New studies in the shell and collective models

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Introduction

Introduction

The well-known form of Woods-Saxon potential is given by:

$$V(r) = -\frac{V_0}{1 + \exp\left(\frac{r-R}{a}\right)}, \tag{1}$$

where V_0 is the potential depth, $R = r_0 A^{1/3}$ is the nuclear radius (A is the mass number, $r_0 \approx 1.27$ fm), the a is the surface diffuseness parameter (typically $0.5 - 0.7$ fm).

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In a 2015 paper authored by Çapak *et al*, a more general form of the Woods-Saxon potential was introduced and applied within the Bohr Hamiltonian framework

$$V(r) = \frac{-V_0'}{1+\exp(a'(r-r'))} \tag{2}$$

In this expression, the parameters V_0', a', and r' are adjustable.

WS bases

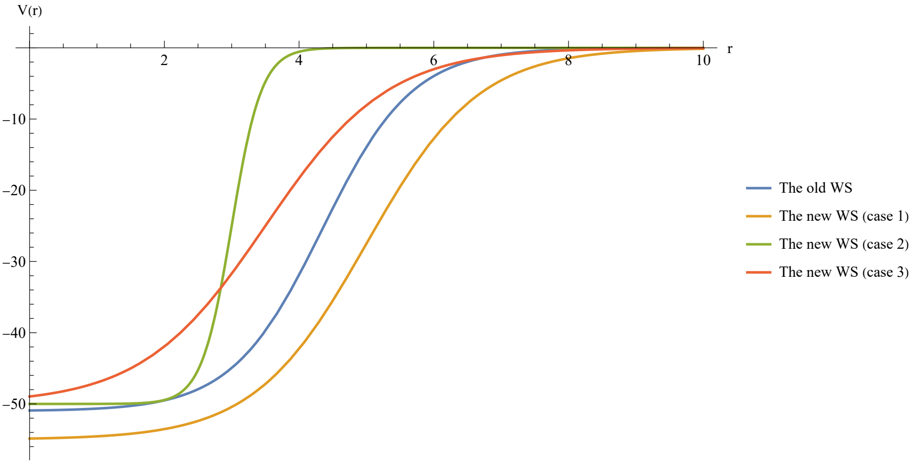
Assuming the total wave function takes the form $\Psi(\boldsymbol{r}) = g(r)Y_{lm}(\theta, \phi)$, where the spherical harmonics are denoted by Y_{lm}, and z-component of the angular momentum is m. The function $g(r)$ is obtained from the following radial Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2} + \left(\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + V(r)\right)u(r) = Eu(r) \tag{3}$$

where $u(r) = g(r)/r$, the mass of the a nucleon is m, the mean-field potential is $V(r)$ and finally the energy is shown by E.

Comparison

In the following one can compare how flexible the new WS can be versus the old WS for a given mass number A.



How to solve WS differential equation

Consider the following general second-order differential equation:

$$-\frac{d^2y(x)}{dx^2} + V(x)y(x) = \lambda y(x), \quad x \in [a,b], \tag{4}$$

where the system's eigenvalue is λ, and the effective potential is $V(x)$. The domain $[a,b]$ is discretized into $N+2$ equally spaced points with spacing $h = \frac{b-a}{N+1}$, assuming Dirichlet boundary conditions like $y(a) = y(b) = 0$. A second-order finite difference formula may then be used to approximate the second derivative:

$$\frac{d^2y}{dx^2} \approx \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2}. \tag{5}$$

How to solve WS differential equation

When this is substituted into the differential equation, a linear algebraic system is produced

$$-\frac{1}{h^2}y_{i-1} + \left(\frac{2}{h^2} + V_i\right)y_i - \frac{1}{h^2}y_{i+1} = \lambda y_i. \tag{6}$$

The matrix representation of this system is in the form of

$$\mathbf{A}\mathbf{y} = \lambda\mathbf{y}, \tag{7}$$

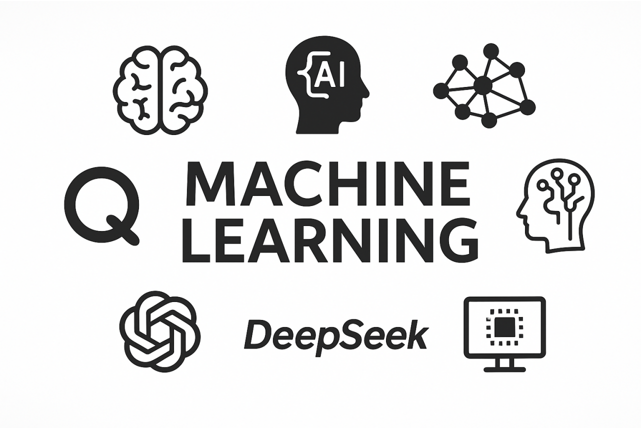
where $\mathbf{A}$ is a symmetric tridiagonal matrix of the form:

$$\mathbf{A} = \frac{1}{h^2}\begin{pmatrix} 2+h^2V_1 & -1 & 0 & \dots & 0 \\ -1 & 2+h^2V_2 & -1 & \dots & 0 \\ 0 & -1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \dots & 0 & -1 & 2+h^2V_N \end{pmatrix}. \tag{8}$$

When the matrix $\mathbf{A}$ is constructed, the original boundary value issue is transformed into an eigenvalue problem.

Machine learning

Machine learning



Motivations

Why well-known shell and collective models should be revisited

- **The presence of significant approximations:** Approximation is a commonly used strategy for simplifying mathematical operations. However, in some shell model calculations, the approximations used can result in the loss of significant amounts of information.
- **The complexity of numerical computations:** More sophisticated mathematical tools with many adjustable parameters are needed. Using them makes computations more complex.
- **Optimization Challenges:** Adjusting parameters has always been one of the main challenges, especially in matrix computations.

Machine learning and nuclear models

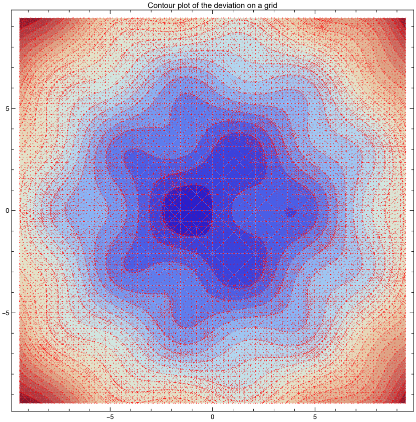
To achieve more accurate predictions, we rely on more precise assumptions, avoid crude approximations, and make use of phenomenological bases. Optimization techniques from machine learning, such as gradient descent and Nesterov accelerated gradient, are applied.

