Pairing effects on pure rotational energy of nuclei

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Introduction

Rotational band $E_x(J^+)$ = J(J+1)/2I indicates that the intrinsic state of the nucleus is deformed and rotates with the moment of inertia (MoI).

From a microscopic standpoint, nuclei are well described in the self-consistent mean-field (MF) theories, but the rotational symmetry is spontaneously broken. Using angular momentum projection(AMP) to restore the symmetry and get more exact approximation.

However, rotational spectra have also been observed in light nuclei including those far off the β-stability. It will deserve reinvestigating from a general perspective how the rotational energy of nuclei arises, not restricting ourselves to well-deformed heavy nuclei.

Meanwhile, the rotational energy of nuclei should be formed from the effective Hamiltonian, including the nucleonic interaction. We will decompose the rotational energy into contributions of the individual terms of the Hamiltonian.

It is known that the pair correlations in nuclei significantly influence the rotational energy.

Theory

definition of rotational energy

$$E_{rot} = \langle J|\hat{H}|J\rangle - \langle 0|\hat{H}|0\rangle$$

consider an axially-symmetric intrinsic state, which is an eigenstate of J_z with the eigenvalue M = 0.

to calculate the expectation

$$\langle J|\hat{\mathcal{S}}|J\rangle = \frac{\int_0^{\pi/2} d\beta \sin\beta\, d_{00}^{(J)}(\beta)\, \langle\Phi_0|\hat{\mathcal{S}}\, e^{-i\hat{J}_y\beta}|\Phi_0\rangle}{\int_0^{\pi/2} d\beta \sin\beta\, d_{00}^{(J)}(\beta)\, \langle\Phi_0|e^{-i\hat{J}_y\beta}|\Phi_0\rangle}.$$

$$|\Phi_0\rangle = \sum_J |J0\rangle\, \langle J0|\Phi_0\rangle.$$

J0 mean the z-component of J is 0 (M=0)

Using these expansion series:

$$d_{00}^{(J)}(\beta) = \sum_{n=0}^{\infty} c_{2n}\beta^{2n}; \quad c_{2n} = \frac{(-)^n}{(2n)!}\langle J0|\hat{J}_y^{2n}|J0\rangle\,.$$

$$\mathcal{S}^{01}(\beta) := \frac{\langle\Phi_0|\hat{\mathcal{S}}\, e^{-i\hat{J}_y\beta}|\Phi_0\rangle}{\langle\Phi_0|e^{-i\hat{J}_y\beta}|\Phi_0\rangle} = \sum_{n=0}^{\infty} s_{2n}\beta^{2n}; \quad s_{2n} = \frac{(-)^n}{(2n)!}\langle\Phi_0|\hat{\mathcal{S}};\underbrace{\hat{J}_y;\cdots;\hat{J}_y}_{2n}|\Phi_0\rangle_{\text{cum}}$$

$$\langle \exp \sum_{j=1}^{N} \xi_j X_j\rangle = \exp\langle \exp\left(\sum \xi_j X_j\right) - 1\rangle_c$$

here use

where

$$s_0 = \langle\Phi_0|\hat{\mathcal{S}}|\Phi_0\rangle\,, \quad s_2 = -\frac{1}{2!}C[\hat{\mathcal{S}},\hat{J}_y^2], \quad s_4 = \frac{1}{4!}\left(C[\hat{\mathcal{S}},\hat{J}_y^4] - 6\,C[\hat{\mathcal{S}},\hat{J}_y^2](\sigma[\hat{J}_y])^2\right).$$

$$C[\hat{A},\hat{B}] := \langle\Phi_0|\hat{A}\hat{B}|\Phi_0\rangle - \langle\Phi_0|\hat{A}|\Phi_0\rangle\,\langle\Phi_0|\hat{B}|\Phi_0\rangle\,, \quad \sigma[\hat{A}] := \sqrt{C[\hat{A},\hat{A}]}.$$

Theory

finally we have

$$\langle J|\hat{S}|J\rangle = \frac{\sum_{m,n=0}^{\infty} c_{2m}s_{2n}\Lambda_{2m+2n}}{\sum_{\ell=0}^{\infty} c_{2\ell}\Lambda_{2\ell}},$$

$$N_{2n} := \int_0^{\pi/2} d\beta \sin\beta\, \beta^{2n} \langle\Phi_0|e^{-i\hat{J}_y\beta}|\Phi_0\rangle, \quad \Lambda_{2n} := \frac{N_{2n}}{N_0}, \quad (n = 0, 1, 2, \cdots).$$

We hope to write it in term of $\langle 0|\hat{S}|0\rangle$

we get

$$\langle J|\hat{S}|J\rangle = \langle 0|\hat{S}|0\rangle + \frac{J(J+1)}{2\,\mathcal{I}[S]} + \cdots;$$

$$\langle 0|\hat{S}|0\rangle := \sum_{n=0}^{\infty} s_{2n}\Lambda_{2n}, \quad \frac{1}{\mathcal{I}[\hat{S}]} := \sum_{n=1}^{\infty} s_{2n}\left[-\frac{1}{2}(\Lambda_{2n+2} - \Lambda_{2n}\Lambda_2)\right].$$

