Symmetry restoration and generator coordinate method

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Outline

Introduction

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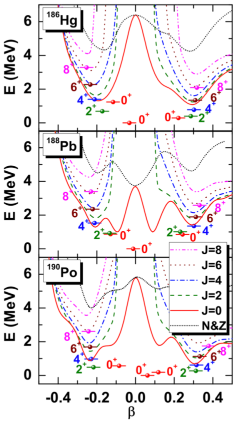


Figure: Deformation energy curves projected onto particle number (N&Z), or additional onto angular momentum (J), as well as the projected GCM states in the $N = 106$ isotones. JMY, M. Bender, and P.-H. Heenen, Phys. Rev. C 87, 034322 (2013).

- Particle number is not conserved in HFB state
- Angular momentum is not conserved in deformed HFB state

Symmetry restoration

Spontaneous symmetry breaking

- The exact many-body Hamiltonian H is invariant under a number of symmetry operations, that is, it commutes with the corresponding symmetry operator S :

$$[H, S] = 0.$$

  Therefore, we can always find wave functions that are simultaneous eigenfunctions of H and S. Examples are the three components of the linear momentum P, the particle number N, and the angular momentum operators $\mathbf{J}^2$, $\boldsymbol{J_z}$.

- Many-body correlations are treated by allowing for symmetry breaking in the wave function (density) of intrinsic frame, like the BCS state, HFB state which are not invariant under the rotation operator $e^{i\varphi\hat{N}}$ of $U(1)$ symmetry, as well as the deformed HFB state which does not have a definite angular momentum J.

$$e^{i\varphi\hat{N}}|\mathrm{BCS}\rangle \neq e^{i\varphi N_0}|\mathrm{BCS}\rangle.$$

Beyond the mean field approach

There are, however, two reasons to go beyond the mean field approach:

- In nuclear physics we are also interested in quantities such as transition probabilities and electromagnetic moments, which can never be calculated from a symmetry-violating Nilsson wave function alone.
- The nucleus is a finite system. The phase-transition is therefore always smeared out. We often find a gradual transition from conservation to weak violation, and eventually a strong breaking of the symmetry. In cases of weak symmetry violation we have to go beyond the mean field approach and incorporate the symmetries properly.

Particle number projection

- Particle number N_0 or number parity $(-1)^{N_0}$: The wave function with the correct particle number N_0 can be constructed as

$$\left|\Psi^{N_0}(q)\right\rangle \equiv \hat{P}^{N_0}|\Phi(q)\rangle,$$

which defines a particle-number projection operator

$$\hat{P}^{N_0} \equiv \frac{1}{2\pi}\int d\varphi e^{-i\varphi N_0}\hat{S}(\varphi), \quad \hat{S}(\varphi) \equiv e^{i\varphi\hat{N}}$$

with the gauge angle $\varphi_N \in [0, 2\pi]$. In this case, the rotated quasiparticle operator $\beta^\dagger_k(\boldsymbol{q}, g)$ becomes $\beta^\dagger_k(\boldsymbol{q}, \varphi)$, which can be determined with the Baker-Campbell-Hausdorff(BCH) formula

$$\begin{aligned}
\beta^\dagger_k(\boldsymbol{q}, \varphi) &\equiv \hat{S}(\varphi)\beta^\dagger_k(\boldsymbol{q})\hat{S}^\dagger(\varphi) \\
&= \sum_p \left[V_{pk}(\boldsymbol{q})\hat{S}(\varphi)c_p\hat{S}^\dagger(\varphi) + U_{pk}(\boldsymbol{q})\hat{S}(\varphi)c^\dagger_p\hat{S}^\dagger(\varphi)\right] \\
&\equiv \sum_p \left[V_{pk}(\boldsymbol{q}, \varphi)c_p + U_{pk}(\boldsymbol{q}, \varphi)c^\dagger_p\right]
\end{aligned}$$

Particle number projection

Homework: Prove that the single-particle operators $(c_p^\dagger, c_p)$ under the rotation transformation $e^{i\varphi\hat{N}}$ are given by

$$e^{i\varphi\hat{N}} c_p e^{-i\varphi\hat{N}} = c_p e^{-i\varphi}, \quad e^{i\varphi\hat{N}} c_p^\dagger e^{-i\varphi\hat{N}} = c_p^\dagger e^{i\varphi}$$

where $\hat{N} = \sum_k c_k^\dagger c_k$. Note that the BCH formula reads

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \cdots$$

Angular momentum projection

- The corresponding group is the special orthogonal group of order 3, i.e. $\mathrm{SO}(3)$, with a continuous rotation $\hat{R}(\phi,\theta,\psi)=e^{i\phi\hat{J}_z}e^{i\theta\hat{J}_y}e^{i\psi\hat{J}_z}$ in three-dimensional Euclidean space, where $\hat{J}_i$ is the component along the i-th axis of the angular momentum $\hat{\boldsymbol{J}}$, being generators of the Lie algebra of the $\mathrm{SO}(3)$ group, and the three Euler angles $\Omega=(\phi,\theta,\psi)$. The wave function with angular momentum J, z-projection M, and intrinsic z-projection K is constructed as

$$\left|\Psi^J_{MK}(\boldsymbol{q})\right\rangle \equiv \hat{P}^J_{MK}|\Phi(\boldsymbol{q})\rangle$$

