

# 利用投影的多维形状约束协变密度 泛函理论研究 $^{96}\text{Zr}$ 的八极关联

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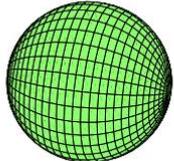
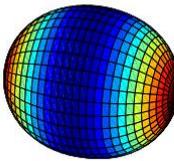
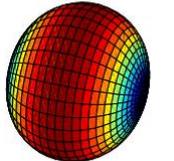
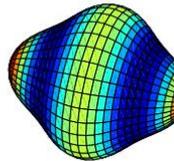
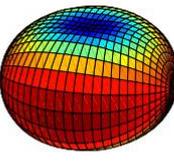
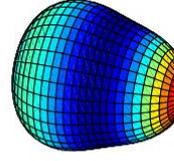
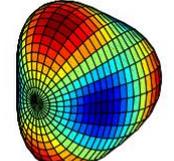
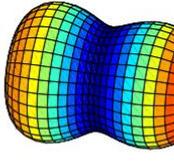
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- 研究背景和意义
- p-MDCRHB模型
- 结果和讨论
- 总结和展望

# 原子核的形状

原子核形变参数可通过表面多极展开定义：

$$R(\theta, \varphi) = R_0 \left[ 1 + \beta_{00} + \sum_{\lambda=1}^{\infty} \sum_{\mu=-\lambda}^{\lambda} \beta_{\lambda\mu}^* Y_{\lambda\mu}(\theta, \varphi) \right].$$

(a) $\beta_{\lambda\mu} = 0$	(b) $\beta_{20} > 0$	(c) $\beta_{20} < 0$	(d) $\beta_{40} > 0$
			
(e) $\beta_{22} \neq 0$	(f) $\beta_{30} \neq 0$	(g) $\beta_{32} \neq 0$	(h) $\beta_{20} \gg 0$
			

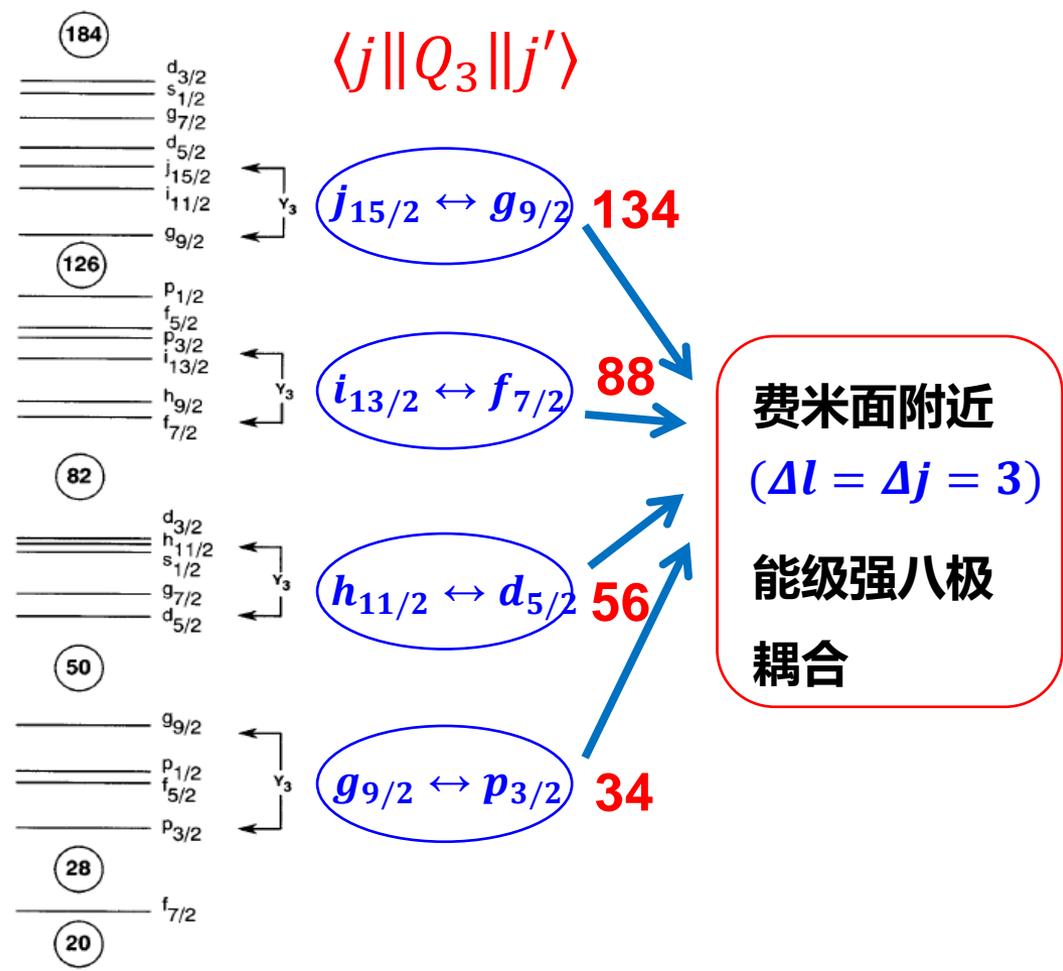
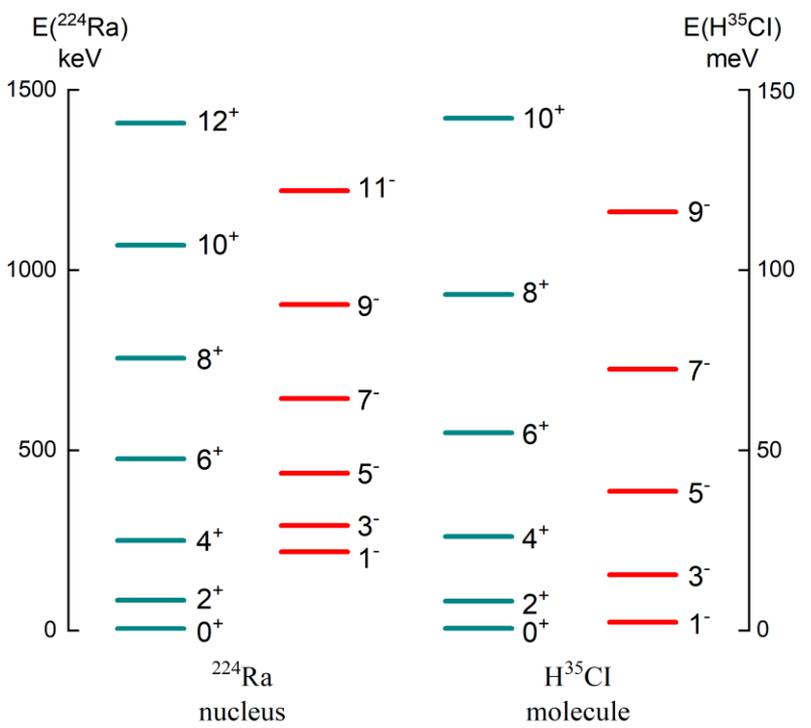
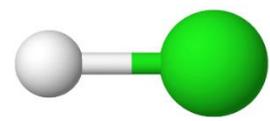
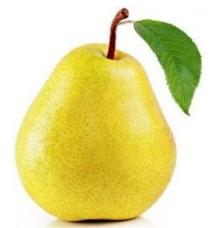
Bing-Nan Lu, 2012

大多数原子核是轴对称形变

一些原子核 ( $^{224}\text{Ra}$ ,  $^{144}\text{Ba}$ ,  $^{146}\text{Ba}$ ,  $^{228}\text{Th}$ ) 表现出八极形变

# 原子核的八极关联/形变

From Z.P. Li



Asaro et. al., PR 92, 1495 (1953).  
 Stephens et. al., PR100, 1543 (1955).  
 Lee & Inglis, PR 108, 774 (1957).