Ignore high order(n≥2), but sometime are not negligible which will discuss later

J=0, d function become 1 and vanish the sum of c

Theory

Effective Hamiltonian $$\hat{H} = \hat{K} + \hat{V}_{\rm nucl} + \hat{V}_{\rm Coul} - \hat{H}_{\rm c.m.}.$$

$$\hat{V}_{\rm nucl} = \hat{V}^{(\rm C)} + \hat{V}^{(\rm LS)} + \hat{V}^{(\rm TN)} + \hat{V}^{(\rm C\rho)}; \quad \hat{V}^{(\rm X)} = \sum \hat{v}_{ij}^{(\rm X)}, \quad (\rm X = C, LS, TN, C\rho)$$

where

$$\hat{v}_{ij}^{(\rm C)} = \sum_n \left(t_n^{(\rm SE)} P_{\rm SE} + t_n^{(\rm TE)} P_{\rm TE} + t_n^{(\rm SO)} P_{\rm SO} + t_n^{(\rm TO)} P_{\rm TO}\right) f_n^{(\rm C)}(r_{ij}),$$

$$\hat{v}_{ij}^{(\rm LS)} = \sum_n \left(t_n^{(\rm LSE)} P_{\rm TE} + t_n^{(\rm LSO)} P_{\rm TO}\right) f_n^{(\rm LS)}(r_{ij})\, \mathbf{L}_{ij} \cdot (\mathbf{s}_i + \mathbf{s}_j),$$

$$\hat{v}_{ij}^{(\rm TN)} = \sum_n \left(t_n^{(\rm TNE)} P_{\rm TE} + t_n^{(\rm TNO)} P_{\rm TO}\right) f_n^{(\rm TN)}(r_{ij})\, r_{ij}^2\, S_{ij},$$

$$\hat{v}_{ij}^{(\rm C\rho)} = \left(t_\rho^{(\rm SE)} P_{\rm SE} \cdot [\rho(\mathbf{r}_i)]^{\alpha^{(\rm SE)}} + t_\rho^{(\rm TE)} P_{\rm TE} \cdot [\rho(\mathbf{r}_i)]^{\alpha^{(\rm TE)}}\right) \delta(\mathbf{r}_{ij}),$$

use semi-realistic interaction M3Y-P6

to analyzing the paring effect, use HF+BCS method , and introduce parameter g

$$\langle \hat{H}_g \rangle = \langle \hat{H}_{\rm dns} \rangle + g \langle \hat{H}_{\rm pair} \rangle$$

Theory

It also investigate the relevance of the spatial correlations between nucleons to the rotational energy

$$\hat{D} := \sum_{i<j} \delta(\mathbf{r}_{ij}).$$

pair-distribution function is defined as

$$\mathcal{G}(x_1, x_2) := \frac{\langle \psi^\dagger(x_1)\psi^\dagger(x_2)\psi(x_2)\psi(x_1)\rangle}{\langle \hat{\rho}(x_1)\rangle \ \langle \hat{\rho}(x_2)\rangle},$$

degree of proximity (DoP) is

$$\begin{aligned}\langle \hat{D}\rangle &= \frac{1}{2}\sum_{\tau_1\tau_2}\sum_{\sigma_1\sigma_2}\int d^3r \, \langle \psi^\dagger(\mathbf{r}\sigma_1\tau_1)\psi^\dagger(\mathbf{r}\sigma_2\tau_2)\psi(\mathbf{r}\sigma_2\tau_2)\psi(\mathbf{r}\sigma_1\tau_1)\rangle \\ &= \frac{1}{2}\sum_{\tau_1\tau_2}\sum_{\sigma_1\sigma_2}\int d^3r \, \langle \hat{\rho}(\mathbf{r}\sigma_1\tau_1)\rangle \ \langle \hat{\rho}(\mathbf{r}\sigma_2\tau_2)\rangle \, \mathcal{G}(\mathbf{r}\sigma_1\tau_1, \mathbf{r}\sigma_2\tau_2).\end{aligned}$$

result

Influence of pairing on deformation

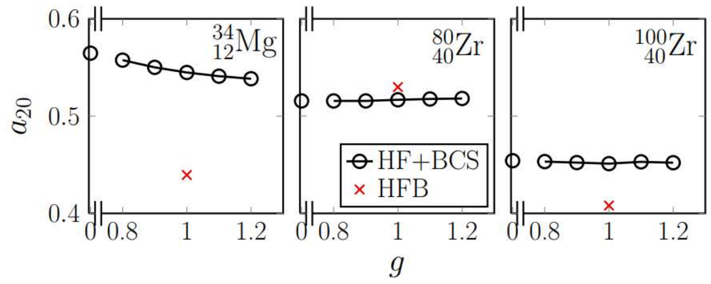


FIG. 1. The g dependence of the deformation parameter a_{20} in the HF+BCS results with $\langle \hat{H}_g \rangle$ for $^{34}_{12}$Mg and $^{80,100}_{40}$Zr. The red crosses represent the a_{20} values in the HFB solutions.