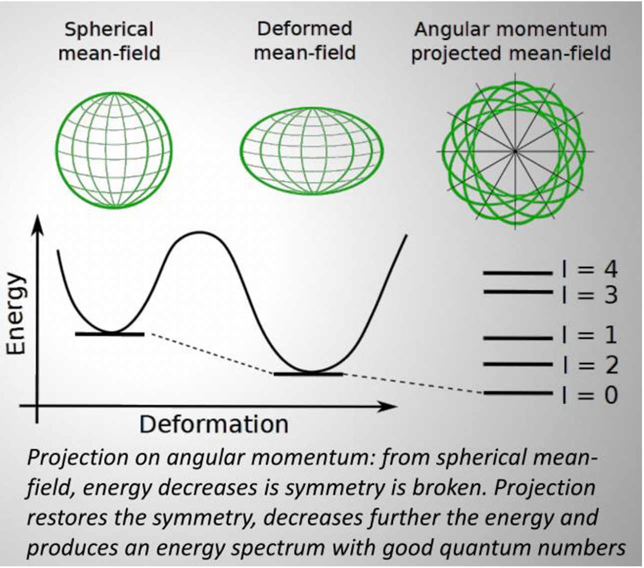
where the operator $\hat{P}^J_{MK}$ is introduced as

$$\hat{P}^J_{MK} \equiv \frac{2J+1}{8\pi^2}\int_0^{2\pi}d\phi\int_0^{\pi}d\cos\theta\int_0^{2\pi}d\psi D^{J*}_{MK}(\phi,\theta,\psi)\hat{R}(\phi,\theta,\psi),$$

where $D^{J*}_{MK}(\Omega)$ is the complex conjugate of Wigner D-matrix of dimension $2J+1$ in the spherical basis with elements

$$D^J_{MK}(\phi,\theta,\psi)\equiv\langle JM|\hat{R}(\phi,\theta,\psi)|JK\rangle=e^{iM\phi}d^J_{MK}(\theta)e^{iK\psi}$$

Angular momentum projection



Generator coordinate method (GCM)

GCM

- The GCM is based on the assumption that the trial wave function Ψ_α of a nuclear state labeled with α is written as a continuous superposition of the basis functions $\Phi(q)$, with a continuous parameter set q,

$$\Psi_\alpha = \int dq f_q^\alpha \Phi(q),$$

where the parameters q denote a set of collective variables–the so-called generator coordinates and they do not appear in the nuclear state wave function Ψ_α. The weight $f(q)$ also called "generator function" is folded into the basis functions to produce the wave function Ψ_α. The internal degrees of freedom are supposed to be taken into account by the functions $\Phi(q)$.

GCM

- In practical applications, the generator coordinate q is discretized. The continuous integral over q becomes a sum of discretized states. In the PGCM, the trial wave function is constructed as

$$\left|\Psi_{\alpha}^{JNZ}\right\rangle = \sum_{K=-J}^{J} \sum_{n=1}^{N_q} f_{K,q_n}^{J\alpha} \left|JMK, \boldsymbol{q}_n\right\rangle$$

where $|JMK, \boldsymbol{q}_n\rangle$ are symmetry-projected quasiparticle vacua,

$$|JMK, \boldsymbol{q}_n\rangle = \hat{P}_{MK}^{J} \hat{P}^{N} \hat{P}^{Z} \left|\Phi\left(\boldsymbol{q}_n\right)\right\rangle$$

The basis functions $|\Phi(\boldsymbol{q})\rangle$ labeled by the generator-coordinate parameters $\boldsymbol{q}$ are a set of quasiparticle vacua determined from HFB or (VAP-HFB) calculations with constraints on the quantities q. The projection operators produce basis states that are not orthonormal to each other.