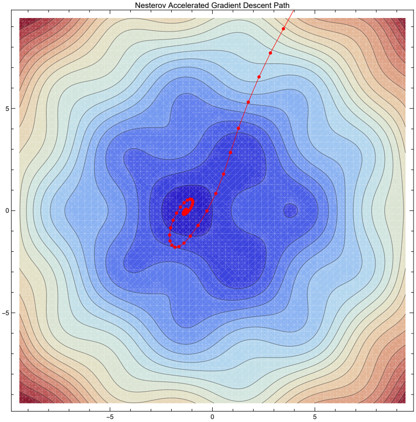
To evaluate the accuracy of the model, the difference between the theoretical and the experimental values of the energies is calculated, and the root mean square of these differences is used as a measure of error.

The model parameters are updated step by step in such a way that they move in the direction of reducing this error. The learning rate determines how large each update step will be.

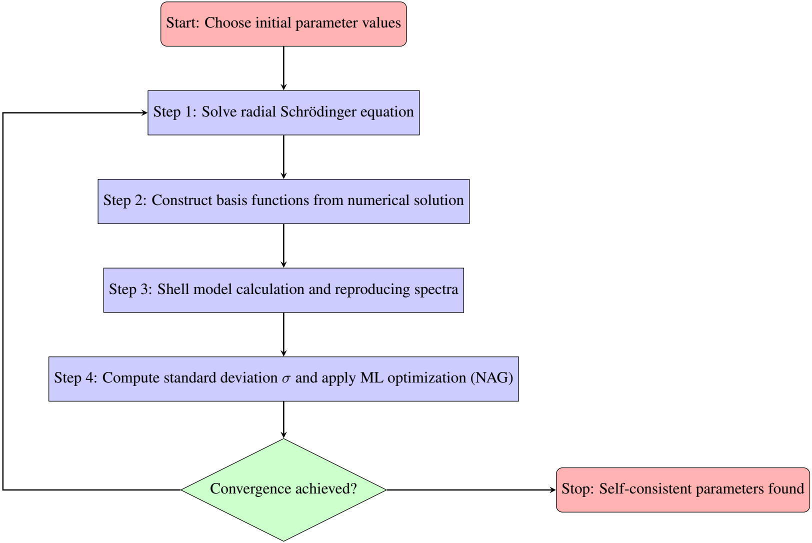
In the accelerated gradient method, in addition to using the gradient of the error to adjust the parameters, a “momentum” term is also included. This momentum helps the parameter updates proceed faster and more smoothly towards reducing the error. As an example, the learning rate may be set to 0.1, and the momentum factor to 0.9.

Graphical comparison





The strategy



Shell model

2p, 2n, pn nuclei

The surface delta (SDI) interaction

the matrix components linked to a particular interaction model called the simplified surface delta interaction (SDI)

$$\langle a\, b;\; J\, T|V_{\mathrm{SDI}}|c\, d;\; J\, T\rangle = K_{abcd}\mathcal{N}_{ab}(JT)\mathcal{N}_{cd}(JT)[1+(-1)^{l_a+l_b+l_c+l_d}]\widehat{j_a}\widehat{j_b}\widehat{j_c}\widehat{j_d}$$
$$\times\left\{[1+(-1)^T]\begin{pmatrix} j_a & j_b & J \\ \frac{1}{2} & \frac{1}{2} & -1\end{pmatrix}\begin{pmatrix} j_c & j_d & J \\ \frac{1}{2} & \frac{1}{2} & -1\end{pmatrix}\right.$$
$$\left.-(-1)^{l_a+l_c+j_b+j_d}[1+(-1)^{l_c+l_d+J+T}]\begin{pmatrix} j_a & j_b & J \\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}\begin{pmatrix} j_c & j_d & J \\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}\right\}, \quad (9)$$

where $\mathcal{N}_{ab}(JT) = \sqrt{1-\delta_{ab}(-1)^{J+T}}/1+\delta_{ab}$, $\hat{j} = \sqrt{2j+1}$ and the standard $3j$ symbols are used. A_T (which will come into the V_0 parameter) are strength parameters for isospins $T = 0, 1$, and K_{abcd} can be calculated as

$$K_{abcd} \equiv -\frac{V_0(T)\,\kappa_{ac}\kappa_{bd}}{16\pi}, \quad (10)$$

where $\kappa_{ab} = g_{n_a l_a}(R)g_{n_b l_b}(R)R$ in which $g_{nl}(r)$ is the basis considered in the problem

The matrix elements

The WS base with the definition

$$\mathcal{M}^{\mathrm{WS}}_{abcd}(JT) = -\sum_{J'} \hat{j}'^{2} \begin{Bmatrix} j_a & j_b & J \\ j_c & j_d & J' \end{Bmatrix} \langle ad; J'T|V^{\mathrm{WS}}_{\mathrm{SDI}}|cb; J'T\rangle_{V_0(T)=1}, \tag{11}$$

we have the following relations

$$\langle p_1\, p_2^{-1};\ J|V^{\mathrm{WS}}_{\mathrm{SDI}}|p_3\, p_4^{-1};\ J\rangle = A_1\, \mathcal{M}^{\mathrm{WS}}_{a_1a_2a_3a_4}(J1), \tag{12}$$

$$\langle n_1\, n_2^{-1};\ J|V^{\mathrm{WS}}_{\mathrm{SDI}}|n_3\, n_4^{-1};\ J\rangle = A_1\, \mathcal{M}^{\mathrm{WS}}_{a_1a_2a_3a_4}(J1), \tag{13}$$

$$\begin{aligned} \langle p_1\, p_2^{-1};\ J|V^{\mathrm{WS}}_{\mathrm{SDI}}|n_3\, n_4^{-1};\ J\rangle = \tfrac{1}{2}\Big\{ & A_1\sqrt{[1+(-1)^J\delta_{a_1a_2}][1+(-1)^J\delta_{a_3a_4}]}\,\mathcal{M}^{\mathrm{WS}}_{a_1a_2a_3a_4}(J1) \\ & - A_0\sqrt{[1-(-1)^J\delta_{a_1a_2}][1-(-1)^J\delta_{a_3a_4}]}\,\mathcal{M}^{\mathrm{WS}}_{a_1a_2a_3a_4}(J0)\Big\}, \end{aligned} \tag{14}$$

$$\begin{aligned} \langle p_1\, n_2^{-1};\ J|V^{\mathrm{WS}}_{\mathrm{SDI}}|p_3\, n_4^{-1};\ J\rangle &= -\tfrac{1}{2}\sum_{J'} \widehat{J'}^{2} \begin{Bmatrix} j_{p_1} & j_{n_2} & J \\ j_{p_3} & j_{n_4} & J' \end{Bmatrix} \\ &\times \Big[\langle a_1\, a_4;\ J'\, T=1|V^{\mathrm{WS}}_{\mathrm{SDI}}|a_3\, a_2;\ J'\, T=1\rangle + \langle a_1\, a_4;\ J'\, T=0|V^{\mathrm{WS}}_{\mathrm{SDI}}|a_3\, a_2;\ J'\, T=0\rangle\Big] \\ &= \tfrac{1}{2}\Big[A_1\mathcal{M}_{a_1a_2a_3a_3}(J1) + A_0\mathcal{M}_{a_1a_2a_3a_3}(J0)\Big] = \langle n_1\, p_2^{-1};\ J|V^{\mathrm{WS}}_{\mathrm{SDI}}|n_3\, p_4'^{-1};\ J\rangle, \end{aligned} \tag{15}$$

