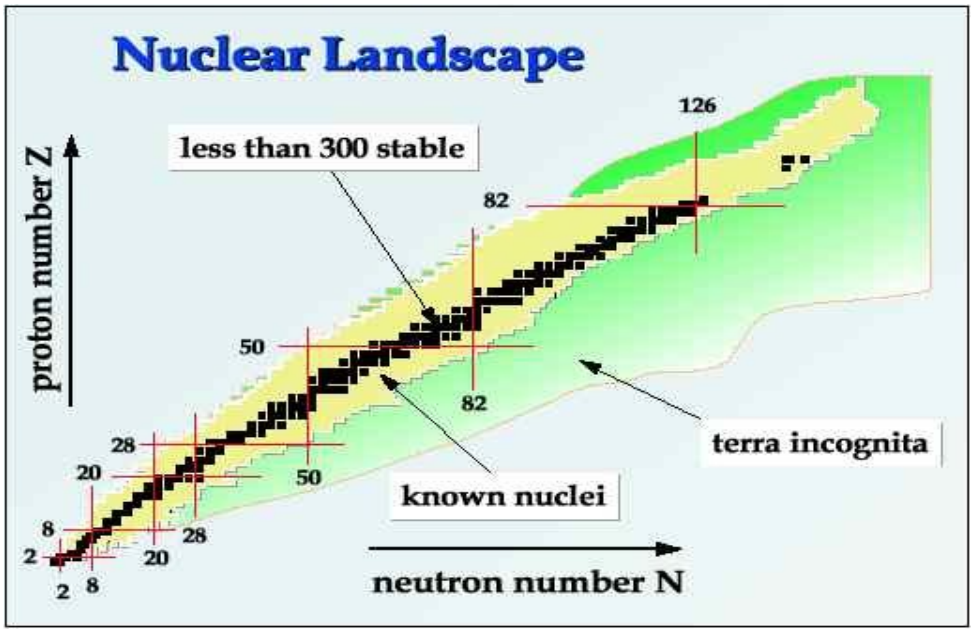
- Improve the agreement with experimental data exploring new parametrizations and functional forms
  - Skyrme (Sly, Brussels, UNEDF)
  - Gogny D1M
  - Density dependent relativistic lagrangians,
  - BCPM (a true EDF inspired by realistic nuclear matter EoS)
- Incorporate in a consistent manner **time odd fields** which are important for odd nuclei, odd-odd nuclei, high spins and beta decay
- Provide a consistent framework to add beyond mean field correlations, both for symmetry restoration and for fluctuations in the collective degrees of freedom
- Achieve true predictive power for extrapolations in unknown regions of the nuclear chart

Computational challenges for the nuclear EDF

The shape of the nucleus is an interesting magnitude and it is common to explore the energy associated to different shapes. This leads to the solution of Constrained HFB equations for a large number of constraint's values: quadrupole, octupole, hexadecapole, etc

odd-A systems described by blocked HFB that requires many initial configurations.





Over 6000 nuclei to consider

The ideal method to solve the highly-non-linear HFB equations has to be robust and lead to a low iteration count.

The traditional iterative solution does not have these properties. Often fails to converge and is not adequate to handle many constraints.

Computational challenges: Solution of the HFB equation

Look at the problem as an energy minimization problem depending upon the parameters of the Thouless theorem and search for the minimum using the gradient method.

- This is an old idea that has problems: the gradient gives you the direction but not the step size. To estimate the step size the curvature is required but it is difficult to compute (RPA cost). The conjugate gradient method (Egido, NPA594, 70(1995)) is and alternative but adding approximate second order curvature information (the curvature matrix is approximated by its diagonal form) if far cheaper: (G.F. Bertsch and LMR PRC 84, 014312 (2011)).
  Any form of the gradient method handles very well multiple constraints

- Recent proposals involving derivative free algorithms (POUNDERS) are also available PRC 82, 024313 (2010)

- Succesive diagonalization methods are still in use with appropriate annealing strategies

- Any progress in multidimensional minimization will help

Extend those techniques to finite temperature HFB and also to Projection After Variation (PAV) where the projected energy is minimized instead.