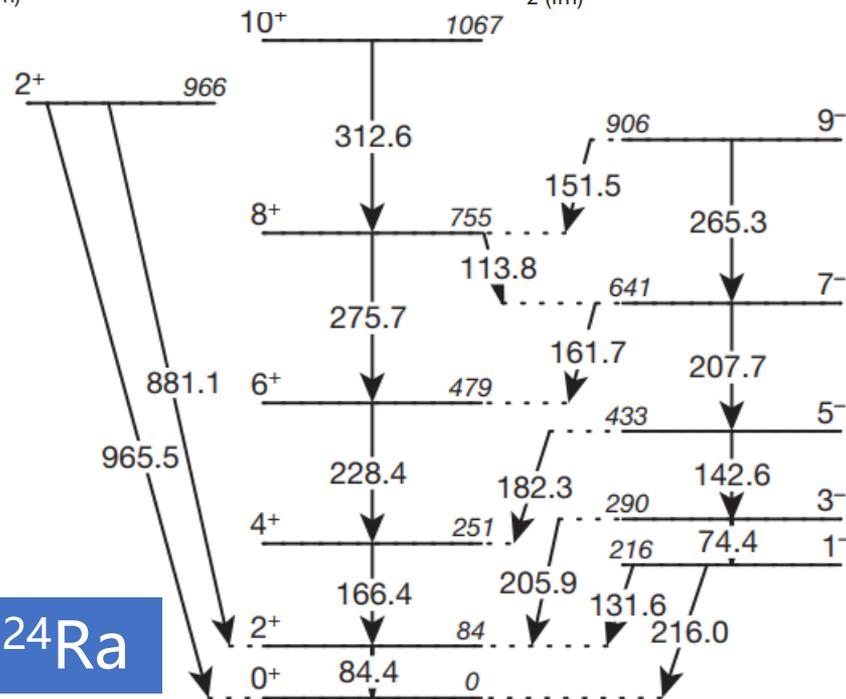
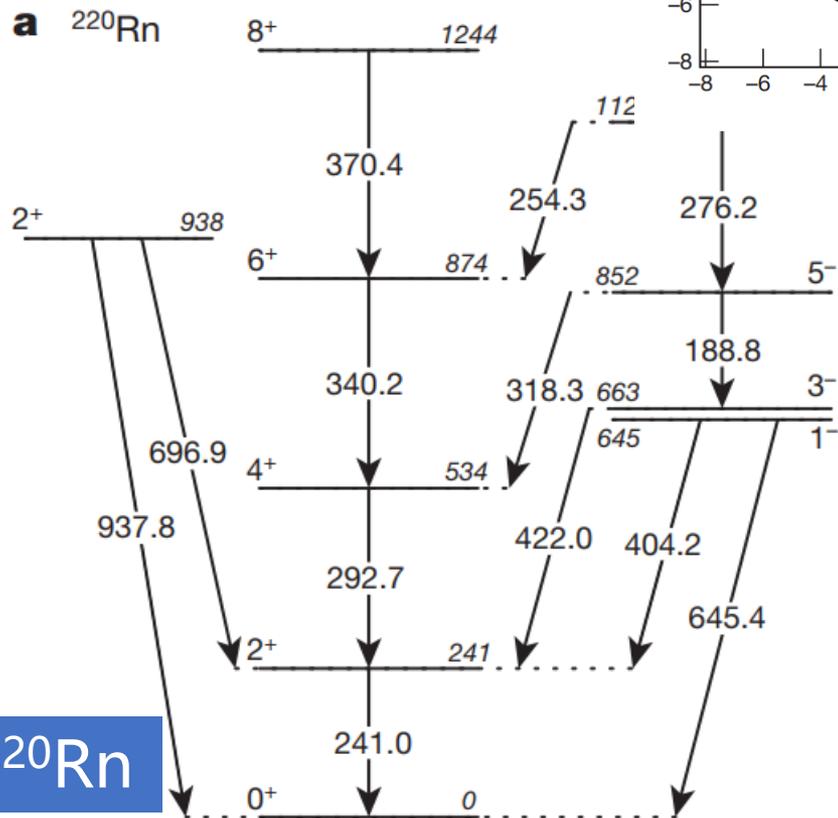
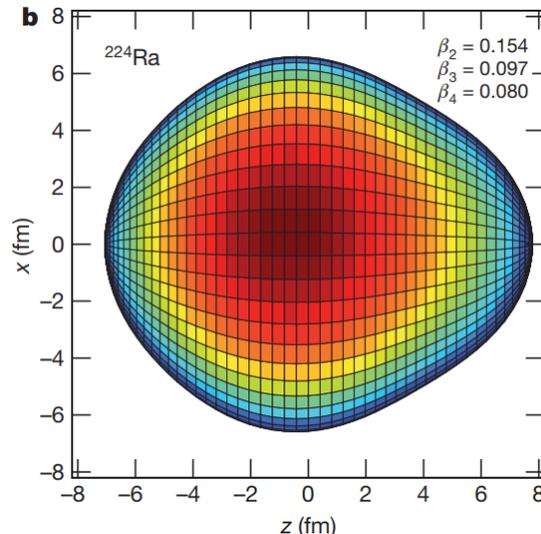
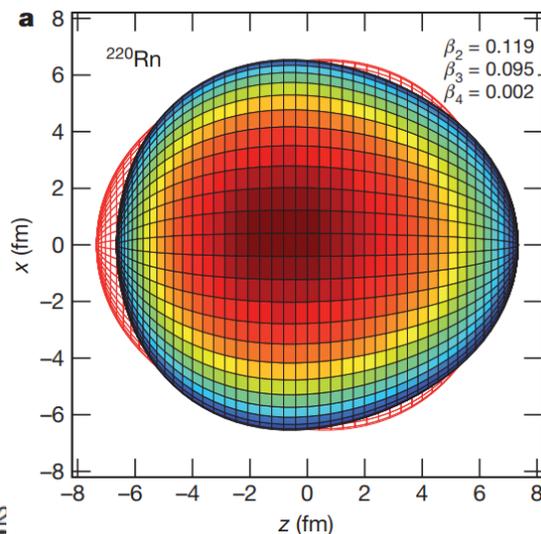
Butler & Nazarewicz, RMP68, 349 (1996).

# 原子核的八极关联/形变

转动谱,  $B(E3)$

八极振动 & 稳定八极形变

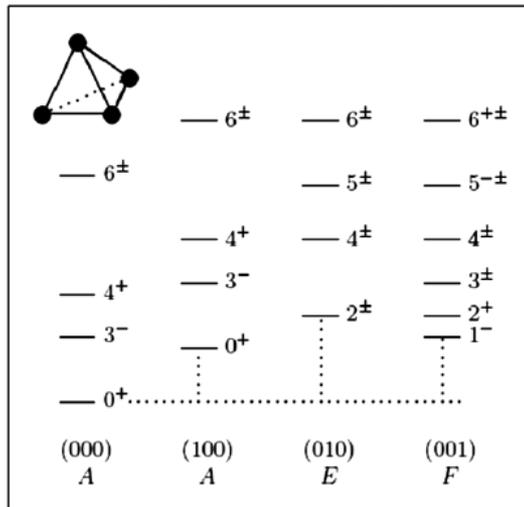
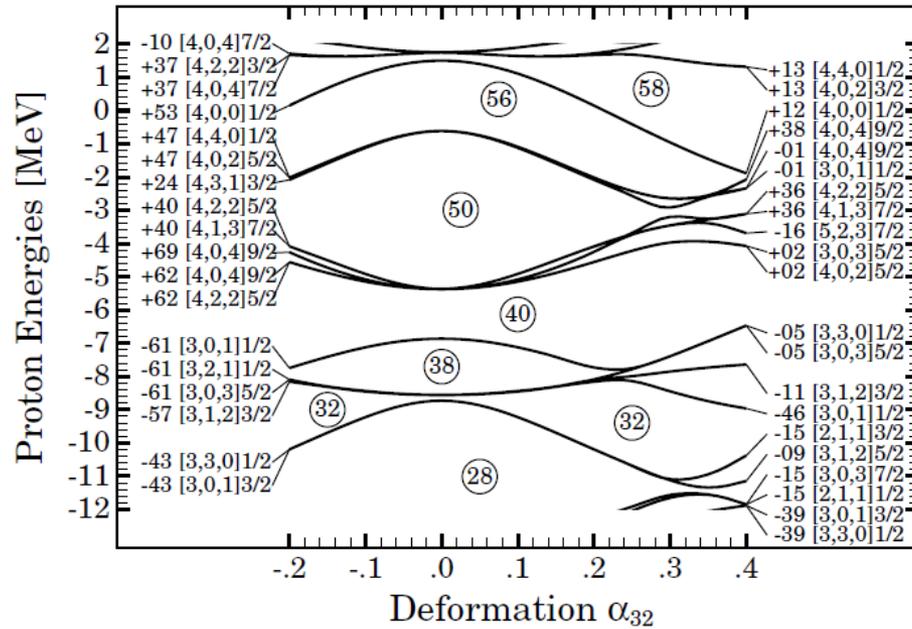
L. P. Gaffney, P. A. Butler, M. Scheck et al., Nature 497 (2013) 199.