2p, 2n, pn nuclei

Table: The optimized parameters and the resulting standard deviations for the nuclei considered in the text.

	The new WS						The old WS		
Nuclei	V_0'	a'	r'	A_0	A_1	σ	A_0	A_1	σ
^{18}O	50	0.38351	7.93264	—	75.0027	2.299	—	$(16\pi)^3 8.28508$	2.396
^{18}F	51.1014	0.41904	2.62582	66.0776	44.0777	1.675	$(16\pi)^3 2.01591$	$(16\pi)^3(-0.849643)$	1.766
^{38}Ar	185	1.21225	6.51978	—	10.0585	1.902	—	$(16\pi)^2 1.58594$	1.905

Effective charges

The effective charges concept slightly modify the fundamental definition of electric charge

$$e^{\mathrm{p}}_{\mathrm{eff}} = (1+\chi)e, \tag{16}$$
$$e^{\mathrm{n}}_{\mathrm{eff}} = \chi e, \tag{17}$$

where χ is called the polarization parameter, and it can be given physical interpretations. One of its key features is that the closer it is to zero, the more desirable it is, since it approaches the original definition of electric charge.

2p, 2n, pn nuclei

Table: Comparison between theoretical predictions of the old and the new WS results of $B(\mathrm{E2})$ transitions for different nuclei studied in the text with the experimental data. All $B(\mathrm{E2})$ vales are in $e^2\mathrm{fm}^4$.

Nucleus	Transition	Exp.	The new WS	The old WS
^{18}O	$2_1^+ \to 0_{gs}^+$	9.303	8.737	8.884
	$4_1^+ \to 2_1$	3.334	5.442	5.562
	$2_2^+ \to 0_{gs}^+$	3.643	3.311	1.840
	$2_3^+ \to 0_{gs}^+$	6.025	1.104	1.112
^{18}F	$3_1^+ \to 1_{gs}^+$	16.252	16.261	5.605
	$3_2^+ \to 1_{gs}^+$	1.933	1.392	34.898
	$3_3^+ \to 1_{gs}^+$	0.42	0.002	10.130
^{38}Ar	$2_1^+ \to 0_{gs}^+$	25.801	25.840	27.990
	$0_2^+ \to 2_1^+$	9.562	1.293	1.244
	$2_2^+ \to 0_{gs}^+$	12.977	14.578	8.459
	$2_4^+ \to 0_{gs}^+$	0.835	0.832	0.466
	$4_1^+ \to 2_1^+$	7.589	4.623	5.155

2p, 2n, pn nuclei

Table: Comparison between the value of the polarization constant and the deviation parameter for $B(\mathrm{E2})$ values.

Nucleus	χ(The new WS)	χ(The old WS)	σ(The new WS)	σ(The old WS)
^{18}O	0.400757	0.042642	2.697	2.852
^{18}F	0.03451	−0.433699	0.395	20.771
^{38}Ar	0.575314	−0.913149	3.993	4.482

Tamm-Dancoff approximation

Tamm-Dancoff approximation

In Tamm-Dancoff approximation, the shell model Hamiltonian can be represented as

$$H = H_{\mathrm{HF}} + V_{\mathrm{RES}}, \tag{18}$$

where the first term is the one-body contribution to the excitation energy

$$\langle ab^{-1}|H_{\mathrm{HF}}|cd^{-1}\rangle = \delta_{ac}\delta_{bd}(\varepsilon_a - \varepsilon_b), \tag{19}$$

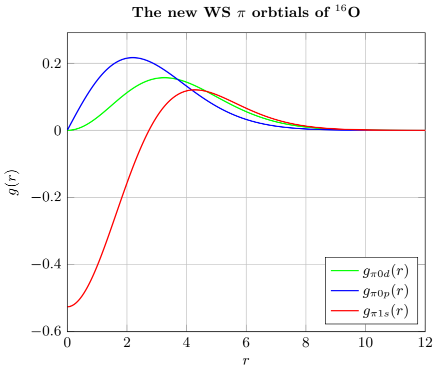
where the single-particle energy is ε. The last part of the interaction is written using the Pandya transformation

$$\langle ab^{-1}; J|V_{\mathrm{RES}}|cd^{-1}; J\rangle = -\sum_{J'} \hat{J'}^2 \begin{Bmatrix} j_a & j_b & J \\ j_c & j_d & J' \end{Bmatrix} \langle ad; J'|V|cb; J'\rangle. \tag{20}$$

Furthermore, considering the residual interaction matrix components isospin formalism, we derive

$$\langle ab^{-1}; JT|V_{\mathrm{RES}}|cd^{-1}; JT\rangle = -\sum_{J'T'} \begin{Bmatrix} j_a & j_b & J \\ j_c & j_d & J' \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & T \\ \frac{1}{2} & \frac{1}{2} & T' \end{Bmatrix} \langle ad; J'T'|V|cb; J'T'\rangle. \tag{21}$$

Tamm-Dancoff approximation in WS bases



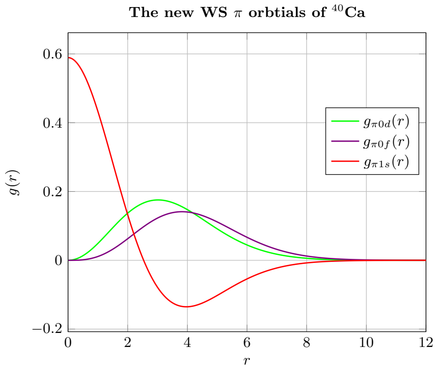
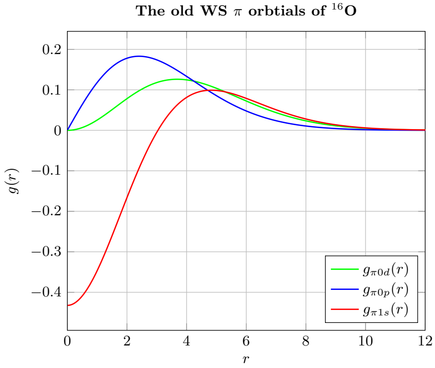


Figure: The π orbitals used in new WS basis for ^{16}O and ^{40}Ca.