Expansion on a basis: convergence and all that

Quasiparticle operators are expanded on a (finite) basis

- Gaussian
- Harmonic oscillator
- Wood-Saxon
- Sturmians
- Lagrange interpolation (aka spatial meshes)
- Bsplines
- DVR ...

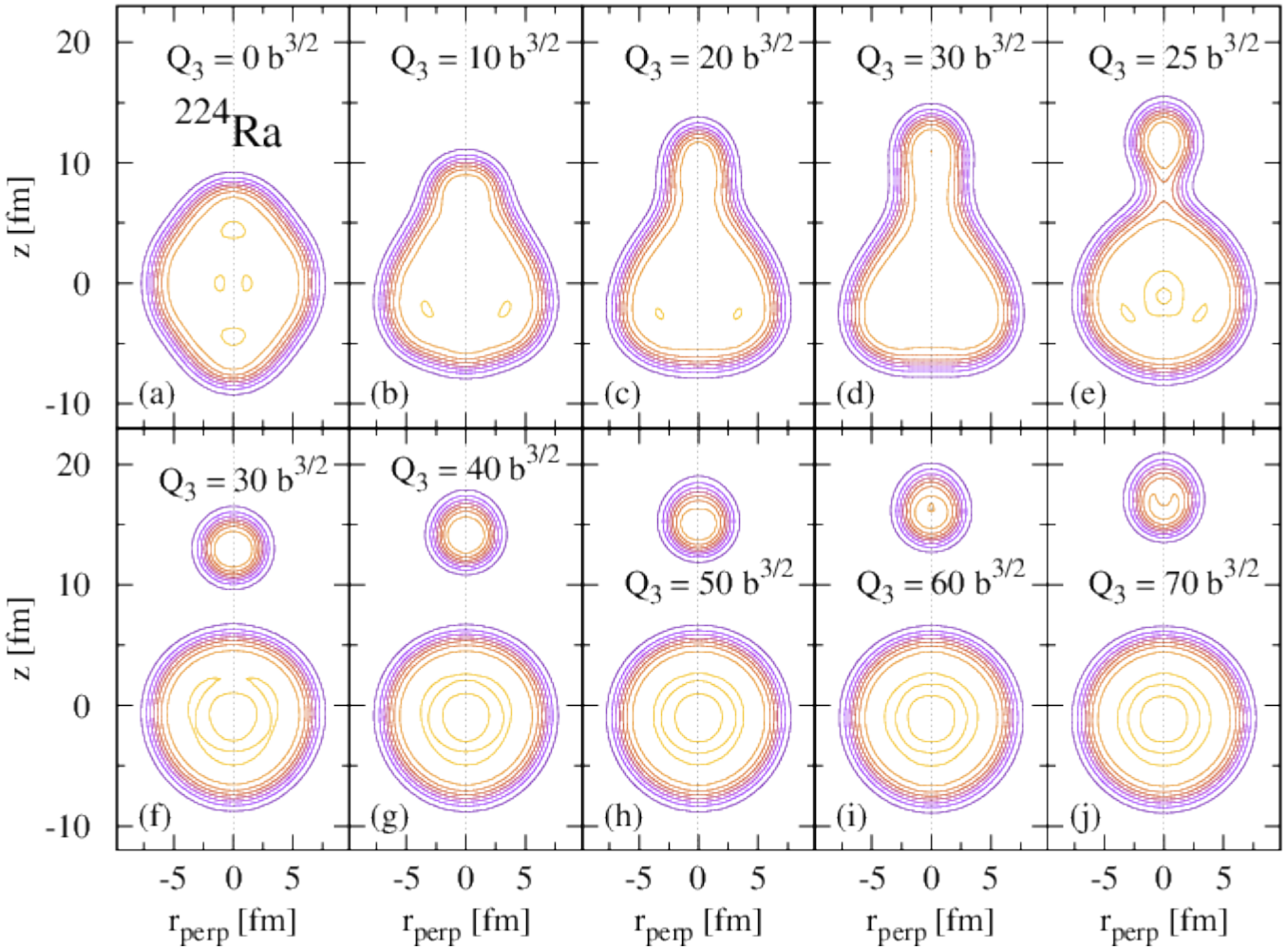
The basis should

- Adapt to any relevant nuclear geometry (extreme deformations like fission)
- Facilitate the computation of (two body) matrix elements
- Extrapolate easily to the infinite basis limit

The harmonic oscillator basis is a popular choice in nuclear physics because

- Varying the oscillator lengths gives some freedom to adapt to the geometry
- Many analytical results are at hand for the computation of matrix elements