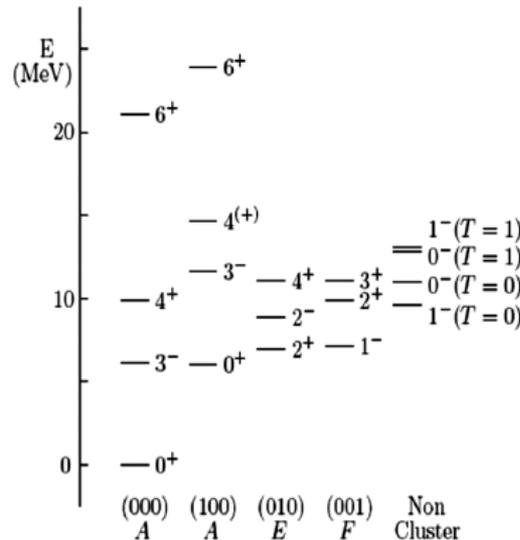
$^{220}\text{Rn}$

$^{224}\text{Ra}$

# 原子核的八极关联/形变



low-lying spectrum of  $^{16}\text{O}$

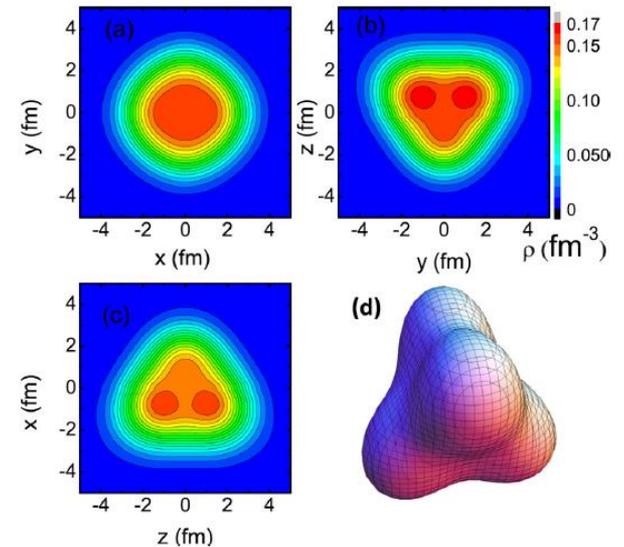


Bijker & Iachello, PRL 112 (2014) 152501.<sup>6</sup>

$T_D^d$  symmetry

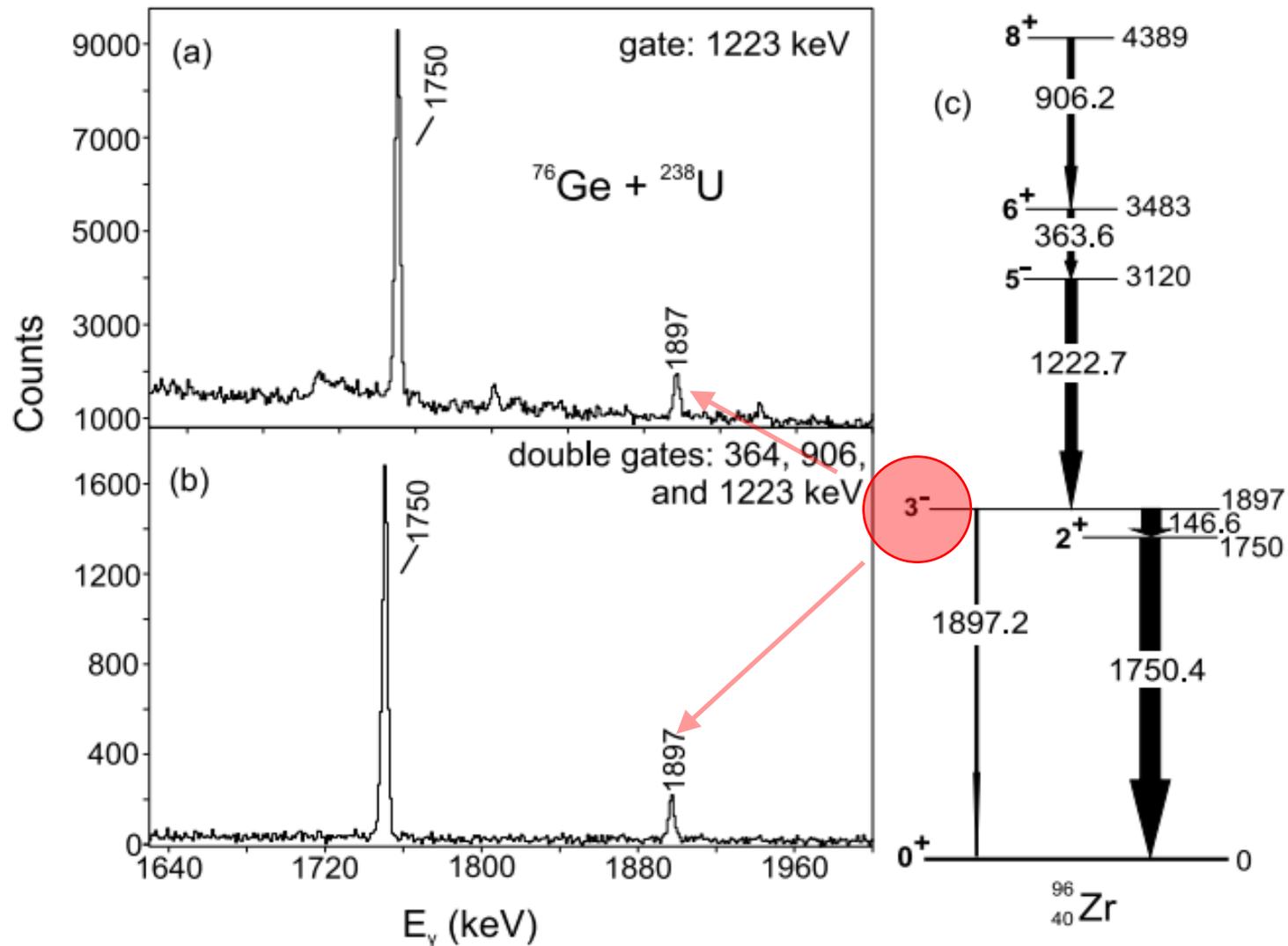
Tetrahedral magic numbers:  
16, 20, 32, 40, 56, 64, 70, 90,  
112 and 136

Dudek et al., PRL 88 (2002) 252502.  
Dudek et al., PS 89 (2014) 054007.



Wang et al., PLB 790 (2019) 498.

# $^{96}\text{Zr}$ 形状的实验研究



L.W. Iskra, R. Broda, R.V.F. Janssens et al., PLB 788 (2019) 396.