GCM

Variation of the energy with respect to the weight function $f^{J\alpha}_{K,q}$ leads to the Hill-Wheeler-Griffin (HWG) equations

$$\sum_{K',\boldsymbol{q}'}\left[\mathcal{H}^J_{KK'}(\boldsymbol{q},\boldsymbol{q}')-E^J_\alpha\mathcal{N}^J_{KK'}(\boldsymbol{q},\boldsymbol{q}')\right]f^{J\alpha}_{K',\boldsymbol{q}'}=0$$

where the Hamiltonian and norm kernels $\mathcal{H}$ and $\mathcal{N}$ are given by the expressions

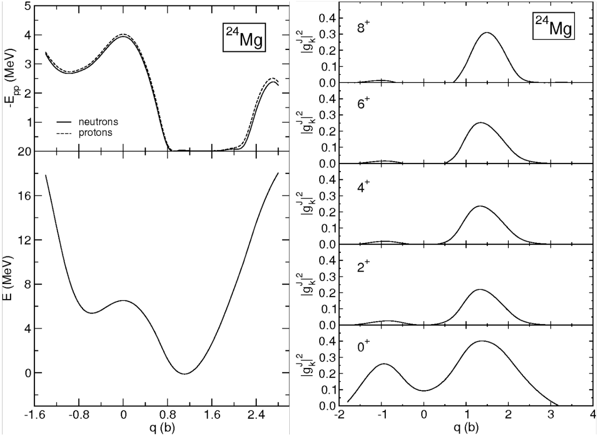
$$\begin{aligned}\mathcal{H}^J_{KK'}(\boldsymbol{q},\boldsymbol{q}')&=\left\langle JMK,\boldsymbol{q}|\hat{H}|JMK',\boldsymbol{q}'\right\rangle\\ \mathcal{N}^J_{KK'}(\boldsymbol{q},\boldsymbol{q}')&=\langle JMK,\boldsymbol{q}\mid JMK',\boldsymbol{q}'\rangle\end{aligned}$$

and E^J_α is the energy of the state with angular momentum J.

GCM

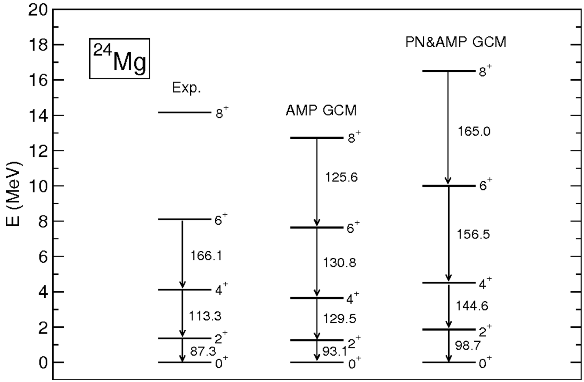
- The HWG equation is solved by diagonalizing the norm kernel to obtain a basis of “natural states” and then diagonalizing the Hamiltonian H in that basis. Because of the overcompleteness of the GCM-basis, the second diagonalization can be numerically unstable. This problem is taken care of by truncating the natural basis to include only states with norm eigenvalues larger than a reasonable value.

GCM: axially deformed nucleus



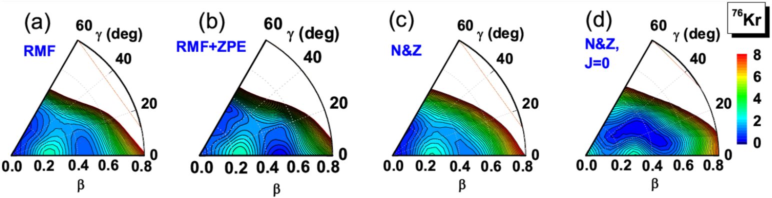
T. Niksic et al., PRC(2006)

GCM axially deformed nucleus



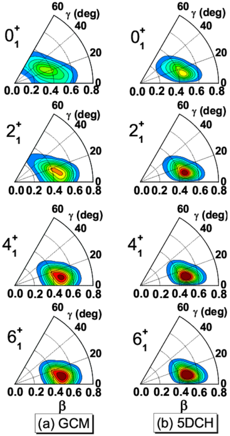
T. Niksic et al., PRC(2006)

GCM: triaxially deformed nucleus



JMY et al., PRC(2014)

GCM: triaxially deformed nucleus



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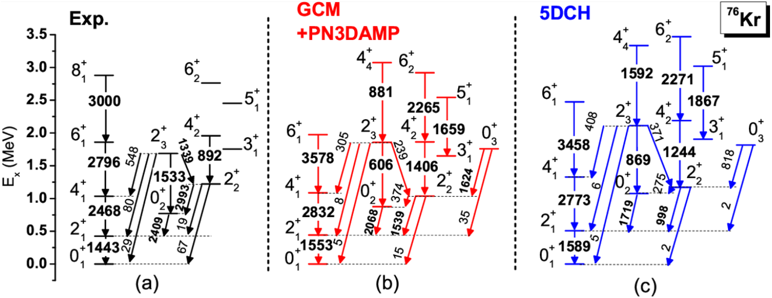

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