- Recent studies show how convenient the basis is for extrapolations to infinite basis (arXiv:1409.5997, S. Koning et al)

Cluster emission

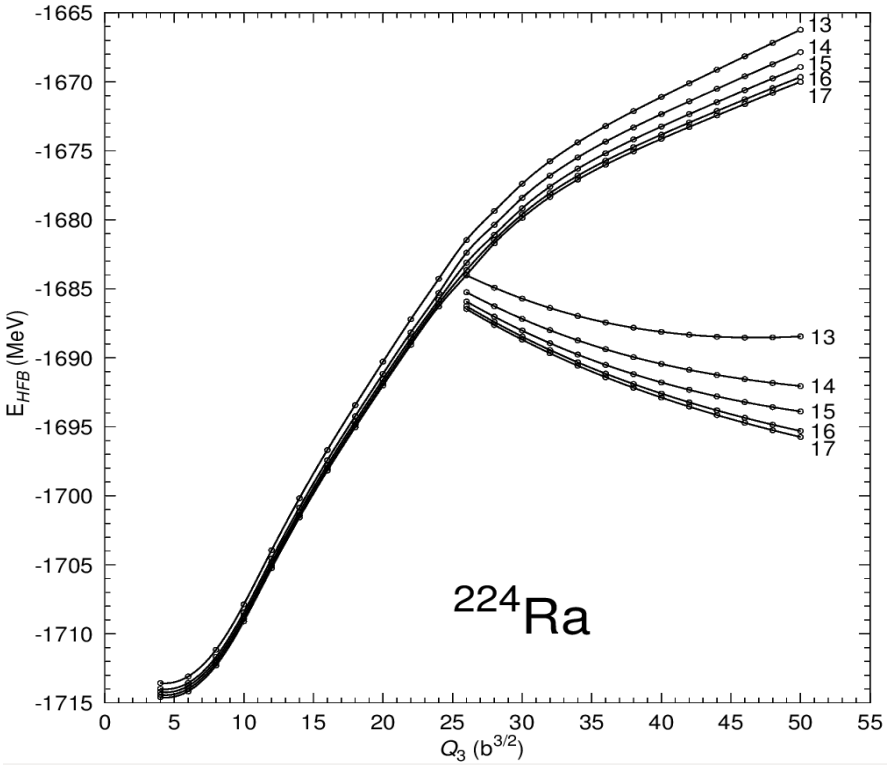


Constraining the octupole moment Q_{30} in a fully self-consistent calculation leads to the above sequence describing the emission of ^{14}C off ^{224}Ra (cluster radiactivity)

We use a HO basis in cilindrical coordinates

$$2n_\perp + |m| + \frac{1}{q} n_z \leq N_0$$

The two oscillator lengths b_{perp} and b_z are optimized for each configuration



Non uniform convergence with N_0 for different Q_3 values

Is it possible to extend recent ideas to extrapolate HO results to this non-spherical case ?

Is it possible to easily generalize to other kinds of basis ?