重离子碰撞实验提取原子核形变信息:

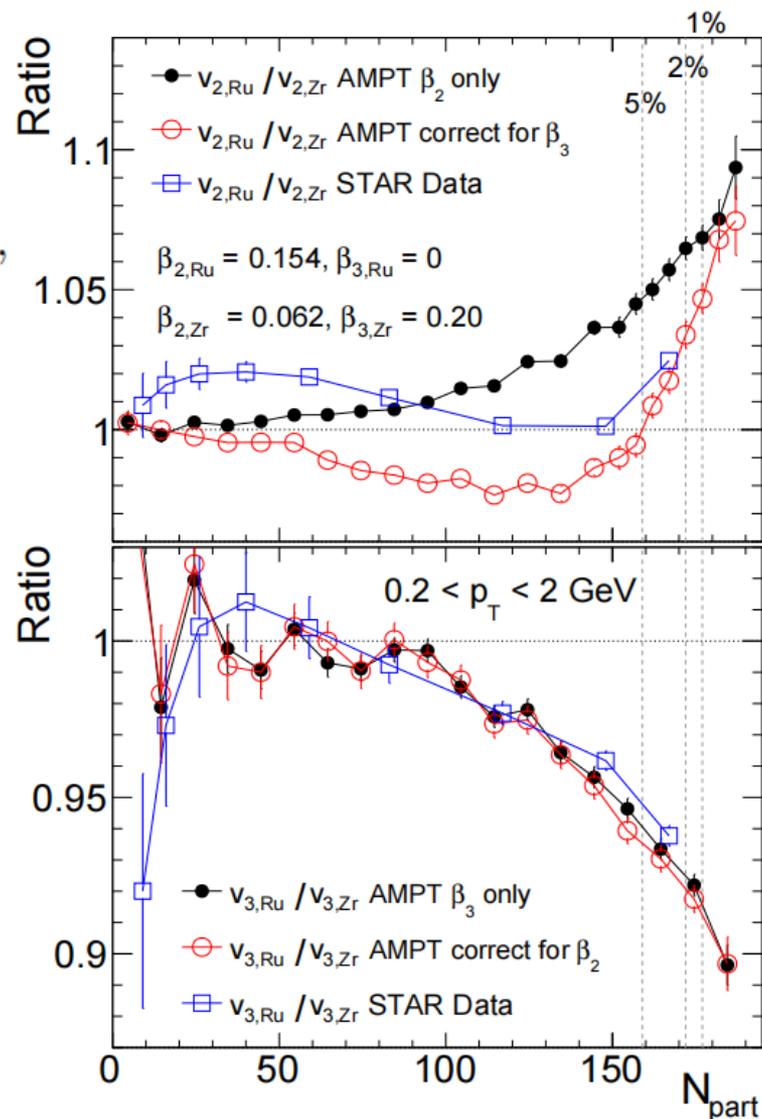
$$\varepsilon_n^2 = a'_n + \sum_{m,k=2}^4 b'_{n;mk} \beta_m \beta_k, \quad v_n^2 = a_n + \sum_{m,k=2}^4 b_{n;mk} \beta_m \beta_k,$$

$$\frac{\varepsilon_{n,Y}^2}{\varepsilon_{n,X}^2} = 1 + \frac{b'_n}{a'_n} (\beta_{n,Y}^2 - \beta_{n,X}^2) / (1 + \frac{b'_n}{a'_n} \beta_{n,X}^2)$$

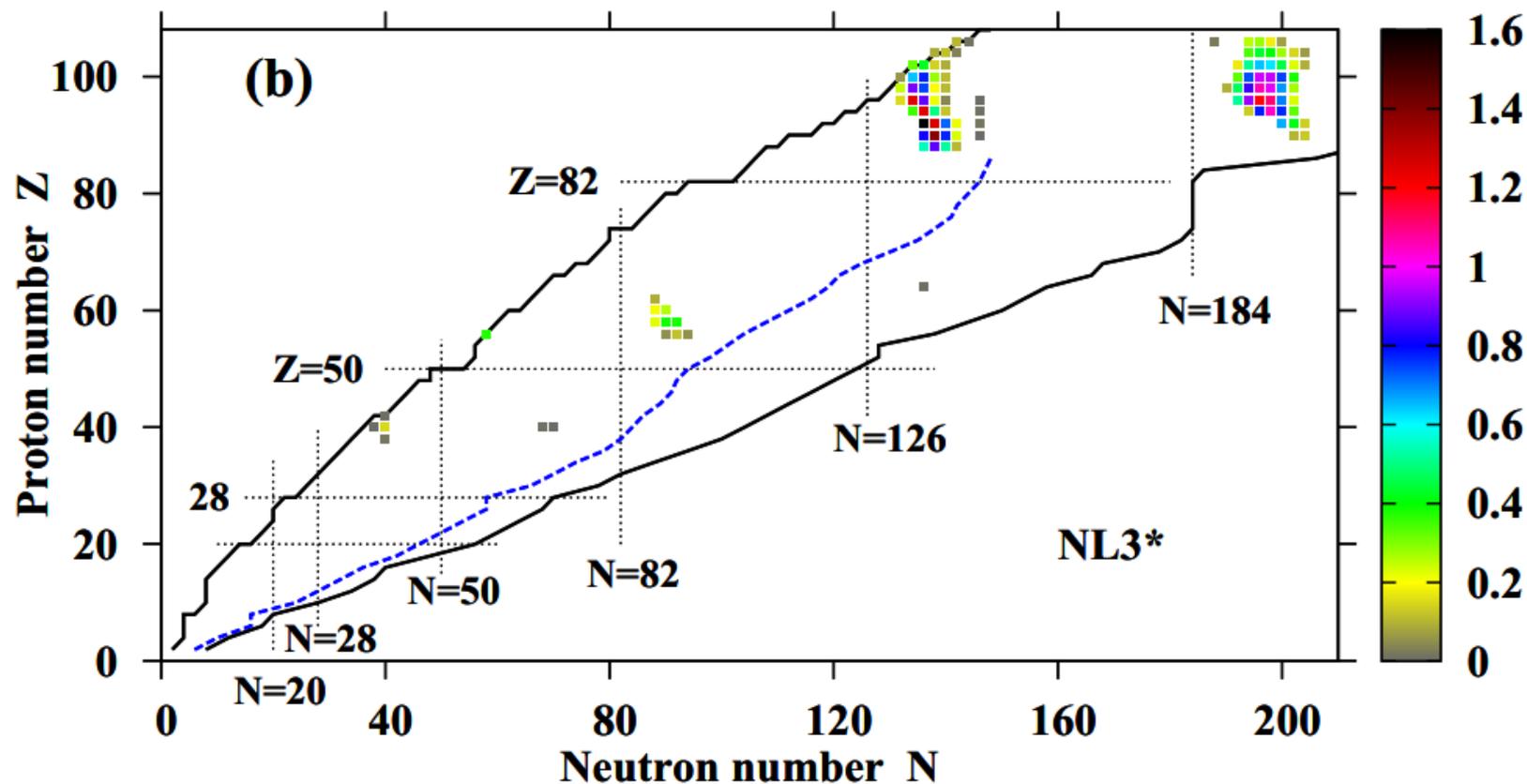
$$\approx 1 + \frac{b'_n}{a'_n} (\beta_{n,Y}^2 - \beta_{n,X}^2),$$

$$\frac{v_{n,Y}^2}{v_{n,X}^2} = 1 + \frac{b_n}{a_n} (\beta_{n,Y}^2 - \beta_{n,X}^2) / (1 + \frac{b_n}{a_n} \beta_{n,X}^2)$$

$$\approx 1 + \frac{b_n}{a_n} (\beta_{n,Y}^2 - \beta_{n,X}^2).$$



平均场模型计算得到的基态没有八极形变.