Tamm-Dancoff approximation in WS bases



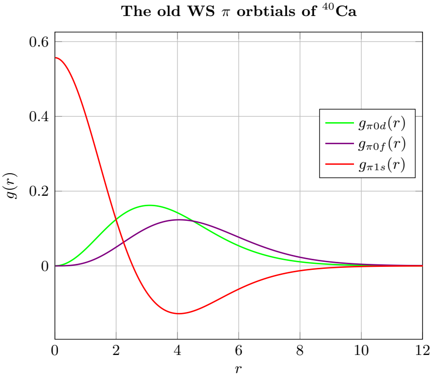


Figure: The same as 1, but for the old WS basis.

Tamm-Dancoff approximation in WS bases

Table: The optimized parameters and the resulting standard deviations for the nuclei considered in the text.

	The new WS						The old WS		
Nuclei	V_0'	a'	r_0'	A_0	A_1	σ	A_0	A_1	σ
^{16}O	171.999	0.176525	10.0935	2.24362	−0.308074	1.166	−1.34154	−0.540814	1.145
^{40}Ca	173.929	0.1991	7.9991	1.08156	0.381825	1.246	0.99404	1.0009	1.408

Tamm-Dancoff approximation in WS bases

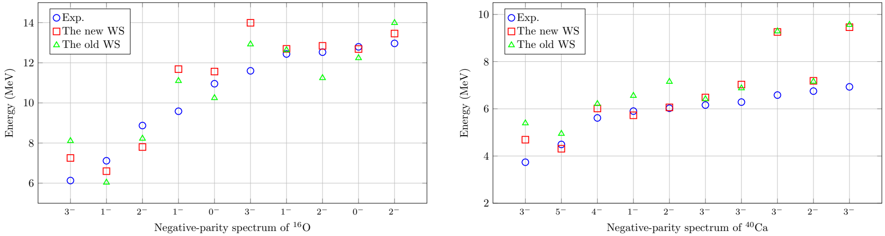


Figure: Graphical comparison of theoretical predictions using the new and the old form of WS with the experimental values.

Tamm-Dancoff approximation in WS bases

The octupole transition probability is $205.286\ e^2\ \text{fm}^6$ for ^{16}O, and $2946.240\ e^2\ \text{fm}^6$ for ^{40}Ca. After reproduction of these values in different WS bases, we obtain

$$\chi_{\text{The new WS}}(^{16}\text{O}) = -0.0785275, \qquad \chi_{\text{The old WS}}(^{16}\text{O}) = -295.895, \tag{22}$$

$$\chi_{\text{The new WS}}(^{40}\text{Ca}) = 0.515877, \qquad \chi_{\text{The old WS}}(^{40}\text{Ca}) = 1.13046. \tag{23}$$

proton-neutron Tamm-Dancoff approximation in WS bases

Beta decay formalism I

The half-life of beta decay is calculated using

$$t_{1/2} = \frac{\ln 2}{T_{fi}}, \tag{24}$$

where T_{fi} represents the transition probability. This is

$$t_{1/2} = \frac{\kappa}{f_0(B_{\mathrm{F}} + B_{GT})}, \tag{25}$$

where Fermi and Gamow-Teller reduced probabilities have the following expressions: $\kappa = 6147\mathrm{s}$, f_0 is an integral calculated across phase space

$$B_{\mathrm{F}} = \frac{g_{\mathrm{V}}^2}{2J_i + 1}|\mathcal{M}_{\mathrm{F}}|^2, \qquad B_{\mathrm{GT}} = \frac{g_{\mathrm{A}}^2}{2J_i + 1}|\mathcal{M}_{\mathrm{GT}}|^2, \tag{26}$$

in which J_i represents the initial state's angular momentum, g_{V} is the vector coupling constant, and g_{A} is the axial-vector coupling constant, which emerges in weak

Beta decay formalism II

interaction processes. The constants are $g_{\mathrm{V}} = 1$ and $g_{\mathrm{A}} = 1.25$, with Fermi and Gamow-Teller matrix elements

$$\mathcal{M}_{\mathrm{F}} = (\xi_f J_f \| \mathbf{1} \| \xi_i J_i) = \delta_{J_i J_f} \sum_{ab} (a \| \mathbf{1} \| b)(\xi_f J f \| [c_a^\dagger \tilde{c}_b]_0 \| \xi_i J_i), \tag{27}$$

$$\mathcal{M}_{\mathrm{GT}} = (\xi_f J_f \| \boldsymbol{\sigma} \| \xi_i J_i) = \frac{\delta_{J_i J_f}}{\sqrt{3}} \sum_{ab} (a \| \boldsymbol{\sigma} \| b)(\xi_f J_f \| [c_a^\dagger \tilde{c}_b]_1 \| \xi_i J_i), \tag{28}$$

ξ represents all other quantum numbers in the state, with the exception of total angular momentum J. For $c_{-\alpha} = c_{a,-m\alpha}$, $\tilde{c}_\alpha = (-)^{j_a + m_\alpha} c_{-\alpha}$. In terms of angular momenta, the $\mathbf{1}$ and $\boldsymbol{\sigma}$ carry zero and one, respectively. The reduction theorem simplifies the computation of the reduced matrix elements for these.
Take the $\log$ of both sides of Eq. (25) to compute the theoretical $\log ft$. Eq. (25) incorporates a phase-space factor to reflect the integrated leptonic phase space. This is sometimes called the Fermi integral.