TABLE I. a_{20} for the HF and HFB solutions at their lowest minima for $^{24}_{12}$Mg, $^{40}_{12}$Mg and $^{104}_{40}$Zr.

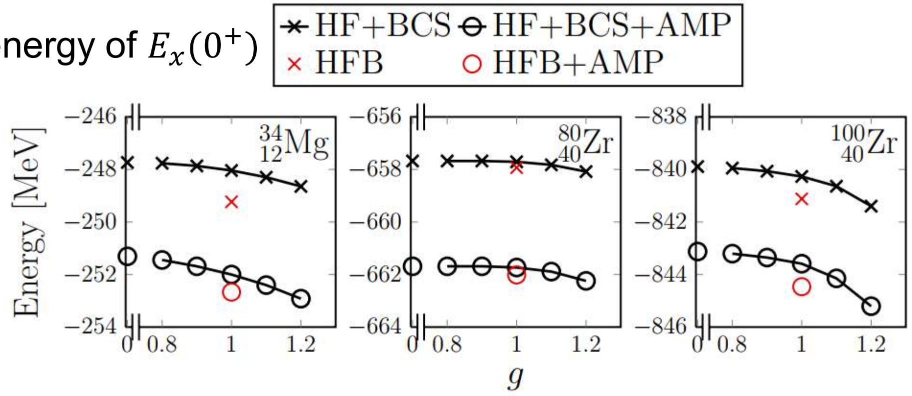
nuclide	HF	HFB
$^{24}_{12}$Mg	0.54	0.54
$^{40}_{12}$Mg	0.47	0.43
$^{104}_{40}$Zr	0.46	0.43

While a_{20} is insensitive to g for the $^{80}_{40}Zr$, $^{100}_{40}Zr$ nuclei, a_{20} slightly decreases as g grows for the $^{34}_{12}Mg$ nucleus. The a_{20} values for the HF+BCS solutions are close to that of the HFB solution for the $^{80}_{40}Zr$ nucleus, while they do not match well for the $^{34}_{12}Mg$ and $^{100}_{40}Zr$ nuclei, indicating influence of the pairing on the HF configurations.

result

comparison of $E_x(2^+)$ with rigid-rotor model and experiment

energy of $E_x(0^+)$



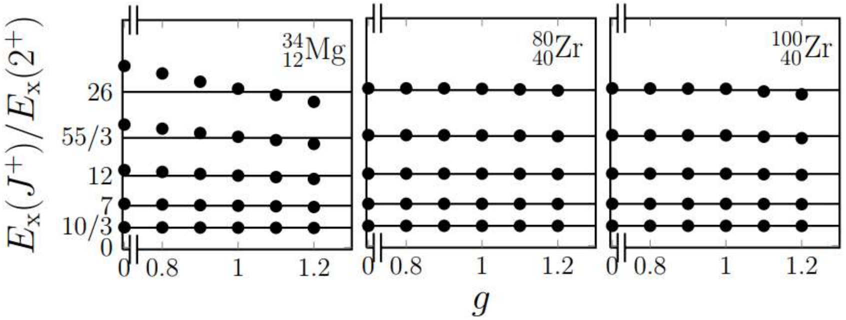


FIG. 3. $E_x(J^+)/E_x(2^+)$ for the HF+BCS solutions of $^{34}_{12}$Mg and $^{80,100}_{40}$Zr. The lines display the rigid-rotor values $J(J+1)/6$.

The ratios $E_x(J^+)\ /E_x(2^+)$ are insensitive to g and close to the J(J + 1)/6 lines except for high J ($\gtrsim$ 10) $^{34}_{12}Mg$. For $^{34}_{12}Mg$ nucleus, the ratios $E_x(J^+)\ /E_x(2^+)$ decrease for high J as g increases. The deviation from the J(J + 1)/6 lines indicates that the higher- c_{2n} terms are not negligible.