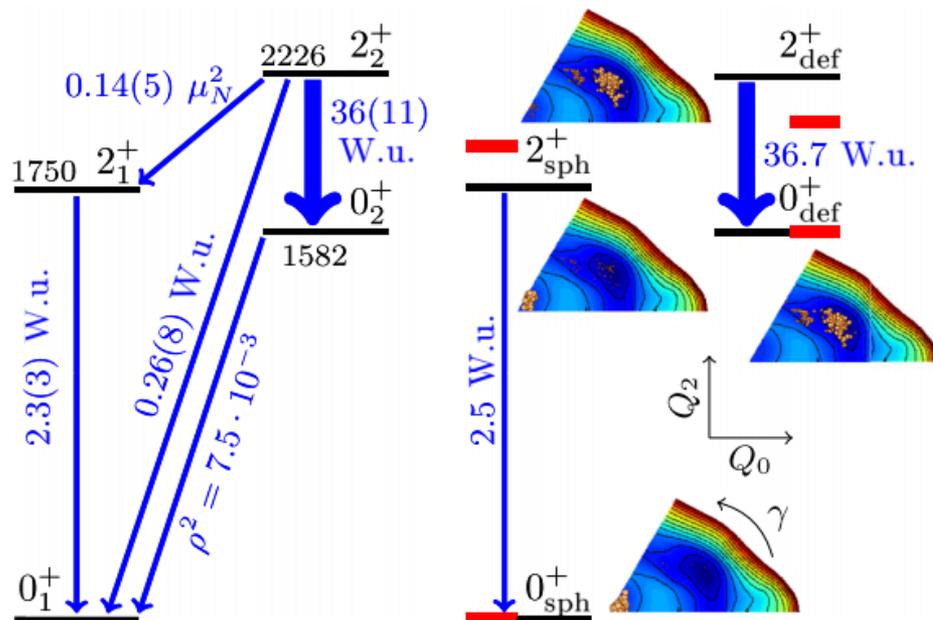


$$\Delta E_{\text{oct}} = E^{\text{oct}}(\beta_2, \beta_3) - E^{\text{quad}}(\beta'_2, \beta'_3 = 0)$$

S. E. Agbemava, A. V. Afanasjev, P. Ring, PRC 93 (2016) 044304.

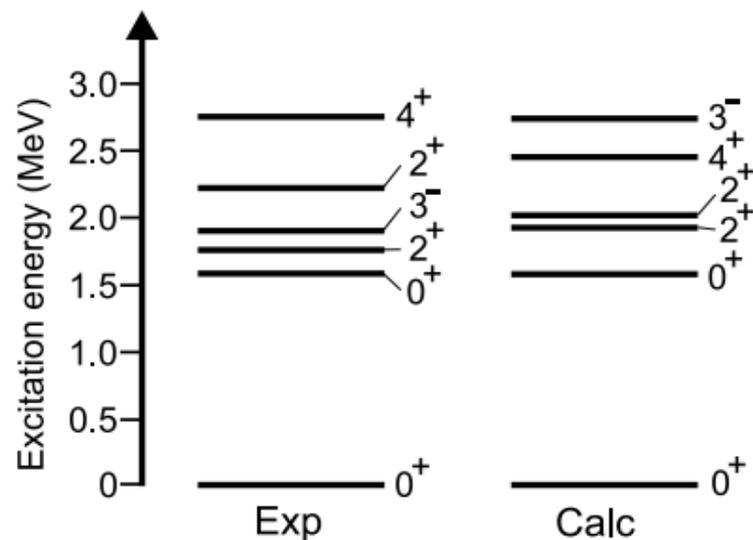
# $^{96}\text{Zr}$ 形状的理论研究

三轴形变的壳模型计算表明 $^{96}\text{Zr}$ 的低激发态存在球形和三轴形变的形状共存, 基态带为球形振动带



C. Kremer, S. Aslanidou, S. Bassauer et al., PRL 117 (2016) 172503.

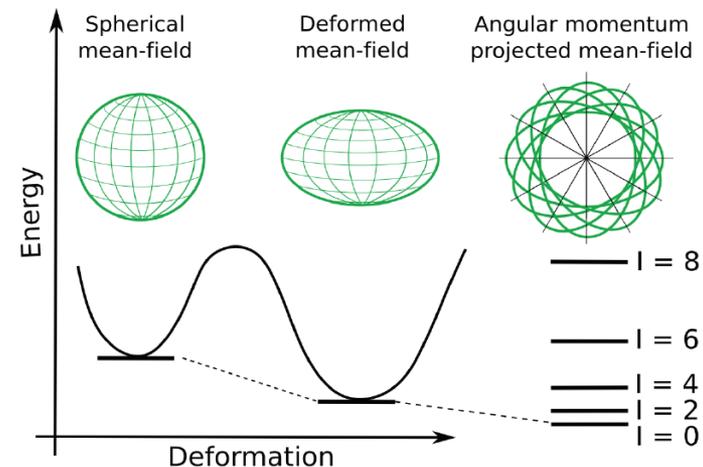
八极形变的 MCSM 给出的  $B(E3:3^- \rightarrow 0^+) = 46.6 \text{ W. u.}$  和实验值  $42(3) \text{ W.u.}$  很接近, 但  $3^-$  激发能偏高



L.W. Iskra, R. Broda and R.V.F. Janssens et al., PLB 788 (2019) 396.

# 基于密度泛函方法研究原子核低激发谱

- 静态平均场模型不能用于描述原子核激发态
- 投影+GCM是原子核谱学研究的常用方法 (PAV)
- 基于相对论平均场的投影+GCM方法:



Basis	$(\beta_{20})$	$(\beta_{20}, \beta_{22})$	$(\beta_{20}, \beta_{30})$	$(\beta_{20}, \beta_{22}, \beta_{30}, \beta_{32})$
HO基展开	Niksic_Vretnar(2006) RMF+BCS+AMP+GCM	Yao_Meng_Ring_Arteaga(2009) (RMF+BCS+AMP+GCM)	Yao_Zhou_Li(2015) RMF+BCS+AMP+PP+PNP+GCM	Wang_Lv(2022) RHB+AMP+P
WS基展开	Sun_Zhou(2021) RHB+AMP	×	×	×

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构造点耦合的拉氏量：

$$\mathcal{L} = \mathcal{L}^{\text{free}} + \mathcal{L}^{4\text{f}} + \mathcal{L}^{\text{hot}} + \mathcal{L}^{\text{der}} + \mathcal{L}^{\text{em}}$$

$$\mathcal{L}^{\text{free}} = \bar{\psi}(i\gamma_{\mu}\partial^{\mu} - m)\psi$$

$$\begin{aligned} \mathcal{L}^{4\text{f}} = & -\frac{1}{2}\alpha_S(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\bar{\psi}\gamma_{\mu}\psi)(\bar{\psi}\gamma^{\mu}\psi) \\ & - \frac{1}{2}\alpha_{TS}(\bar{\psi}\vec{\tau}\psi)(\bar{\psi}\vec{\tau}\psi) - \frac{1}{2}\alpha_{TV}(\bar{\psi}\vec{\tau}\gamma_{\mu}\psi)(\bar{\psi}\vec{\tau}\gamma^{\mu}\psi) \end{aligned}$$

$$\begin{aligned} \mathcal{L}^{\text{der}} = & -\frac{1}{2}\delta_S\partial_{\nu}(\bar{\psi}\psi)\partial^{\nu}(\bar{\psi}\psi) - \frac{1}{2}\delta_V\partial_{\nu}(\bar{\psi}\gamma_{\mu}\psi)\partial^{\nu}(\bar{\psi}\gamma^{\mu}\psi) \\ & - \frac{1}{2}\delta_{TS}\partial_{\nu}(\bar{\psi}\vec{\tau}\psi)\partial^{\nu}(\bar{\psi}\vec{\tau}\psi) \\ & - \frac{1}{2}\delta_{TV}\partial_{\nu}(\bar{\psi}\vec{\tau}\gamma_{\mu}\psi)\partial^{\nu}(\bar{\psi}\vec{\tau}\gamma_{\mu}\psi), \end{aligned}$$

$$\mathcal{L}^{\text{hot}} = -\frac{1}{3}\beta_S(\bar{\psi}\psi)^3 - \frac{1}{4}\gamma_S(\bar{\psi}\psi)^4 - \frac{1}{4}\gamma_V[(\bar{\psi}\gamma_{\mu}\psi)(\bar{\psi}\gamma^{\mu}\psi)]^2$$

$$\mathcal{L}^{\text{em}} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} - e\frac{1-\tau_3}{2}\bar{\psi}\gamma^{\mu}\psi A_{\mu}$$