Beta decay formalism III

For the decay of $\beta^{\pm}$, the phase-space contribution

$$f_0^{\pm} = \int_1^{E_0} F_0(\pm Z_f, \epsilon) p\epsilon(E_0 - \epsilon)^2 \mathrm{d}\epsilon, \tag{29}$$

where the endpoint energy is $E_0 = (E_i - E_f)/m_e c^2$, the initial and final state energies are E_i and E_f, the electron's mass is shown by m_{e}, and $\epsilon \approx 1 - \frac{1}{2}(\alpha Z_i)^2$, F_0 is the Fermi function, and the momentum of the emitted electron is $p = \sqrt{\epsilon^2 - 1}$. The Fermi function has an analytic form in the Primakoff-Rosen approximation, which is not relativistic in nature. Using the fine structure constant $\alpha = 1/137$, we get

$$F_0(Z_f, \epsilon) \approx \frac{\epsilon}{p} F_0^{(\mathrm{PR})}(Z_f) = \frac{2\pi\alpha Z_f}{1 - \exp(-2\pi\alpha Z_f)}.$$

Beta decay formalism IV

This type of transition is characterized using the generic shape function, which captures the intricacies of the transition process while also providing information about the nuclear structure.

$$S^{(\mp)}_{K\mathrm{u}}(Z_f,\epsilon) \approx F_0(\pm Z_f,\epsilon)p\epsilon(E_0-\epsilon)^2 \sum_{k_\mathrm{e}+k_\nu=K+2} \frac{(\epsilon^2-1)^{k_\mathrm{e}-1}(E_0-\epsilon)^{2(k_\nu-1)}}{(2k_\mathrm{e}-1)!(2k_\nu-1)!}, \tag{30}$$

where K denotes the forbidden order, and k_e and k_ν are integers that begin at zero. The integration of the shape function, also known as the phase-space factor, takes the following form in the case of prohibited decays

$$f^{(\pm)}_{K\mathrm{u}} = \left(\frac{3}{4}\right)^K \frac{(2K)!!}{(2K+1)!!} \int_1^{E_0} S^{(\mp)}_{K\mathrm{u}}(Z_f,\epsilon)\,\mathrm{d}\epsilon, \tag{31}$$

Beta decay formalism V

where “u” represents the unique type of forbidden decay and the following relation with the first-forbidden unique type (meaning for the initial and final states, $\Delta J = 2$).

$$f^{(\mp)}_{K=1,\mathrm{u}} = \frac{1}{12} f^{(\mp)}_{1,\mathrm{u}}. \tag{32}$$

The matrix elements of the beta decay are obtained via

$$\mathcal{M}_{1\mathrm{u}} = \frac{m_{\mathrm{e}} c^2}{\sqrt{4\pi}} \zeta (\xi_f \; J_f \| [\boldsymbol{\sigma} \boldsymbol{r}]_2 \| \xi_i \; J_i) \tag{33}$$

$$= \sum_{ab} \mathcal{M}^{(1\mathrm{u})}(ab) (\xi_f \; J_f \| [c^\dagger_a \tilde{c}_b]_2 \| \xi_i \; L_i), \tag{34}$$

where in the Condon-Shortley convention for the phase factor we have $\zeta = 1$.

Beta decay formalism VI

The final piece of equipment required for this study is the ability to manage a transition in the event of a hole case. Configuration mixing occurs when we model each state as a linear combination of a few bases for a given angular momentum Regarding the change from an initial to a final state via beta decay

$$|\Psi_i\rangle = \sum_k A_k |k\rangle, \quad |\Psi_f\rangle = \sum_l B_l |l\rangle, \tag{35}$$

where A_i, B_i represent real constants. The transition amplitude transforms into

$$(\Psi_f \| \mathcal{O}_\lambda \| \Psi_i) = \sum_{kl} A_k B_l (l \| \mathcal{O}_\lambda \| k). \tag{36}$$

The β-decay ^{16}N $\rightarrow^{16}$ O in pnTDA

Table: The optimized parameters and the resulting standard deviations for the nuclei considered in the text.

	The new WS						The old WS		
Nuclei	v_0	a	r_0	A_0	A_1	σ	A_0	A_1	σ
^{16}O	171.999	0.176525	10.0935	2.24362	-0.308074	1.166	-1.34154	-0.540814	1.145
^{16}Na	52.9914	0.332586	4.39587	0.935152	1.0975	0.670	0.598779	1.16397	0.754

The β-decay ^{16}N $\rightarrow^{16}$ O in pnTDA

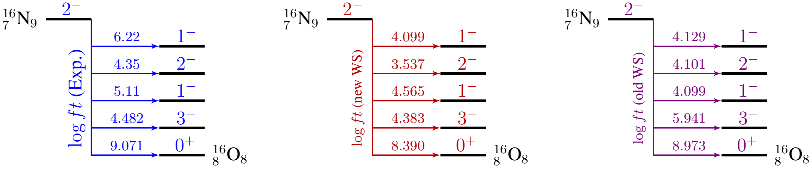


Figure: Comparison between the theoretical predictions of log ft of ^{16}N $\rightarrow$ ^{16}O decay and experimental data.

$$\sigma(\text{New WS}) = 1.089, \qquad \sigma(\text{Old WS}) = 1.232. \tag{37}$$

Random phase approximation in WS bases

Random phase approximation formalism I

The RPA equations can then be written symbolically in matrix form as

$$\begin{pmatrix} \mathsf{A} & \mathsf{B} \\ -\mathsf{B}^* & -\mathsf{A}^* \end{pmatrix} \begin{pmatrix} \mathsf{X}^\omega \\ \mathsf{Y}^\omega \end{pmatrix} = E_\omega \begin{pmatrix} \mathsf{X}^\omega \\ \mathsf{Y}^\omega \end{pmatrix}, \tag{38}$$

where E_ω denotes the excitation energy.
This formalism introduces two key matrices, A and B, which together form the RPA supermatrix. The vectors X and Y collect the forward and backward amplitudes, respectively.

Random phase approximation formalism II

The explicit forms of A and B are obtained through the equation-of-motion method, yielding

$$\begin{aligned} \mathsf{A}_{ab,cd}(J) &\equiv \langle \mathrm{RPA}|[\mathcal{A}_{ab}(JM), H, \mathcal{A}^{\dagger}_{cd}(JM)]|\mathrm{RPA}\rangle \\ &\simeq \langle \mathrm{HF}|[\mathcal{A}_{ab}(JM), H, \mathcal{A}^{\dagger}_{cd}(JM)]|\mathrm{HF}\rangle, \end{aligned} \tag{39}$$

$$\begin{aligned} \mathsf{B}_{ab,cd}(J) &\equiv -\langle \mathrm{RPA}|[\mathcal{A}_{ab}(JM), H, \tilde{\mathcal{A}}^{\dagger}_{cd}(JM)]|\mathrm{RPA}\rangle \\ &\simeq -\langle \mathrm{HF}|[\mathcal{A}_{ab}(JM), H, \tilde{\mathcal{A}}^{\dagger}_{cd}(JM)]|\mathrm{HF}\rangle. \end{aligned} \tag{40}$$

Here, the double commutator is defined as

$$[A, B, C]_{\pm} \equiv \frac{1}{2}\left(\Big[A, [B, C]\Big]_{\pm} + \Big[[A, B], C\Big]_{\pm}\right), \tag{41}$$

with the $(\pm)$ signs corresponding to commutator or anticommutator operations. This formulation highlights how the quasi-boson approximation is applied within the RPA framework.

