Optimized-Basis Generator Coordinate Method: Application to Low-Lying Excited States of sd-Shell Nuclei

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Background

- Collective Motions: Collective motions are characteristic features of many-body systems.
  - Examples: giant resonances and low-lying surface vibrations ...
  - Relevant: nuclear fission ,shape coexistence,Giant Resonances,Alpha Clustering ...
- Method: The Generator Coordinate Method (GCM) is commonly used to describe these collective motions microscopically.
  - Pre-selection of generator coordinates lacks self-consistency.
  - May miss important modes like Q_4, Q_6 or excited-state structures.
  - Prone to overcompleteness and numerical instability.
- The optimized-basis generator coordinate method (OptGCM) :
  - Eliminates the need for pre-defined coordinates; uses full variational optimization.
  - Optimizes both the basis SDs and weights to self-consistently explore the collective subspace.

In the GCM method, the trial wave function is expressed as

$$|\Psi\rangle = \sum_{a=1}^{M} f_a \, |\Phi_a\rangle, \tag{1}$$

The total energy is given by

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi \mid \Psi\rangle} = \frac{\sum_{ab} f_a^* f_b H_{ab}}{\sum_{ab} f_a^* f_b N_{ab}}, \tag{2}$$

In the OptGCM, the total energy is minimized with respect both to the weight coefficients f_a and the single-particle orbitals $\varphi_i^{(a)}$

$$\frac{\partial E}{\partial f_a^*} = 0 \qquad \frac{\delta E}{\delta \varphi_i^{(a)*}} = 0. \tag{3}$$

variation with respect to f_a^* yields

$$\frac{\delta E}{\delta f_a^*} = \frac{1}{\langle\Psi \mid \Psi\rangle} \sum_b (H_{ab} - E N_{ab}) \, f_b. \tag{4}$$

They take the variation before the projection (VBP) for the angular momentum projection . After the optimum set of the basis SDs are so obtained

$$|\Psi_{IM}\rangle = \sum_{a,K} f_{aK} \hat{P}^{I}_{MK} |\Phi_a\rangle . \tag{5}$$

With the total wave function so obtained, they calculate the reduced electric transition probabilities, $B(E2)$. The $B(E_\lambda)$ for a transition between a state with spin I_i and that with I_f is given by

$$B\left(E\lambda, I_i \to I_f\right) = \frac{1}{2I_i + 1} \left|\left\langle I_f \left\| \hat{Q}^{(e)}_{\lambda} \right\| I_i \right\rangle\right|^2 , \tag{6}$$

where

$$\hat{Q}^{(e)}_{\lambda\mu} = e \int dr \hat{\rho}_p(r) r^{\lambda} Y_{\lambda\mu}(\hat{r}) \tag{7}$$

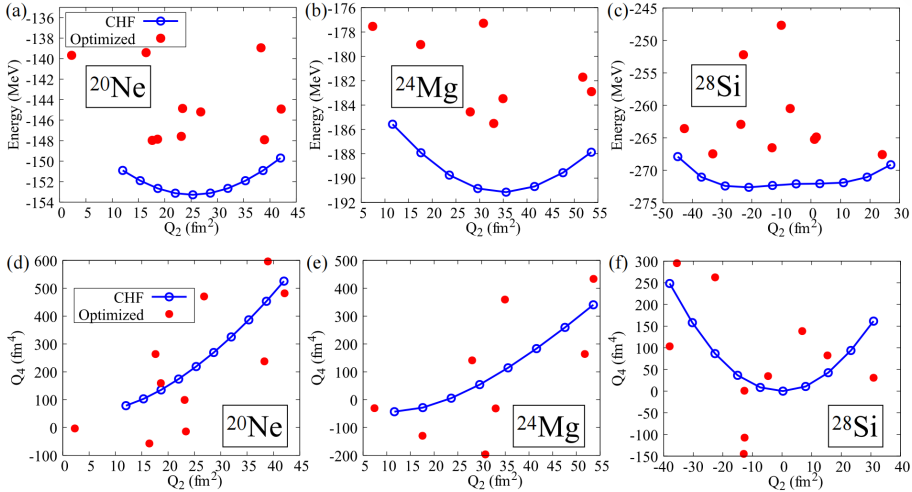

Figure: 上排：使用 CHF（蓝色圆圈）和 OptGCM（红色点）方法获得的 ^{20}Ne、^{24}Mg 和 ^{28}Si 核基态 SD 的能量期望值。这些值随四极矩 Q_2 的期望值变化而变化。下排：使用 CHF（蓝色圆圈）和 OptGCM（红色点）方法获得的 ^{20}Ne、^{24}Mg 和 ^{28}Si 核基态 SD 的四极矩 Q_2 和十六极矩 Q_4。