Relativistic Hartree Bogoliubov 方程:

$$\int d^3 \mathbf{r}' \begin{pmatrix} \hat{h} - \lambda & \Delta \\ -\Delta^* & -\hat{h} + \lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

$$\hat{h}(\mathbf{r}) = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta (M + S(\mathbf{r})) + V(\mathbf{r}),$$

$$\Delta(\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2) = \int d^3 \mathbf{r}'_1 d^3 \mathbf{r}'_2 \sum_{\sigma'_1 \sigma'_2} V(\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2, \mathbf{r}'_1 \sigma'_1, \mathbf{r}'_2 \sigma'_2) \kappa(\mathbf{r}'_1 \sigma'_1, \mathbf{r}'_2 \sigma'_2),$$

点耦合的矢量势和标量势:

$$S = \alpha_S \rho_S + \alpha_{TS} \vec{\rho}_{TS} + \beta_S \rho_S^2 + \gamma_S \rho_S^3 + \delta_S \Delta \rho_S + \delta_{TS} \vec{\rho}_{TS} \cdot \vec{\tau},$$

$$V = \alpha_V \rho_V + \alpha_{TV} \vec{\rho}_{TV} \cdot \vec{\tau} + \gamma_V \rho_V^3 + \delta_V \Delta \rho_V + \delta_{TV} \vec{\rho}_{TV} \cdot \vec{\tau}.$$

有限力程可分离对力:

$$V(\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2, \mathbf{r}'_1 \sigma'_1, \mathbf{r}'_2 \sigma'_2) = -G \delta(\mathbf{R} - \mathbf{R}') P(\mathbf{r}) P(\mathbf{r}') \frac{1 - P_\sigma}{2},$$

形变参数:

$$\beta_{\lambda\mu}^{\tau} = \frac{4\pi}{3N_{\tau}R^{\lambda}} Q_{\lambda\mu}^{\tau} \quad \longleftarrow \quad Q_{\lambda\mu}^{\tau} = \int d^3\mathbf{r} \rho_V^{\tau}(\mathbf{r}) r^{\lambda} Y_{\lambda\mu}(\Omega)$$

角动量和宇称投影:

$$|\Psi_{\alpha,q}^{JM\pi}\rangle = \sum_K f_{\alpha}^{JK\pi} \hat{P}_{MK}^J \hat{P}^{\pi} |\Phi(q)\rangle$$

$$\hat{P}_{MK}^J = \frac{2J+1}{8\pi^2} \int d\Omega D_{MK}^{J*}(\Omega) \hat{R}(\Omega)$$

$$\hat{P}^{\pi} = \frac{1}{2}(1 + \pi \hat{P})$$

粒子数约束:

$$\mathcal{H}' = \mathcal{H} - \lambda_p [Z(\mathbf{r}; q, q'; \Omega) - Z_0] - \lambda_n [N(\mathbf{r}; q, q'; \Omega) - N_0]$$

Hill-Wheeler 方程:

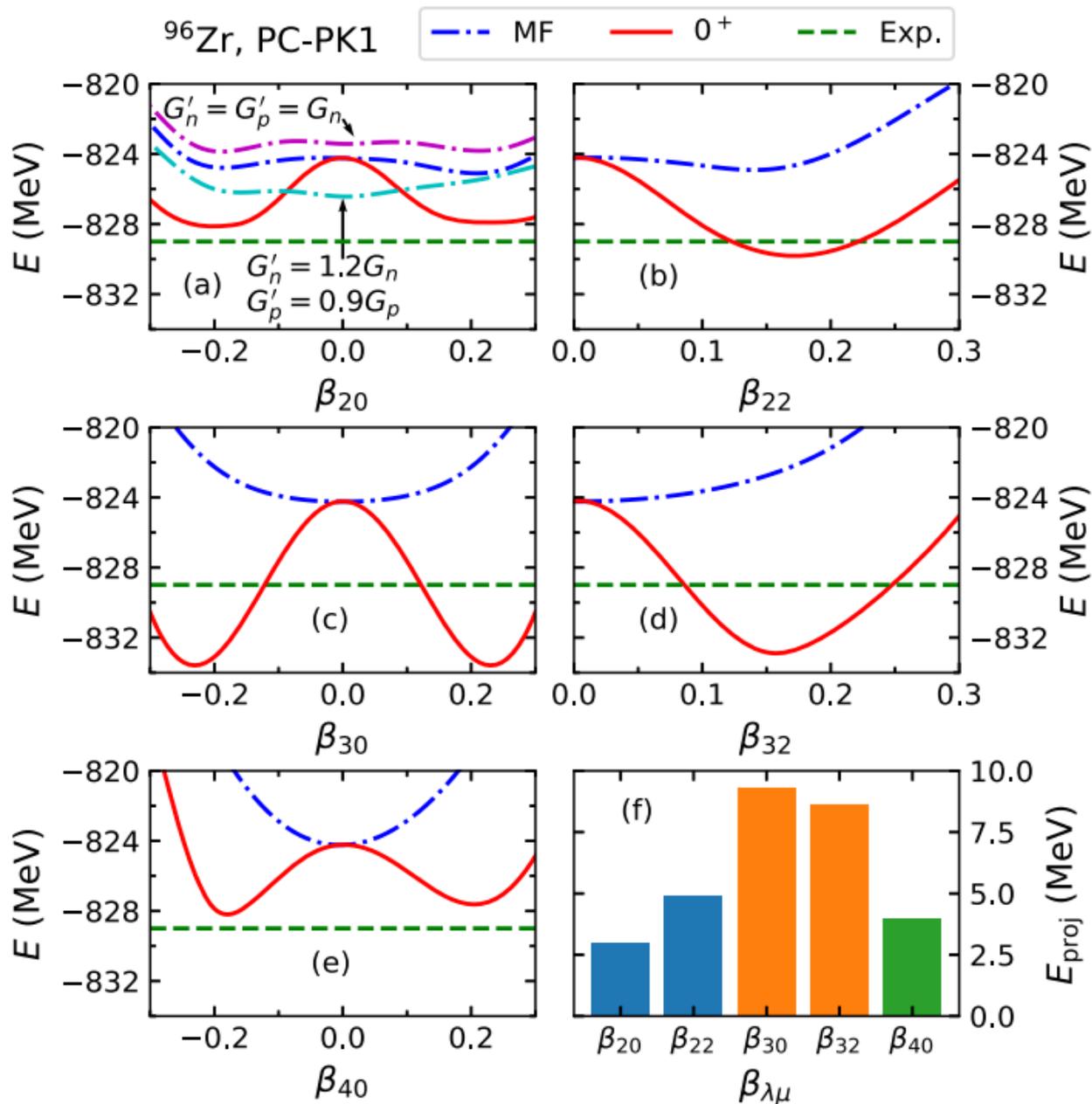
K. Wang and B.N. Lu, CTP 74  
(2022) 015303.

$$\sum_{K'} \left\{ \mathcal{H}'_{KK'}^{J\pi}(q; q) - E_{\alpha}^{J\pi} \mathcal{N}_{KK'}^{J\pi}(q; q) \right\} f_{\alpha}^{JK'\pi} = 0$$