Random phase approximation formalism III

In particular, the matrix A reduces to the familiar Tamm–Dancoff matrix,

$$\mathsf{A}_{ab,cd}(JT) = \delta_{ac}\delta_{bd}(\varepsilon_a - \varepsilon_b) - \sum_{J'T'} \begin{Bmatrix} j_a & j_b & J \\ j_c & j_d & J' \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & T \\ \frac{1}{2} & \frac{1}{2} & T' \end{Bmatrix} \langle ad; J'T'|V|cb; J'T'\rangle, \tag{42}$$

where ε denotes single-particle energies, and standard $6j$ notation is used.
The matrix B, on the other hand, encodes the ground-state correlations and is given by

$$\begin{aligned} \mathsf{B}_{ab,cd}(JT) &= (-1)^{j_b+j_c+J+1+T}\sqrt{(1+\delta_{ac})(1+\delta_{bd})} \\ &\times \sum_{J'T'} (-1)^{J'+T'}\widehat{J'}^2\widehat{T'}^2 \begin{Bmatrix} j_a & j_b & J \\ j_d & j_c & J' \end{Bmatrix} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & T \\ \frac{1}{2} & \frac{1}{2} & T' \end{Bmatrix} \langle ac; J'T'|V|bd; J'T'\rangle. \end{aligned} \tag{43}$$

Random phase approximation in WS bases

Table: The optimized parameters and the resulting standard deviations for the nuclei considered in the text.

	The new WS						The old WS		
Nuclei	V_0'	a'	r'	A_0	A_1	σ	A_0	A_1	σ
^{16}O	171.996	0.289112	5.59822	5.81171	−1.35229	1.261	−6.79284	−3.50546	1.369
^{40}Ca	173.999	0.153103	7.99329	56.6924	5.98731	1.240	72.9826	11.9835	1.243

Random phase approximation in WS bases

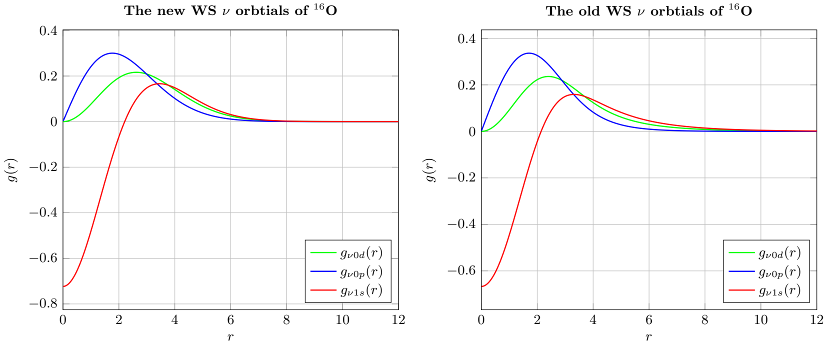


Figure: Optimized neutron (ν) orbitals in ^{16}O. These orbitals are used in RPA calculation.

Random phase approximation in WS bases

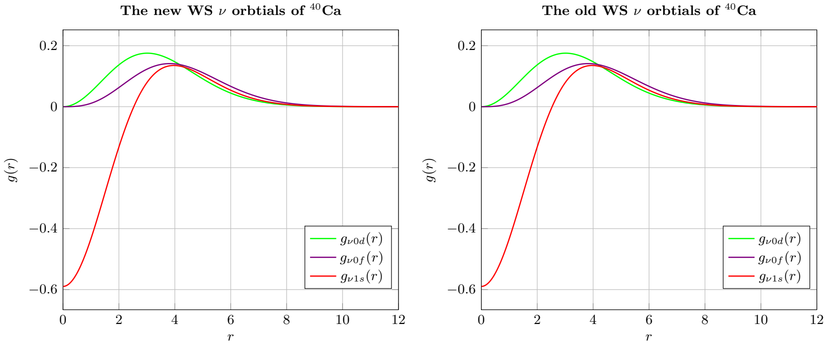


Figure: The same as 5, but for ^{40}Ca.

Random phase approximation in WS bases

By reproducing the octupole transition probability, the polarization parameter in ^{16}O is found to be

$$\chi_{\text{New WS}}(^{16}\text{O}) = 0.283327, \qquad \chi_{\text{Old WS}}(^{16}\text{O}) = 371.413. \tag{44}$$

Similarly, the corresponding calculations for ^{40}Ca yield

$$\chi_{\text{New WS}}(^{40}\text{Ca}) = 0.22997, \qquad \chi_{\text{Old WS}}(^{40}\text{Ca}) = 0.647105. \tag{45}$$

Collective model

AQOA Hamiltonian and Solutions I

Therefore the corresponding Hamiltonian gets the form of

$$H = -\sum_{\lambda=2,3} \frac{\hbar^2}{2B_\lambda} \frac{1}{\beta_\lambda^3} \frac{\partial}{\partial \beta_\lambda} \beta_\lambda^3 \frac{\partial}{\partial \beta_\lambda} + \frac{\hbar^2 \hat{L}^2}{6(B_2\beta_2^2 + 2B_3\beta_3^2)} + V(\beta_2, \beta_3), \tag{46}$$

where β_2 and β_3 are the quadrupole and octupole deformation. B_2 and B_3 are the corresponding masses, which are associated with these distortions. $\hat{L}$ is the angular momentum operator, along the principal axes of rotation in the intrinsic reference frame.

AQOA Hamiltonian and Solutions II

The solutions to the Schrödinger equation can be found in the following way

$$\Phi_L^{\pm}(\beta_2, \beta_3, \theta) = (\beta_2\beta_3)^{-3/2}\Psi_L^{\pm}(\beta_2, \beta_3)|LM0, \pm\rangle, \tag{47}$$

where θ denotes the set of Euler angles, which are essential for comprehending and depicting the orientation of the body-fixed coordinate system delineated by the axes x', y' and z' about the fixed laboratory coordinate system represented by the axes x, y, and z. In this framework, the mathematical notation $|LM0, \pm\rangle$ is utilized to demonstrate the dynamics of the rotation linked to an axially symmetric nucleus, particularly emphasizing the angular momentum projection M as it aligns with the laboratory-fixed z axis, while concurrently preserving a projection K that is equal to 0 along the body-fixed z' axis

$$|LM0, \pm\rangle = \sqrt{\frac{2L+1}{32\pi^2}}(1 \pm (-1)^L)\mathcal{D}^L_{0,M}(\theta) \tag{48}$$

in which $\mathcal{D}(\theta)$ stands for Wigner functions of Euler angles. The positive parity states having $L = 0, 2, 4, \dots$ are indicated by the $+$ label, while the $-$ label refers to ones with $L = 1, 3, 5, \dots$.