result

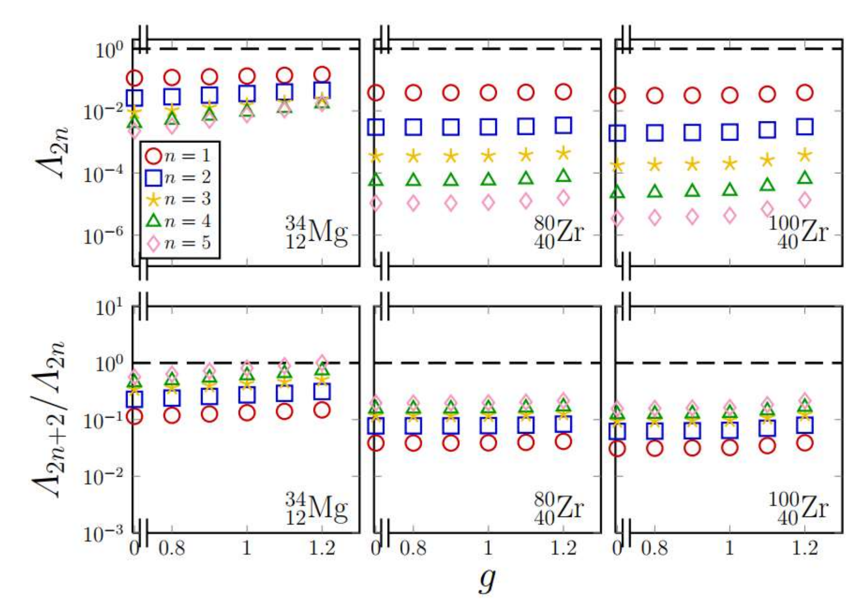
Influence of higher-order terms in cumulant expansion:

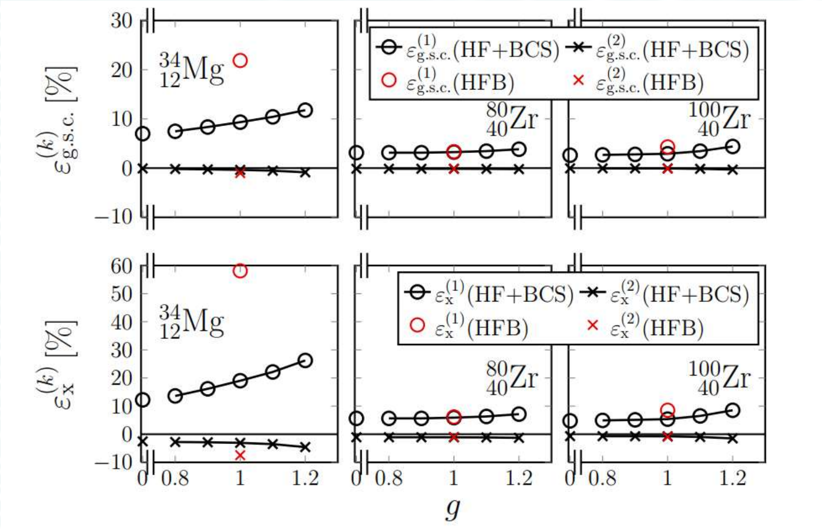
Introduce the quantities to describe the fraction of higher-order contribution

$$\varepsilon^{(k)}_{\mathrm{g.s.c.}} := \frac{-\sum_{n=1}^{k} s_{2n}\Lambda_{2n} - \Delta E_{\mathrm{g.s.c.}}}{\Delta E_{\mathrm{g.s.c.}}},$$

$$\varepsilon^{(k)}_{\mathrm{x}} := \frac{3\sum_{n=1}^{k} s_{2n}\left[-\frac{1}{2}(\Lambda_{2n+2} - \Lambda_{2n}\Lambda_2)\right] - E_{\mathrm{x}}(2^+)}{E_{\mathrm{x}}(2^+)}.$$

where $\Delta E_{\mathrm{g.s.c.}} := \langle \Phi_0 | \hat{H}' | \Phi_0 \rangle - \langle 0 | \hat{H}' | 0 \rangle = -\sum_{n=1}^{\infty} s_{2n}\Lambda_{2n}.$

