Cross-section of deformed 24 Mg from the Generator Coordinate Method

Jennifer Boström Jimmy Rotureau Andrea Idini Jimmy Ljungberg Gillis Carlsson

Division of Mathematical Physics, Lund University, Sweden

Microscopic methods

- Nuclear structure calculation
- Calculate spectra
- Construct optical potential

Possibilites of microscopic methods

- Predictive power
- Exotic nuclei
	- Neutron-rich
	- Radioactive beams
- Shell effects
	- Spectroscopic factor shows the degree of single-particle behaviour

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Method summary

- Method includes
	- Collective modes
	- Correlations
	- Particle-hole excitations
- Explores the huge complete Hilbert space in a systematic way
- Gives wavefunction from which observables can be calculated
- Can be extended

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Generator Coordinate Method

• Generate a basis from one or more generator coordinates

$$
|\phi(x_1, x_2, \dots)\rangle
$$

• Use a linear combination as ansatz

$$
\int f(x_1,x_2,\dots) \,|\phi(x_1,x_2,\dots)\rangle \,d\vec{x}
$$

(discretized)

• Solve the Hill-Wheeler equation

$$
Hh = EOh
$$

Overview of method

- Fit an effective Hamiltonian to the results of an Energy Density Functional (SLy4)
- Solve the effective Hamiltonian in mean field with pairing (HFB) with constraints as generator coordinates
- Introduce randomized particle-hole excitations (similar to temperature)
- Project the resulting HFB states to good quantum numbers
- Solve the resulting Hill-Wheeler equation

Ljungberg et al. Phys. Rev. C 106, 014314 (2022)

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Generator coordinates

- We proceed by solving a constrained HFB equation
- Generator coordinates used:
	- deformation *β*, *γ*
	- pairing strengths G_n , G_p
	- cranking i_x
- Results in a basis of HFB states
- Randomized particle-hole excitations

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Projection

- HFB breaks symmetries, e.g.
	- Particle number
	- Angular momentum
- Restore using projection
- Particle number

$$
P^{N} = \frac{1}{2\pi} \int_{0}^{2\pi} e^{i(\hat{N} - N)\theta} d\theta
$$

• Angular momentum

$$
P_{MK}^{I} = \frac{2I+1}{8\pi^2} \int D_{MK}^{I}^{*}(\Omega) \hat{\mathbf{R}}(\Omega) d\Omega
$$

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Method summary

- Solution in terms of linear combination of projected HFB states
- Includes
	- Collective modes through generator coordinates
	- Correlations through projection and mixing
	- Particle-hole excitations through temperature
- Explores the Hilbert space through choice of generator coordinates
- Gives wavefunction from which observables can be calculated

Odd case

- Single quasiparticle excitation on each HFB state
- Then do the same thing:
	- Project the resulting HFB+1qp states
	- Same effective Hamiltonian
	- Solve the resulting Hill-Wheeler equation Gives $\left|\Psi_k^{\pm}\right|$ $\left. \frac{\pm}{k} \right\rangle$ for $A \pm 1$
- Spectroscopic amplitudes 1

$$
\Big\langle \Psi^+_k \Big| a_\alpha^\dagger \Big| \Psi_0 \Big\rangle
$$

 1 Boström et al. J. Phys.: Conf. Ser. 2586 012080 (2023)

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Green's function

Calculate the Green's function

$$
G_{\alpha,\beta}^{I}(E) = \sum_{i} \frac{\left\langle \Psi_0 \middle| a_{\alpha} \middle| \Psi^{+I}_{i} \right\rangle \left\langle \Psi^{+I}_{i} \middle| a_{\beta}^{\dagger} \middle| \Psi_0 \right\rangle}{E - \left(E^{+I}_{i} - E_0 \right) + i\eta} + \text{holes}
$$

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Dyson equation

• Dyson equation for self-energy Σ (*E*)

$$
G(E) = G_0(E) + G_0(E) \Sigma(E) G(E)
$$

• Solved for
$$
\Sigma(E)
$$
 as

$$
\Sigma(E) = G_0(E)^{-1} - G(E)^{-1}
$$

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Non-local optical potential

• Construct the potential

$$
V_{a,b}\left(E\right) = \sum_{a,b}^{\infty} + \sum_{a,b}\left(E\right)
$$

• Expressed in momentum-space

$$
V(k, k') = \sum_{a,b}^{N} V_{a,b} \psi_a(k) \psi_b^*(k')
$$

- Lippmann-Schwinger equation $T = V + VG_{\text{free}}T$
- Phase shifts and cross-sections

24 Mg spectra

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25 Mg spectroscopic factors (positive parity)

Calculated energies colored by spectroscopic factor, compared to experimental energies as stars.