Obviously this would be of great relevance in fission studies where a large variety of shapes are considered and the relative energy is of relevance

M. Warda and L.M. Robledo, Phys Rev C84, 044608 (2011)

A more flexible basis

Given a positive definite weight ρ(x) in a given interval [a,b] it is always possible to find a complete set of orthogonal polynomials satisfying

$$\int_a^b dx \rho(x) p_n(x) p_m(x) = \delta_{nm}$$

When ρ(x) is a gaussian we recover the HO basis $\varphi_n(x) = N_n \exp(-\frac{1}{2}x^2) H_n(x)$

We propose (*) to consider for the weight a linear combination of gaussians

$$\rho^{1/2}(x) = \sum_k c_k \exp((x - x_{0k})^2/\sigma_k^2)$$

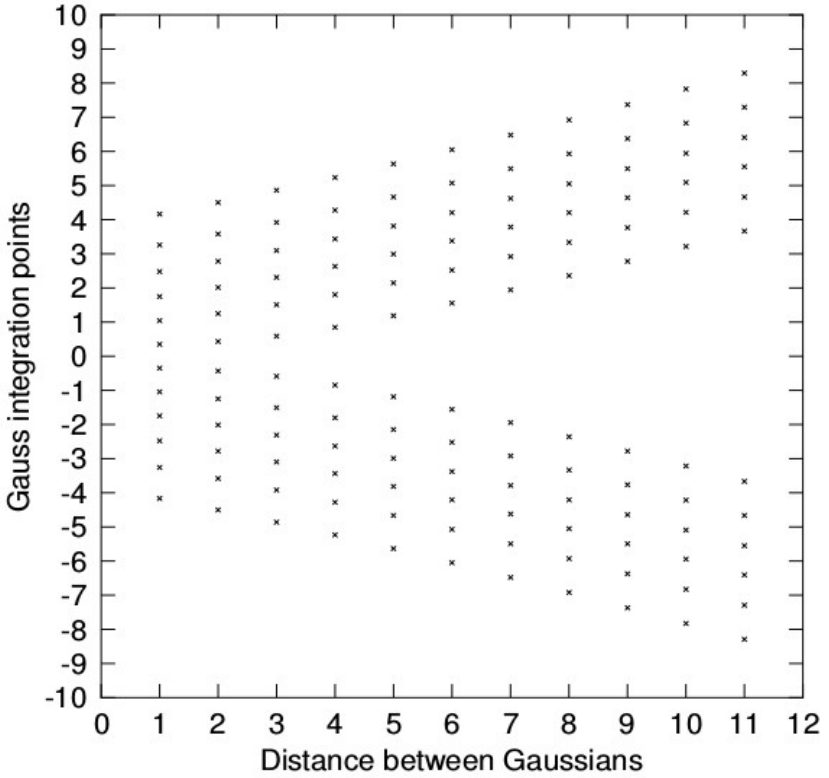
that follow the shape of the potential. Remember that many functions can be expressed as Gauss transforms (Coulomb for instance !).

To visualize the properties of the basis we consider the interpolating Lagrange mesh associated with any orthogonal polynomial (**).

For an orthogonal basis with N elements the **Lagrange mesh** is made of the N Gauss integration points that are the zeroes of $p_N(x)$