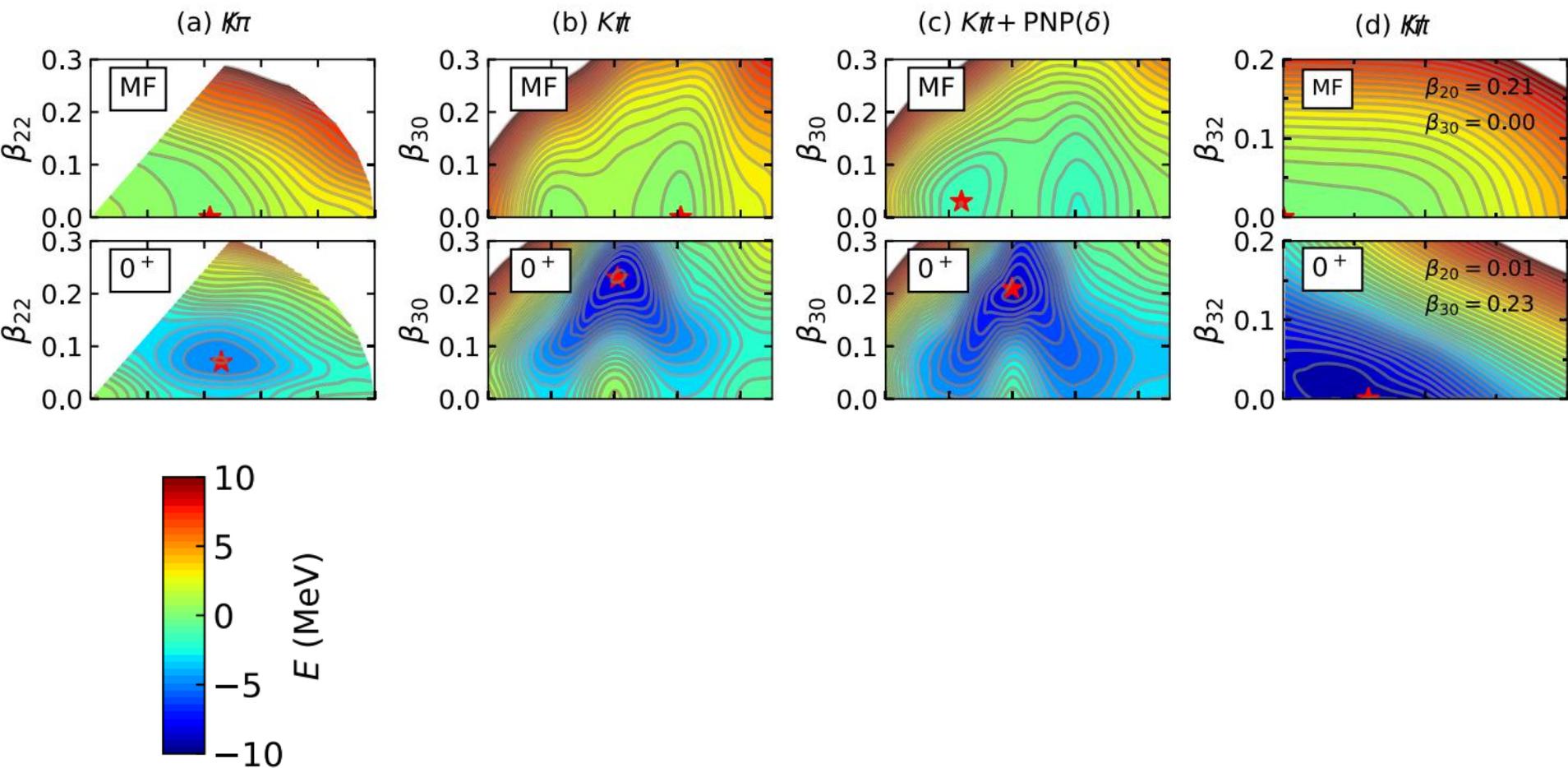
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# 各形变对结合能的影响 (1DPES)