Preliminary ²⁴Mg neutron cross-sections

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Preliminary 24 Mg differential neutron cross-section

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Summary

- Lack of important correlations in many cross-section calculations
- Major step towards including many-body correlations in deformed nuclei
- Paper in progress

Effective Hamiltonian

$$
\hat{H} = \hat{H}_0 + \hat{H}_Q + \hat{H}_P
$$

- \hat{H}_0 Single particle part
- \bullet \hat{H}_Q Generalized quadrupole interaction
- \bullet \hat{H}_P Uniform seniority pairing

Effective Hamiltonian fit (^{24}Mg)

Hill-Wheeler equation after projection

• The Hill-Wheeler equation is constructed

$$
\sum_j H_{ij} h_j^n = E_n \sum_j O_{ij} h_j^n
$$

• Which gives the final wavefunctions

$$
\left|\Psi_{n}^{A}\right\rangle =\sum_{a,K}h_{aK}^{n}P_{MK}^{I}P^{Z}P^{N}\left|\phi_{a}\right\rangle
$$

• We can now evaluate matrix elements between these states

Completeness

To insert
$$
\sum_{i} \left| \Psi^{\pm}{}_{i}^{I} \right\rangle \left\langle \Psi^{\pm}{}_{i}^{I} \right|
$$
 in Green's function

$$
a_{\alpha}^{\dagger} | \Psi_{0} \rangle = \sum_{i} \left| \Psi^{+}{}_{i}^{I} \right\rangle \left\langle \Psi^{+}{}_{i}^{I} \right| a_{\alpha}^{\dagger} \left| \Psi_{0} \right\rangle
$$

No guarantee that this holds

Completing

At $E \to \infty$, correlations vanish \to should approach HF

$$
G_{\alpha,\beta}(E) = \sum_{i} \frac{\sigma_{i,\alpha}^* \sigma_{i,\beta}}{E - \epsilon_i + i\eta} + \sum_{i}^{M} \frac{c_{i,\alpha}^* c_{i,\beta}}{E - \epsilon'_i + i\eta}
$$

 $(\sigma_{i,\alpha} = \left\langle \Psi^{\pm}_{i} \left| a_{\alpha}^{\dagger} \right| \Psi_{0} \right\rangle)$

As few as possible while still giving HF at $E \to \infty$

• Completely determines spectroscopic factors and energies

Backbending for ⁴⁸Cr

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$^{24}\mathsf{Mg}\ 0^+$ wavefunction beta-gamma plane

Related to probability amplitude

Signature selection

Preliminary ²⁴Mg neutron cross-section

Preliminary ²⁴Mg neutron cross-section

Imaginary part

$$
\eta(E) = \frac{a}{\pi} \frac{(E - E_{\rm F})^2}{(E - E_{\rm F})^2 + b^2}
$$

Spectroscopic amplitudes

$$
\left\langle \Psi_k^+ \middle| a_\alpha^\dagger \middle| \Psi_0 \right\rangle =
$$
\n
$$
\sum_{abxK} (h_{a x K})^* h_b \left\langle \Phi_a \middle| \beta_x P^{A+1} P_{KM}^I a_\alpha^\dagger P_{00}^0 P^A \middle| \Phi_b \right\rangle =
$$
\n
$$
\sum_{abxK} (h_{a x K})^* h_b \left\langle \Phi_a \middle| \beta_x a_{\alpha K}^\dagger P_{00}^0 P^A \middle| \Phi_b \right\rangle
$$
\n
$$
a_{\alpha K}^\dagger = \sum_l \left(U_{\alpha K,l}^a \right)^* \beta_l^\dagger + V_{\alpha K,l}^a \beta_l
$$