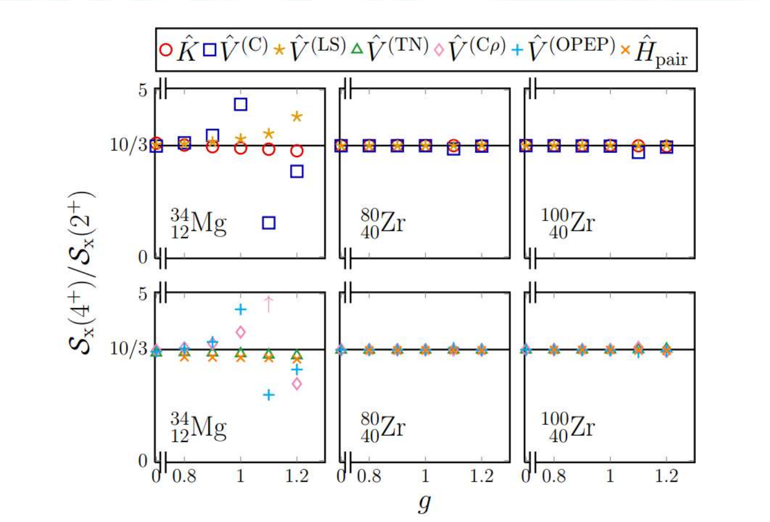


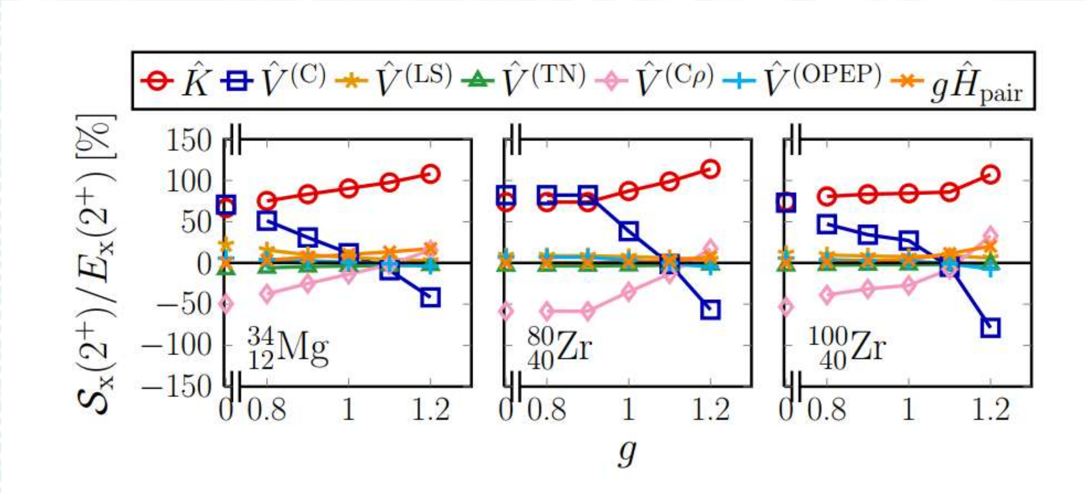


For $^{80}_{40}Zr$, $^{100}_{40}Zr$ nuclei the contributions of the higher- s_{2n} terms are negligible, but not for $^{34}_{12}Mg$.

result

contribution of constituent terms of effective Hamiltonian $\hat{\mathcal{S}} \in \{\hat{H}', \hat{K}, \hat{V}^{(\mathrm{C})}, \hat{V}^{(\mathrm{LS})}, \hat{V}^{(\mathrm{TN})}, \hat{V}^{(\mathrm{C}\rho)}, \hat{V}^{(\mathrm{OPEP})}, \hat{H}_{\mathrm{pair}}\}.$