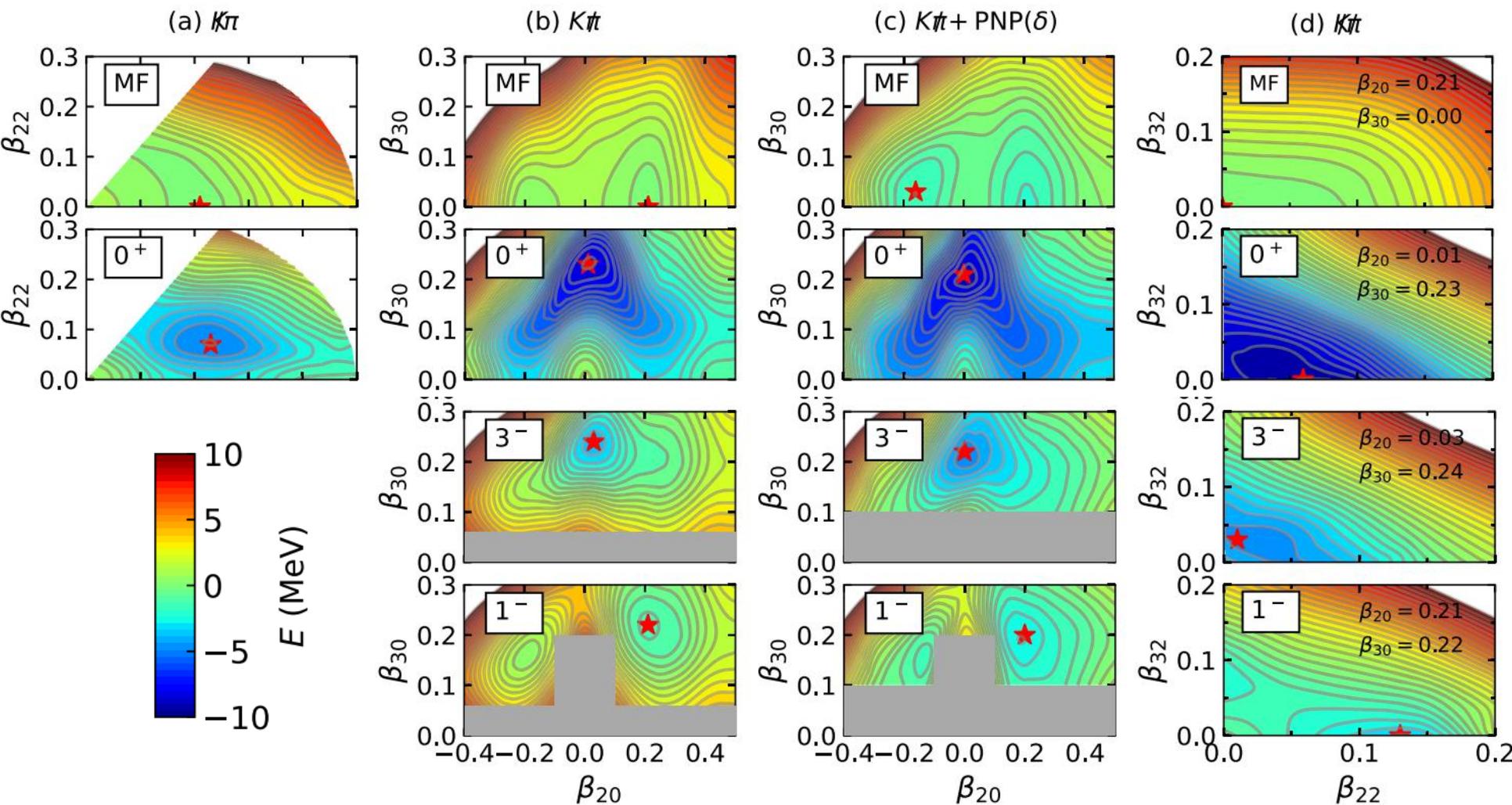


# $^{96}\text{Zr}$ 的基态和激发态 (2DPES)



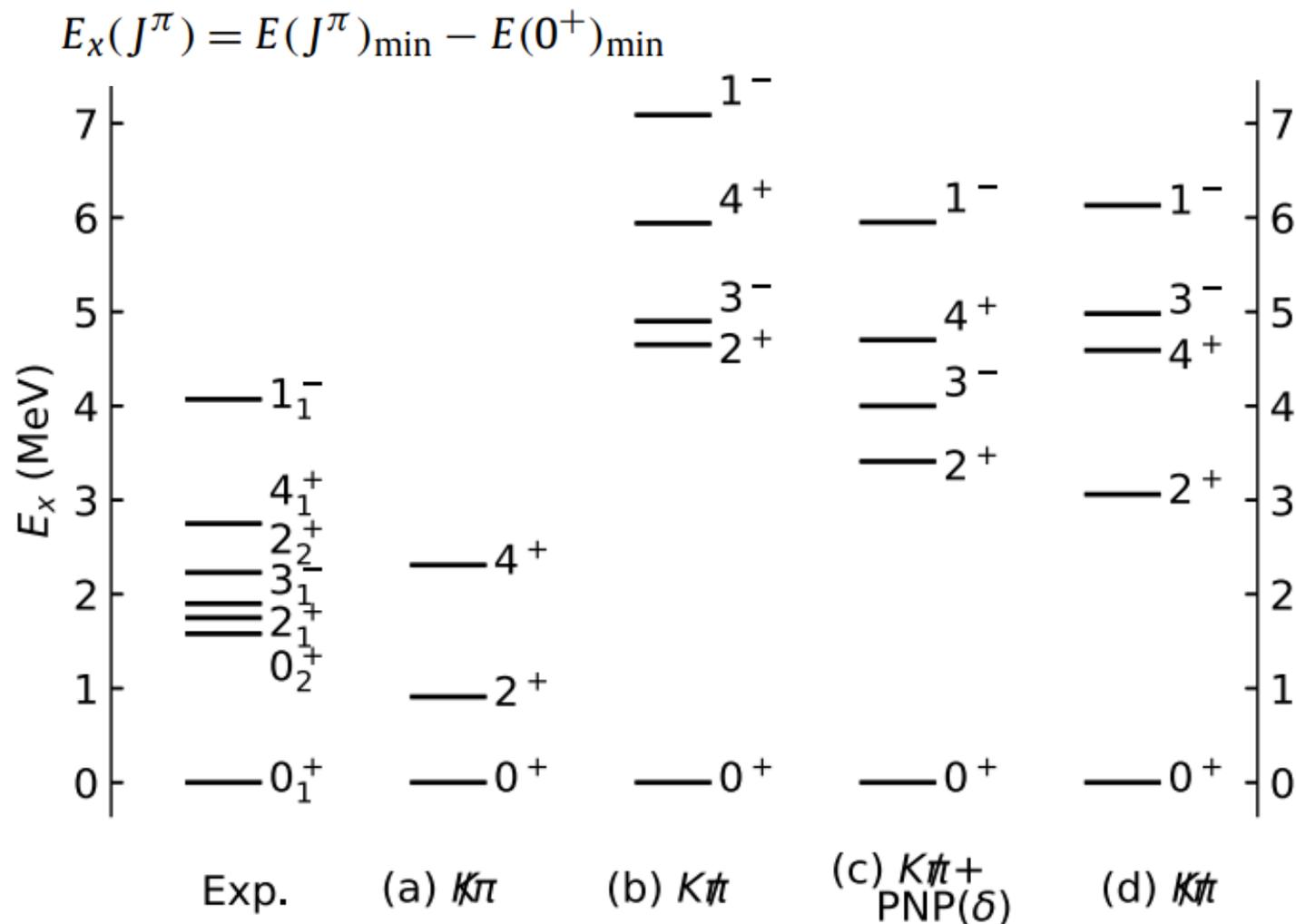
平均场层次下没有八极形变，投影给出的基态存在八极关联，需要打破轴对称和反射对称才能确定。

# $^{96}\text{Zr}$ 的基态和激发态 (2DPES)



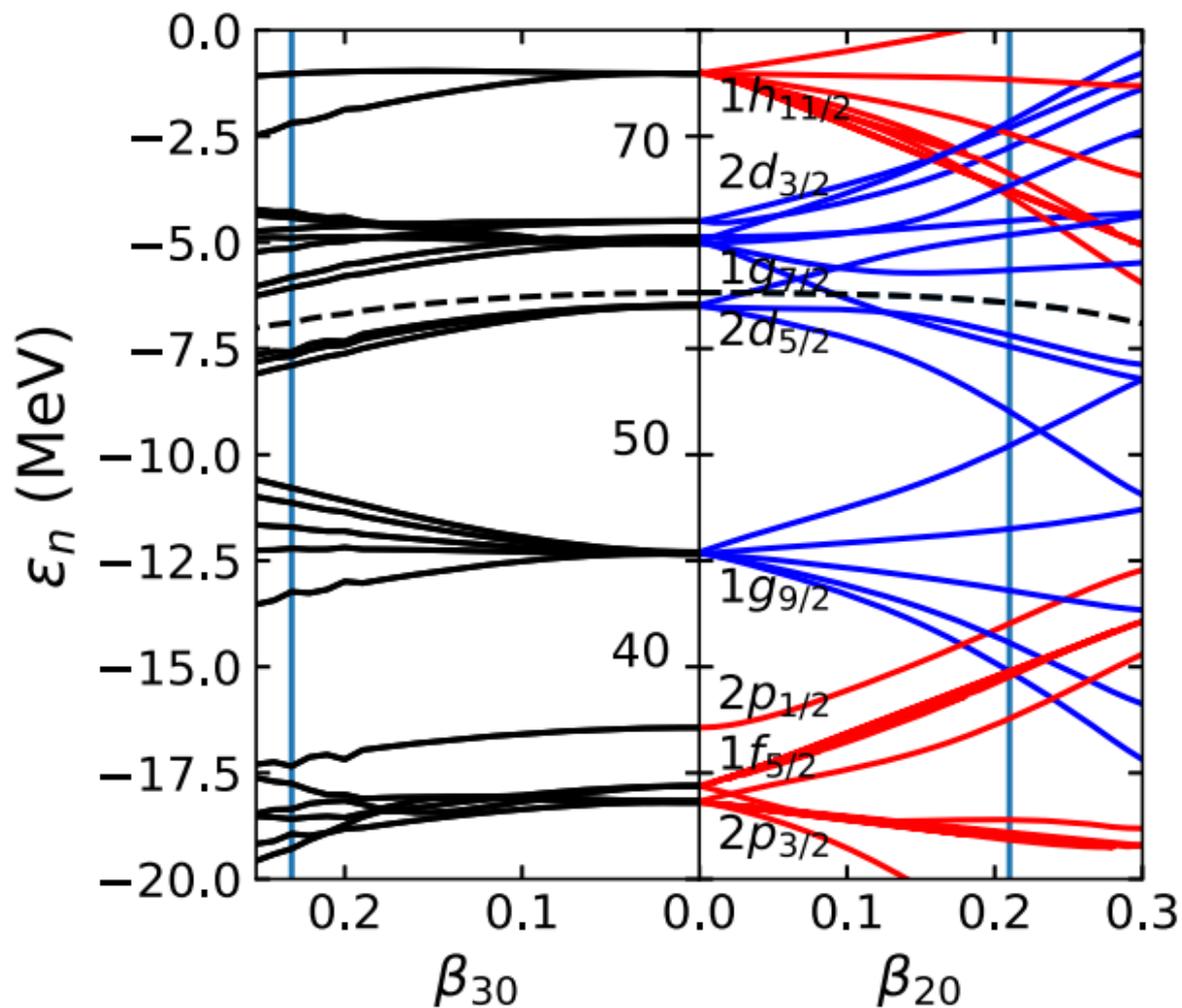
平均场层次下没有八极形变，投影给出的基态存在八极关联，需要打破轴对称和反射对称才能确定。从形变看，基态倾向于八极振动，而非稳定八极形变。

# $^{96}\text{Zr}$ 的低能激发谱



八极能级顺序和实验基本一致，但激发能系统性高出 2-3 MeV。  
非轴对称形变降低除  $3^-$  外的激发能。

# $^{96}\text{Zr}$ 的单粒子能级



八极关联：质子 $2p_{3/2} \rightarrow 1g_{9/2}$ , 中子 $2d_{5/2} \rightarrow 1h_{11/2}$ .

## 总结

- 我们利用变分后投影的相对论协变密度泛函理论研究了  $^{96}\text{Zr}$  的形变
- 投影后的  $^{96}\text{Zr}$  基态表现出八极关联
- 寻找  $^{96}\text{Zr}$  的基态需要同时打破轴对称和反射对称的限制

## 展望

- 考虑粒子数投影和组态混合给出低激发谱
- 高维全空间计算给出真正的基态

**Thank you !**