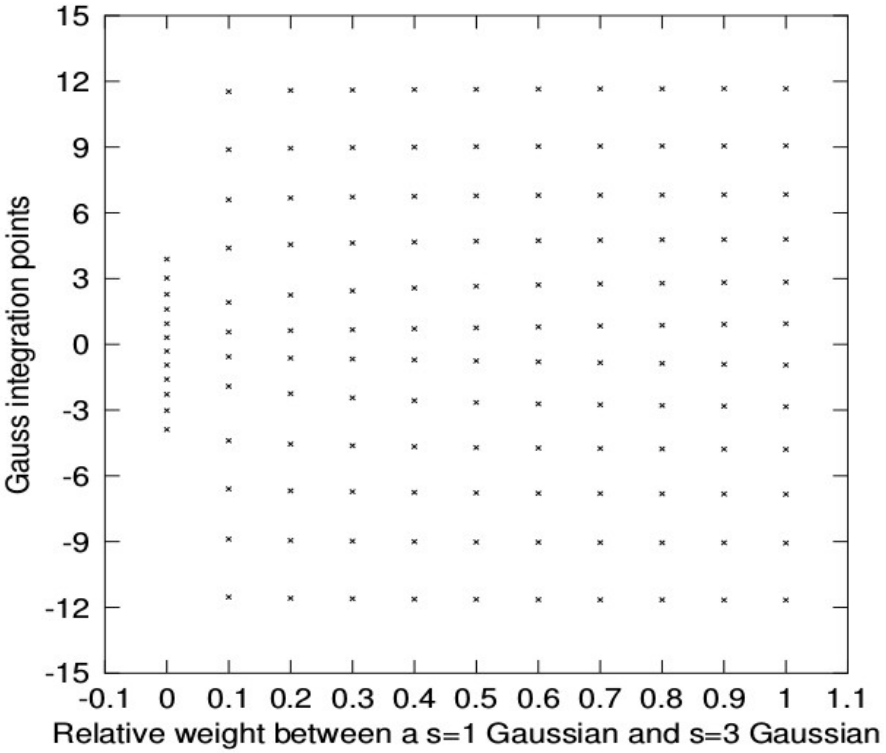
(*) F. Roca-Urgorri and LMR, to be submited
(**) D Baye and P -H Heenen 1986 J. Phys. A: Math. Gen. 19 2041