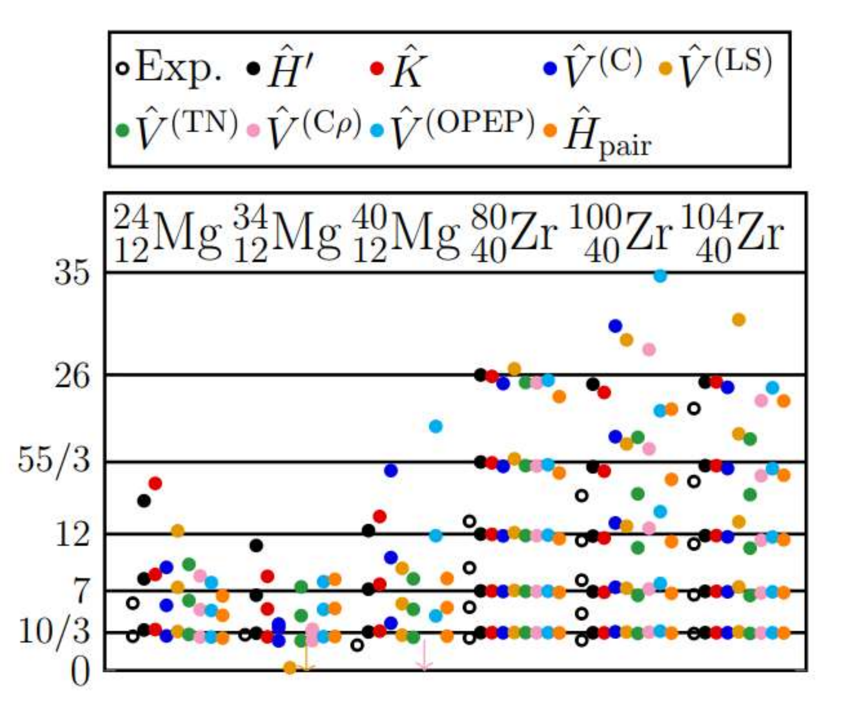


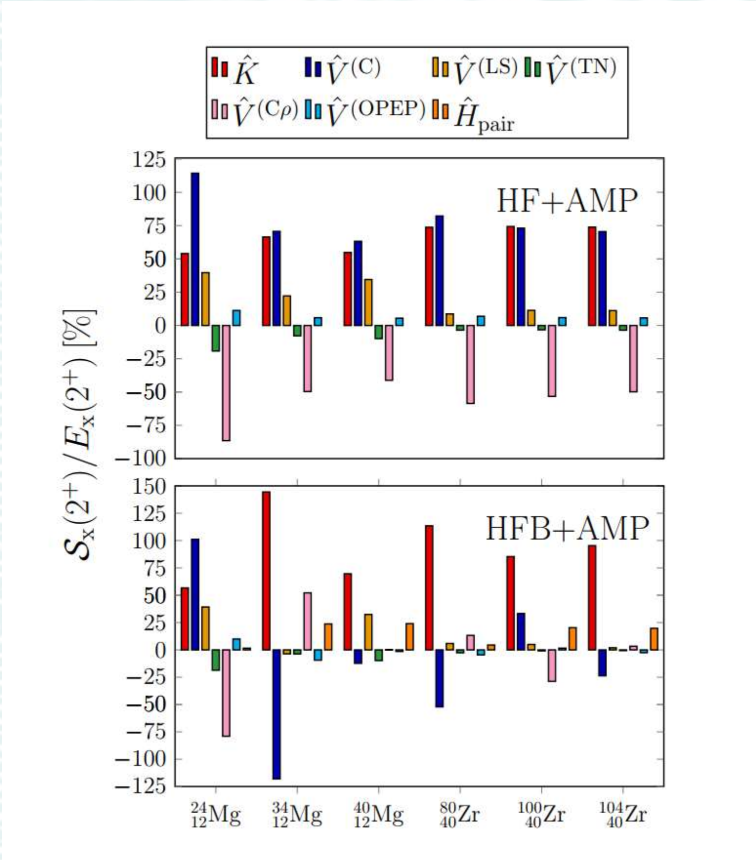


Also indicated that higher- s_{2n} terms are not negligible for $^{34}_{12}Mg$

Even the signs of $H^{pair}, V^{C}, V^{(\mathrm{C}\rho)}$ are inverted near g = 1.1. As g increases, the contribution of gH^{pair} to the rotational energy is enhanced, which is dominated by the central force, also the contributions of the kinetic energies increase result

contribution of constituent terms of effective Hamiltonian (calculation with HFB states)

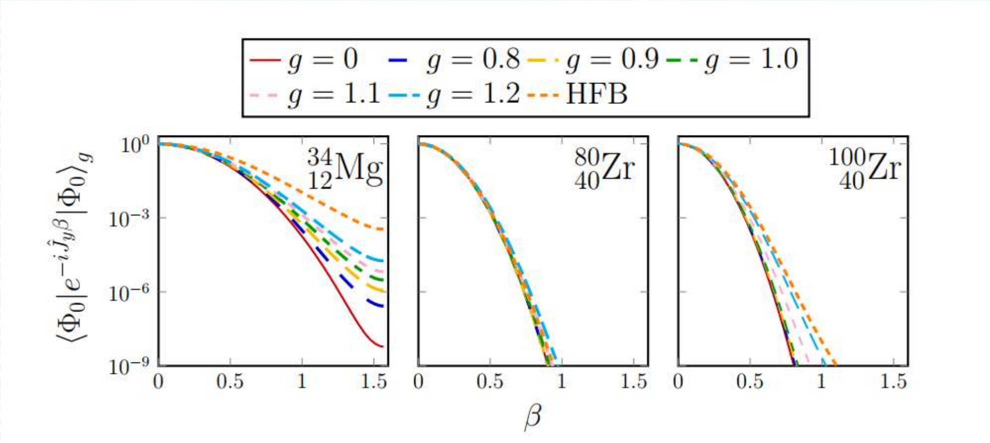




The contribution of the kinetic energy is large.

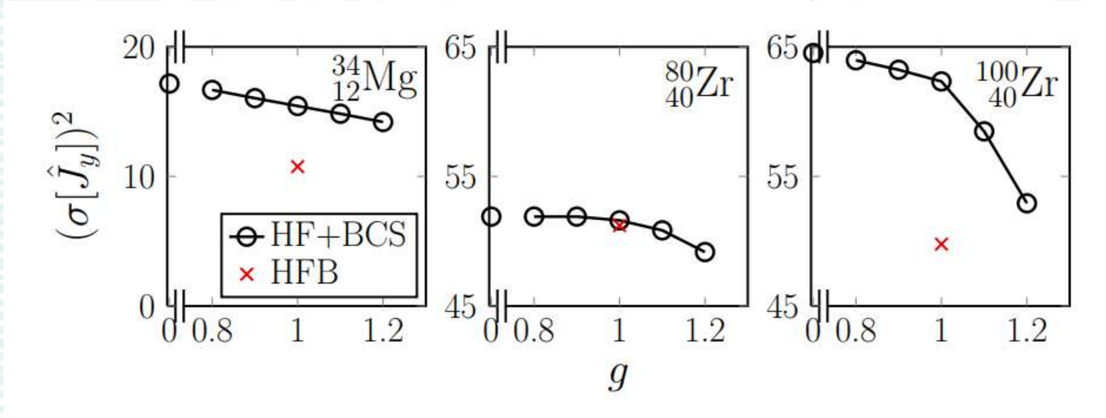
result

Angle dependence of integrands



$^{80}_{40}Zr$, $^{100}_{40}Zr$ have sharp peaks near β=0， and become slightly broader as g increases, where is different with $^{34}_{12}Mg$