AQOA Hamiltonian and Solutions III

The Schrödinger equation may be simplified considering new deformation variables

$$\tilde{\beta}_2 = \beta_2\sqrt{\frac{B_2}{B}}, \qquad \tilde{\beta}_3 = \beta_3\sqrt{\frac{B_3}{B}}, \qquad B = \frac{B_2 + B_3}{2}, \tag{49}$$

the polar coordinates with the aim of the new deformation variables in the range of $0 \leq \tilde{\beta} < \infty$ and $-\pi/2 \leq \phi \leq \pi/2$

$$\tilde{\beta}_2 = \tilde{\beta}\cos\phi, \qquad \tilde{\beta}_3 = \tilde{\beta}\sin\phi, \qquad \tilde{\beta} = \sqrt{\tilde{\beta}_2^2 + \tilde{\beta}_3^2}, \tag{50}$$

the reduced energy $\epsilon = (2B/\hbar^2)E$, and the reduced potential $v = (2B/\hbar^2)V$. Then we have

$$\left[-\frac{\partial^2}{\partial\tilde{\beta}^2} - \frac{1}{\tilde{\beta}}\frac{\partial}{\partial\tilde{\beta}} + \frac{L(L+1)}{3\tilde{\beta}^2(1+\sin^2\phi)} - \frac{1}{\tilde{\beta}^2}\frac{\partial^2}{\partial\phi^2} + v(\tilde{\beta},\phi) + \frac{3}{\tilde{\beta}^2\sin^2 2\phi} - \epsilon_L\right]\Psi_L^{\pm}(\tilde{\beta},\phi) = 0 \tag{51}$$

AQOA Hamiltonian and Solutions IV

As a simplification, let us assume that the potential energy $v(\tilde{\beta}, \phi)$ can be separated into the form $v(\tilde{\beta}, \phi) = u(\tilde{\beta}) + w(\tilde{\phi}^{\pm})$: a function of only, $u(\tilde{\beta})$, and a function of $\tilde{\phi}^{\pm} = \phi \pm \phi_0$, $w(\tilde{\phi}^{\pm})$. Such a hypothesis permits us to separate Eq. (51) into two independent equations. We further assume that $w(\tilde{\phi}^{\pm})$ is a very steep, double-well potential centered around $\pm\phi_0$. Then we have

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}\tilde{\beta}^2} - \frac{1}{\tilde{\beta}}\frac{\mathrm{d}}{\mathrm{d}\tilde{\beta}} + \frac{1}{\tilde{\beta}^2}\left(\frac{L(L+1)}{3(1+\sin^2\phi_0)} + \frac{3}{\sin^2 2\phi_0}\right) + u(\tilde{\beta}) - \epsilon_{\tilde{\beta}}(L)\right]\psi_L(\tilde{\beta}) = 0, \tag{52}$$

and

$$\left[-\frac{1}{\langle\tilde{\beta}^2\rangle}\frac{\mathrm{d}^2}{\mathrm{d}(\tilde{\phi}^{\pm})^2} + w(\tilde{\phi}^{\pm}) - \epsilon_\phi\right]\chi(\tilde{\phi}^{\pm}) = 0 \tag{53}$$

where the total wave function has been assumed as

$$\Psi_L^{\pm}(\tilde{\beta}, \phi) = N_{\tilde{\beta}}\psi_L(\tilde{\beta})N_\phi\left(\chi(\tilde{\phi}^{+}) \pm \chi(\tilde{\phi}^{-})\right)/\sqrt{2} \tag{54}$$

AQOA Hamiltonian and Solutions V

with the normalization factors $N_{\tilde{\beta}}$ and N_ϕ, $\langle\tilde{\beta}^2\rangle$ is the average of $\tilde{\beta}^2$ over $\psi_L(\tilde{\beta})$, and $\epsilon_L = \epsilon_{\tilde{\beta}}(L) + \epsilon_\phi$. The ϕ value of 0 signifies the presence of a pure quadrupole deformation, whereas $\phi = \pm\pi/2$ indicates a pure octupole deformation. The pronounced steepness of the two oscillators ensures that ϕ remains in proximity to $\pm\phi_0$, thereby maintaining a consistent competition between quadrupole and octupole deformation.

AQOA Hamiltonian and Solutions VI

For the $\tilde{\phi}^{\pm}$ component, it is commonly assumed that the potential is centered around the values $\pm\phi_0$. For instance, the equation

$$u(\tilde{\phi}^{\pm}) = \frac{1}{2}c_0(\tilde{\phi}^{\pm})^2 \tag{55}$$

can be rewritten as

$$\left[-\frac{\mathrm{d}}{\mathrm{d}(\tilde{\phi}^{\pm})} + \frac{1}{2}c_0\langle\tilde{\beta}^2\rangle(\tilde{\phi}^{\pm})^2\right]\chi(\tilde{\phi}^{\pm}) = \epsilon_\phi\langle\tilde{\beta}^2\rangle\chi(\tilde{\phi}^{\pm}), \tag{56}$$

This equation represents a simple harmonic oscillator with eigenvalues given by

$$\epsilon_\phi = \sqrt{\frac{2c_0}{\langle\tilde{\beta}^2\rangle}}\left(n_\phi + \frac{1}{2}\right), \qquad n_\phi = 0, 1, 2, \ldots \tag{57}$$

AQOA Hamiltonian and Solutions VII

and eigenfunctions

$$\chi_{n_\phi}(\tilde{\phi}^\pm) = N_{n_\phi}\mathcal{H}_{n_\phi}(b_0\tilde{\phi}^\pm)e^{-b_0^2(\tilde{\phi}^\pm)^2/2}, \quad b_0 = \left(\frac{c_0\langle\tilde{\beta}^2\rangle}{2}\right)^{1/4}, \tag{58}$$

where the normalization constant is given by $N_{n_\phi} = \sqrt{b_0/(\sqrt{\pi}2^{n_\phi}n_\phi!)}$ and Hermite polynomials are $\mathcal{H}$.