A more flexible basis:examples



$$\rho^{1/2}(x) = e^{-(x-x_0)^2} + e^{-(x+x_0)^2}$$

Good for fission studies and reactions

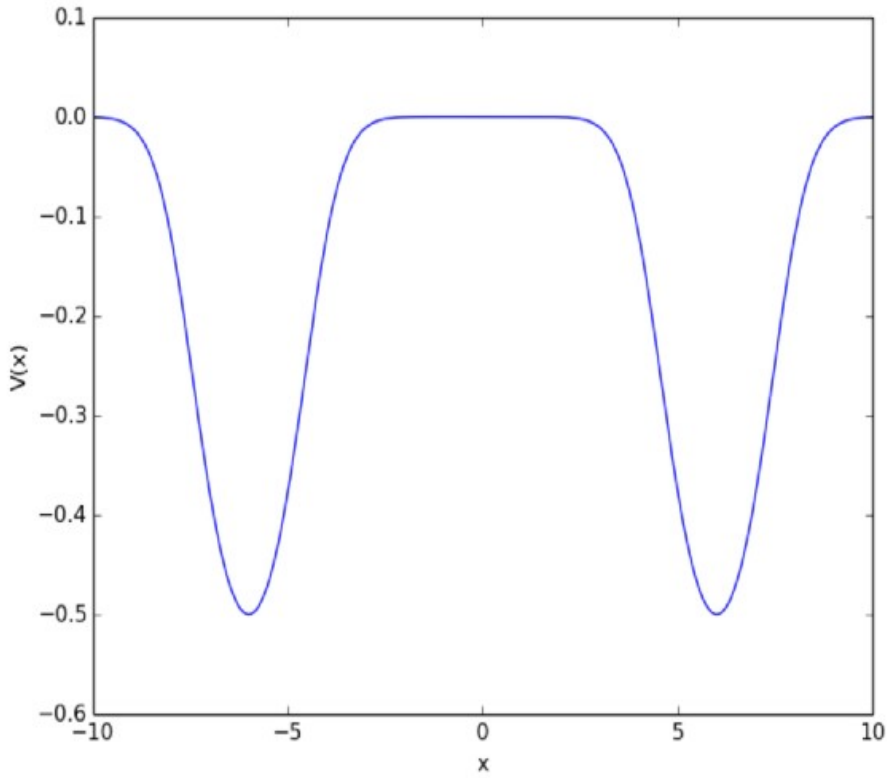


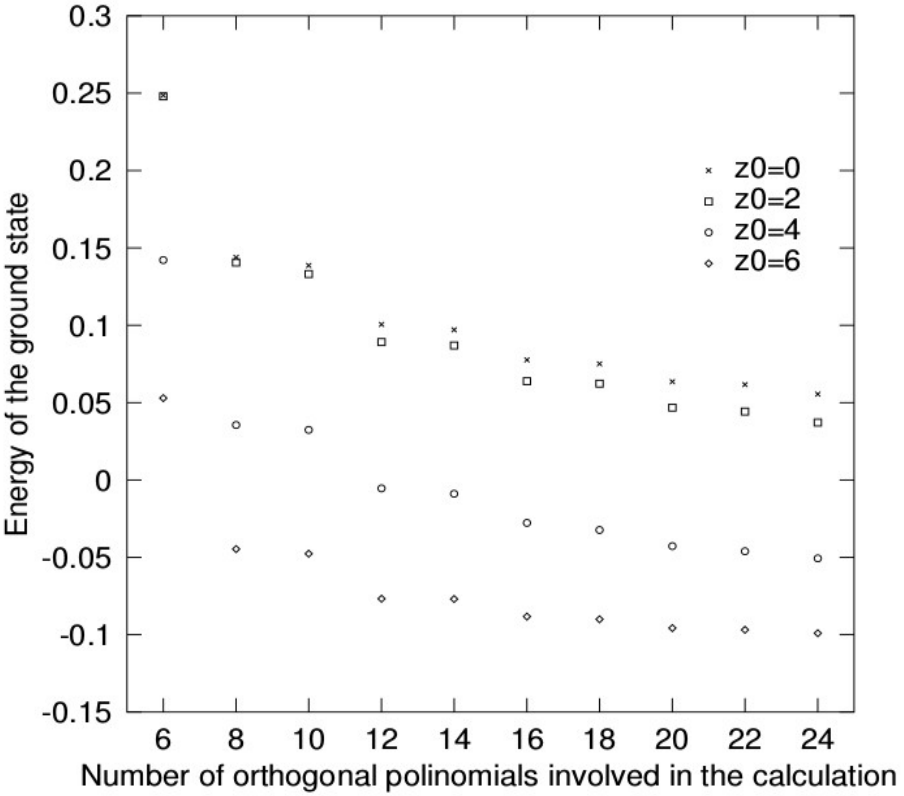
$$\rho^{1/2}(x) = de^{-x^2/\sigma_1^2} + (1-d)e^{-x^2/\sigma_3^2}$$

Good for near continuum states and/or resonances

Most of the analytical results known for the HO basis can be generalized to this case. Computational cost for two body matrix elements of the order of N^2 as in HO.

A more flexible basis:examples





Double well potential with $\rho^{1/2}(x) = e^{-(x-x_0)^2} + e^{-(x+x_0)^2}$

Ground state convergence

Two and three body matrix elements

Three body forces are becoming popular in nuclear physics for **various reasons.**

They require the evaluation of a huge number of matrix elements O(N^6)

$$\nu_{abcdef} = \iiint dx_1 dx_2 dx_3 \varphi_a^*(x_1)\varphi_b^*(x_2)\varphi_c^*(x_3)V(x_1,x_2,x_3)\varphi_d(x_1)\varphi_e(x_2)\varphi_f(x_3)$$

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Exact Tensor Hypercontraction: A Universal Technique for the Resolution of Matrix Elements of Local Finite-Range *N*-Body Potentials in Many-Body Quantum Problems

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Based on the idea that the set of N^2 products of basis states can be expressed as a linear combination of 2N+1 states

$$\Psi_i^*(x)\Psi_j(x) = \Psi_0(x)\sum_k [ij;k]\Psi_k(x)$$

$$\nu_{abcd} = \sum_{pq}[ac;p][bd;q]G^{pq} \quad G^{pq} = \iint dx_1 dx_2 \Psi_0(x_1)\Psi_0(x_2)V(x_1,x_2)\Psi_p(x_1)\Psi_q(x_2)$$