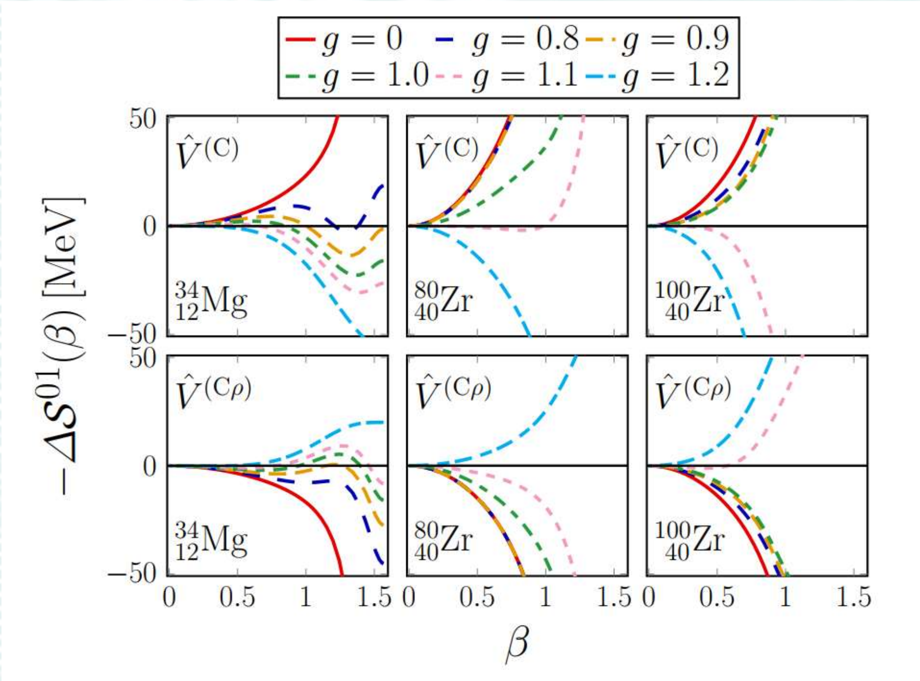
curvature
$$-\frac{d^2}{d\beta^2}\langle\Phi_0|e^{-i\hat{J}_y\beta}|\Phi_0\rangle\Big|_{\beta=0}=(\sigma[\hat{J}_y])^2.$$

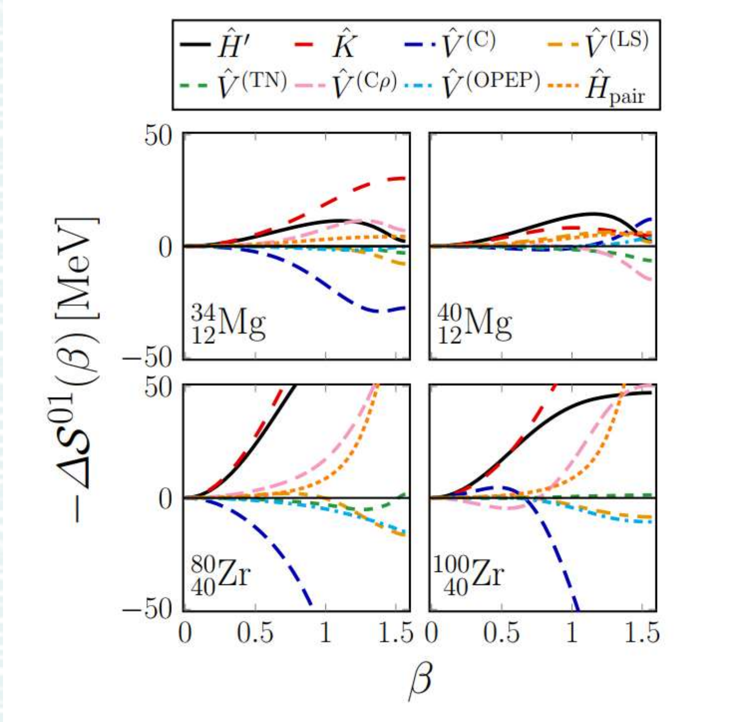


result

investigate the inversion near g = 1.1 for $V^C, V^{(\mathrm{C}_\rho)}$

$$\Delta\mathcal{S}^{01}(\beta) := \mathcal{S}^{01}(\beta) - \mathcal{S}^{01}(\beta = 0)$$