AQOA Hamiltonian and Solutions VIII

Now, we turn to the part of the differential equation involving $\tilde{\beta}$. In this section, we consider the extended sextic (ES) potential

$$u(\tilde{\beta}) = \frac{a}{\tilde{\beta}^2} + b\tilde{\beta}^2 + c\tilde{\beta}^4 + d\tilde{\beta}^6, \tag{59}$$

By substituting this potential and assuming the solution in the form $\psi(\tilde{\beta}) = \frac{\xi(\tilde{\beta})}{\sqrt{\tilde{\beta}}}$, we obtain the following equation:

$$\frac{\mathrm{d}^2\xi(\tilde{\beta})}{\mathrm{d}\tilde{\beta}^2} + \left(\varepsilon - \frac{a_0}{\tilde{\beta}^2} - b\tilde{\beta}^2 - c\tilde{\beta}^4 - d\tilde{\beta}^6\right)\xi(\tilde{\beta}) = 0, \tag{60}$$

$$a_0 = a_0(L, \phi_0) = a - \frac{1}{4} + \frac{L(L+1)}{3(1+\sin^2\phi_0)} + \frac{3}{\sin^2(2\phi_0)}. \tag{61}$$

AQOA Hamiltonian and Solutions IX

We need to perform several algebraic transformations to derive a solution for this differential equation. The first step is the change of variable $x = \tilde{\beta}^2$, which simplifies the equation by lowering the powers of terms:

$$\frac{\mathrm{d}^2\xi(x)}{\mathrm{d}x^2} + \frac{1/2}{x}\frac{\mathrm{d}\xi(x)}{\mathrm{d}x} + \left(-\frac{a_0}{x^2} - b + \frac{\varepsilon}{x} - cx - dx^2\right)\frac{\xi(x)}{4} = 0. \tag{62}$$

We obtain a form with known solutions by eliminating the first-order derivative term in this differential equation. To remove this term, we assume the solution in the form $\xi(x) = f(x)/\sqrt[4]{x}$. Substituting this into the differential equation yields:

$$\frac{\mathrm{d}^2 f(x)}{\mathrm{d}x^2} + \left(-\frac{\frac{a_0}{4} - \frac{3}{16}}{x^2} + \frac{\varepsilon/4}{x} - \frac{b}{4} - \frac{c}{4}x - \frac{d}{4}x^2\right) f(x) = 0. \tag{63}$$

The general solutions to this differential equation are given by:

$$f(x) = x^A \exp\left(Bx + Dx^2\right) h(x), \tag{64}$$

AQOA Hamiltonian and Solutions X

where the parameters are:

$$A = \frac{1}{4}\left(2 + \sqrt{1 + 4a_0}\right), \tag{65}$$

$$B = \frac{-c}{4\sqrt{d}}, \tag{66}$$

$$D = -\frac{\sqrt{d}}{4}, \tag{67}$$

and the governing differential equation for $h(x)$ is:

$$x\frac{\mathrm{d}^2 h(x)}{\mathrm{d}x^2} + \frac{\mathrm{d}h(x)}{\mathrm{d}x}\left(1 + \frac{1}{2}\sqrt{1 + 4a_0} - \frac{c}{2\sqrt{d}}x - \sqrt{d}x^2\right)$$
$$h(x)\left[-\frac{c}{4\sqrt{d}} + \frac{\varepsilon}{4} - \frac{c\sqrt{1 + 4a_0}}{8\sqrt{d}} + x\left(-\frac{b}{4} + \frac{c^2}{16d} - \sqrt{d} - \frac{\sqrt{d}}{4}\sqrt{1 + 4a_0}\right)\right] = 0. \tag{68}$$

AQOA Hamiltonian and Solutions XI

This differential equation has a known solvable form using the Bethe ansatz method. Since, in this Hamiltonian, we are usually interested in node-less solutions, by following the details of the method introduced and utilized in for the ground state $n_{\tilde{\beta}} = 0$, we obtain:

$$h(x) = 1, \tag{69}$$

which leads to the following eigenvalue equation and constraint:

$$\varepsilon = \left(2 + \sqrt{1 + 4a_0}\right) \sqrt{b + \sqrt{d}\left(4 + \sqrt{1 + 4a_0}\right)}, \tag{70}$$

$$c = 2\sqrt{d\left(b + \sqrt{d}\left(4 + \sqrt{1 + 4a_0}\right)\right)}. \tag{71}$$

AQOA Hamiltonian and Solutions XII

To summarize this section of the paper, we present the final form of the solution to this part of the differential equation in the same order as adopted during the solution derivation process

$$\psi(\tilde{\beta}) = N_L \tilde{\beta}^{2A-1} \exp\left[B\tilde{\beta}^2 + D\tilde{\beta}^4\right], \tag{72}$$

where the normalization constant, N_L, is calculated using its definition

$$N_L = \frac{1}{\sqrt{\int_0^\infty |\psi_L(\tilde{\beta})|^2 \tilde{\beta}\, \mathrm{d}\tilde{\beta}}}. \tag{73}$$

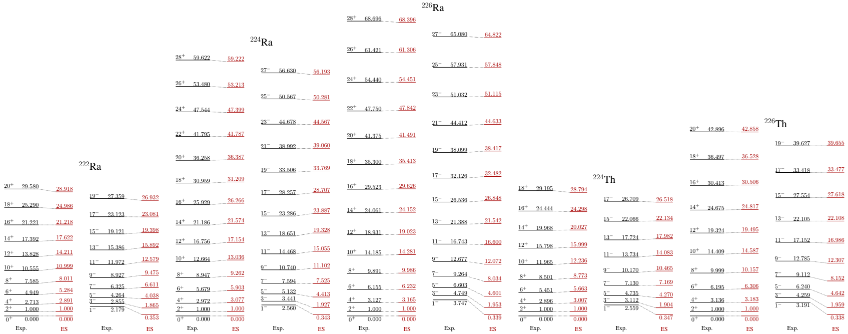
Results for sextic potential

The deviation parameter should be defined as

$$\sigma = \sqrt{\frac{1}{N^*}\left(\frac{E_{\text{Exp.}}(\ell_i^\pi)}{E_{\text{Exp.}}(2^+)} - \frac{E_{\text{Theo.}}(\ell_i^\pi) - E_{\text{Theo.}}(0^+)}{E_{\text{Theo.}}(2^+) - E_{\text{Theo.}}(0^+)}\right)^2}.$$

Isotope	$\ell_{\max}$	σ_{ES}	σ^*_{ES}	σ_{Sextic}	σ_{Davidson}
^{222}Ra	20	0.573	0.587	0.604	0.917
^{224}Ra	28	0.606	0.616	0.801	1.351
^{226}Ra	28	0.947	0.964	1.232	1.360
^{224}Th	18	0.621	0.638	0.691	0.843
^{226}Th	20	0.908	0.930	1.059	0.994

Energy levels



Thank you!