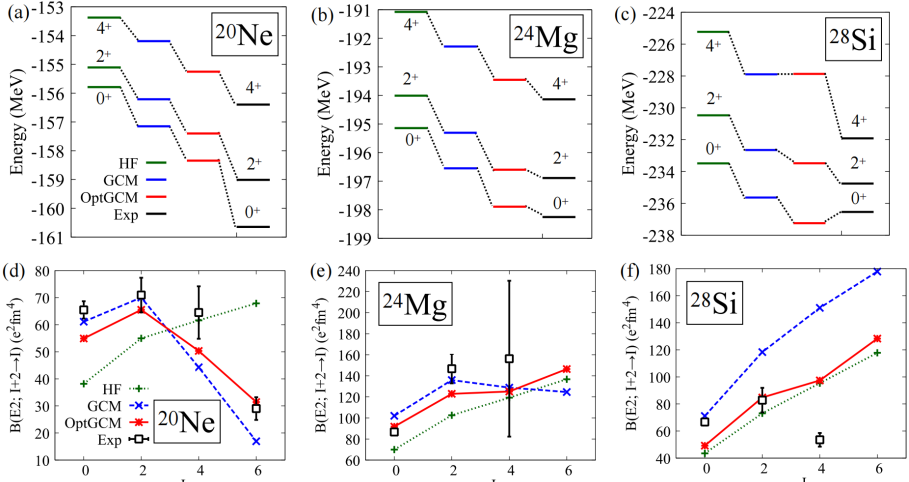

Figure: 图 (a) ^{20}Ne、(b)^{24}Mg 和 (c) ^{28}Si 核的能谱，通过角动量投影的 HF、GCM 和 OptGCM 方法获得，并与实验数据进行比较。下部面板还列出了计算出的 $B(E2)$ 值与实验数据的对比结果。

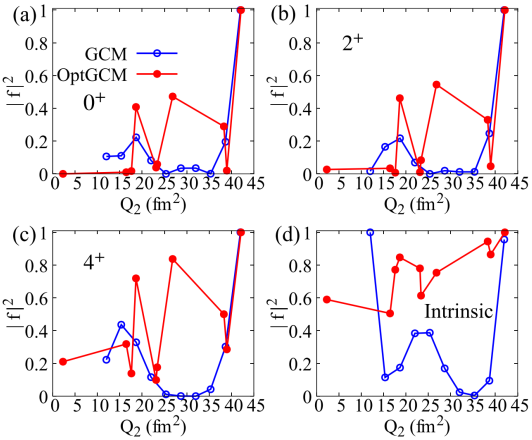

Figure: 权重系数的平方 $|f_a|^2$ 随四极矩 Q_2 变化的函数关系：(a) 0^+、(b) 2^+、(c) 4^+ 及 (d)^{20}Ne 原子核本征态（未投影态）。

- OptGCM 权重分布更集中在势能谷底附近
- 分布形态更不规则、更分散
- 随角动量态变化显著: 在 $0^+, 2^+, 4^+$ 不同角动量态下，OptGCM 的权重分布差异明显。
  说明该方法能为不同自旋态自洽地挑选不同的最优组态，而不是依赖一组固定的生成坐标。
- 内禀态的改进: 未投影态 (d) 已经体现出 OptGCM 更集中于势能谷底附近，这种优化在投影后进一步转化为更合理的集体态。

总结

OptGCM 应用于 sd 壳区核（^{20}Ne、^{24}Mg 和 ^{28}Si）的低激发态结构研究，并在方法上引入了角动量投影

- 基态能量系统性降低
- 基底结构更加丰富：OptGCM 基底在 $Q_2 - Q_4$ 平面分布更广，自动引入高阶形变与高能组态。
- 物理可观测量：激发态能谱更接近实验、跃迁强度（电四极跃迁率 B(E2)）表现良好
- 波函数构成：权重分布更分散，随角动量态显著变化；波函数构成更灵活、更物理。

未来

- ★ 按角动量单独优化基底（VAP）
- ★ 引入配对关联（Hartree-Fock-Bogoliubov (HFB) 态作为基底）...
- ★ ...

Thanks!