As g increases, the behavior of - ΔS^{01}(β) drastically changes, The signs changes from positive (negative) to negative (positive) for S = V^C ($V^{(\mathrm{C}_\rho)}$)

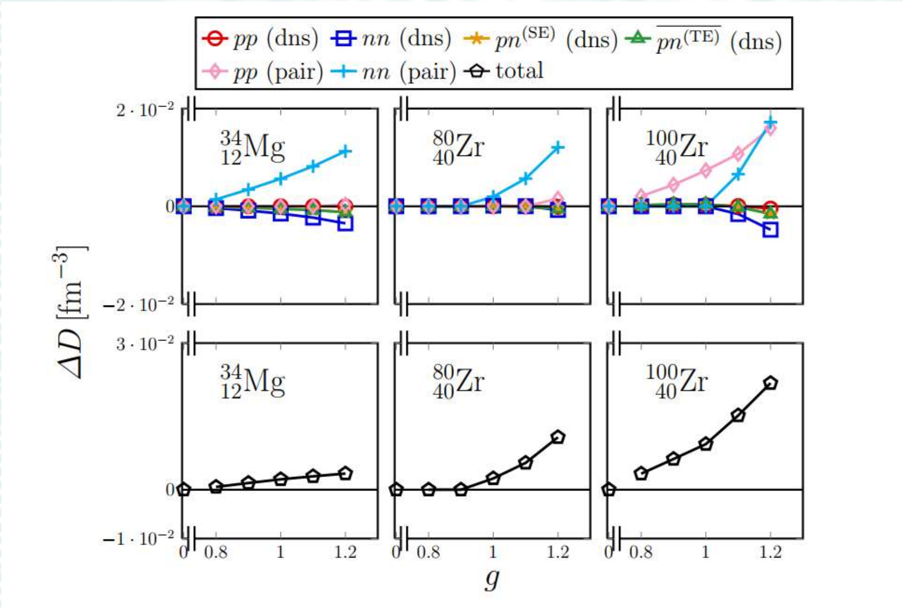
HFB solutions

result

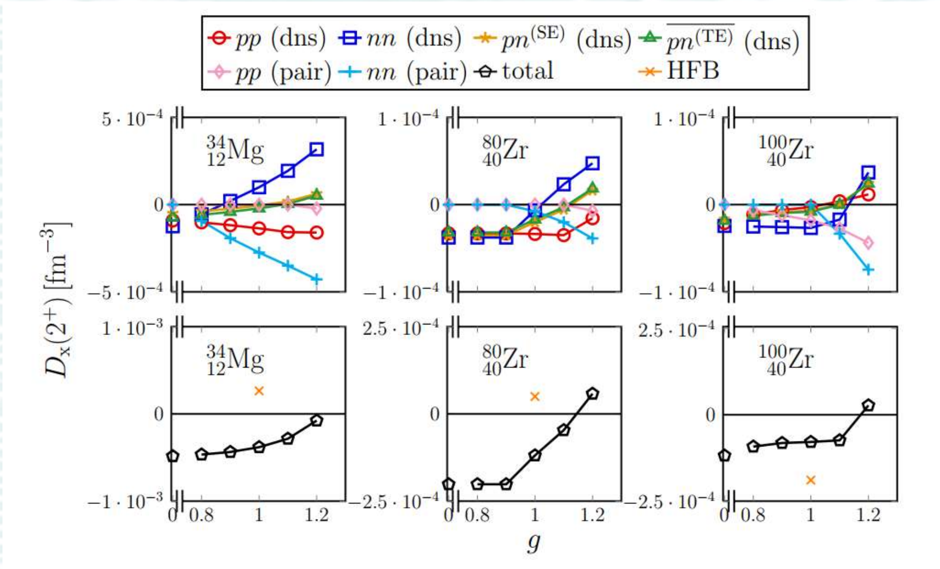
Degree of proximity for nucleons associated with nucleonic interaction

Introduce $\Delta D := \langle \Phi_0|\hat{D}|\Phi_0\rangle_g - \langle \Phi_0|\hat{D}|\Phi_0\rangle_{g=0}$ to describe how pair effect proximity of nucleons

$$D_x(J^+) := \langle J|\hat{D}|J\rangle - \langle 0|\hat{D}|0\rangle ,$$



The black pentagons in the lower panels are the total values of ΔD



For the HF solutions, the $D_x(2^+)$ values are negative. This means that the DoP decreases and the nucleons slightly spread as J goes up. It inverses when g go large.

Conclusion

· Due to the pair correlations, the compositions of the pure rotational energy drastically change, sometimes inverting their signs, and depend strongly on nuclides even for the well-deformed nuclei.

· When the pairing becomes stronger, the contributions of the kinetic energies increase.

· The nucleons slightly spread as J increases at the HF level, while the pair correlations can reduce or invert the effect.

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