Low-energy nuclear spectroscopy with beyond mean-field methods

Benjamin Bally

AG BTPN - 23/06/2016

Energy density functional (EDF) formalism

The basics

$$\mathcal{E}[\Phi] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

H phenomenological interaction

- Minimization: $\delta \mathcal{E}[\Phi] = 0$
- $|\Phi\rangle \begin{cases} \text{Slater determinants} & \rightarrow \text{Hartree-Fock} \\ \text{Bogoliubov quasiparticles} & \rightarrow \text{Hartree-Fock-Bogoliubov} \end{cases}$

Energy density functional (EDF) formalism

The basics

$$\mathcal{E}[\Phi] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$

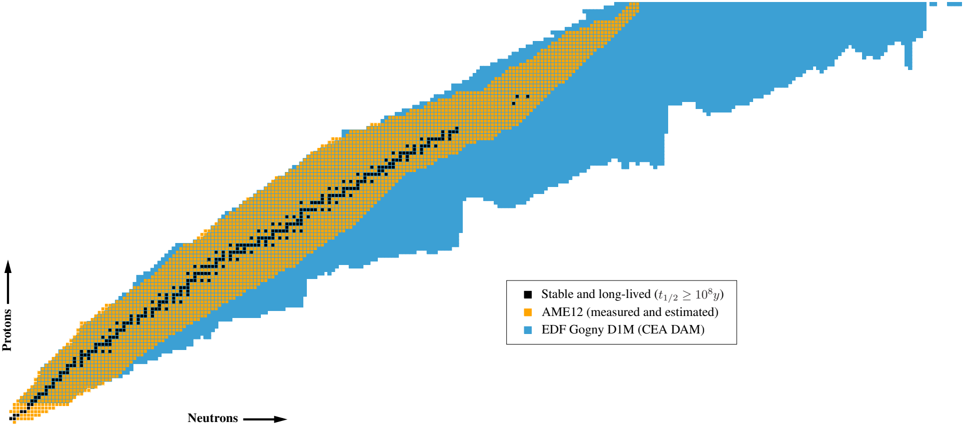
H phenomenological interaction

- Minimization: $\delta \mathcal{E}[\Phi] = 0$
- $|\Phi\rangle \begin{cases} \text{Slater determinants} & \rightarrow & \text{Hartree-Fock} \\ \text{Bogoliubov quasiparticles} & \rightarrow & \text{Hartree-Fock-Bogoliubov} \end{cases}$

Symmetry-breaking scheme

- Allow for symmetry-breaking $|\Phi\rangle$ → larger variational subset
- But unphysical for nuclei (finite-size systems)

Access to the entire nuclear chart



Symmetry Restoration

- Projection method (application of Group Theory)
- Act with a projection operator $P^\lambda|\Phi\rangle \rightarrow$ select component λ
- Particle Number

$$P^N|\Phi\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\phi\, e^{i\phi(\hat{N}-N)}|\Phi\rangle$$

- Angular Momentum

$$P^J_{MK}|\Phi\rangle = \frac{2J+1}{16\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin(\beta) \int_0^{4\pi} d\gamma \times D^{J\,*}_{MK}(\alpha,\beta,\gamma)\,\hat{R}(\alpha,\beta,\gamma)|\Phi\rangle$$

- Important quantum numbers for spectroscopy: N, Z, J, P

Configuration Mixing

- Generate set of states $\Omega_I \equiv \left\{ |\Phi_i\rangle, [\![i = 1, I]\!] \right\}$
- $i \equiv$ generator coordinate, e.g. deformation $\langle \Phi_i | Q | \Phi_i \rangle = q_i$
- More general ansatz

$$|\Psi_\epsilon^{JMNZP}\rangle = \sum_i^I \sum_{K=-J}^J f_{\epsilon,iK}^{JNZP} P^N P^Z P^J_{MK} |\Phi_i\rangle$$

- Variational principle

$$\delta \frac{\langle \Psi_\epsilon^{JMNZP} | H | \Psi_\epsilon^{JMNZP} \rangle}{\langle \Psi_\epsilon^{JMNZP} | \Psi_\epsilon^{JMNZP} \rangle} = 0 \Rightarrow$$

Hill-Wheeler-Griffin equation
$f_{\epsilon,iK}^{JNZP}$ and E_ϵ^{JNZP}

Configuration Mixing

- Generate set of states $\Omega_I \equiv \left\{ |\Phi_i\rangle, [\![i = 1, I]\!] \right\}$
- $i \equiv$ generator coordinate, e.g. deformation $\langle \Phi_i | Q | \Phi_i \rangle = q_i$
- More general ansatz

$$|\Psi_\epsilon^{JMNZP}\rangle = \sum_i^I \sum_{K=-J}^J f_{\epsilon,iK}^{JNZP} P^N P^Z P^J_{MK} |\Phi_i\rangle$$

- Variational principle

$$\delta \frac{\langle \Psi_\epsilon^{JMNZP} | H | \Psi_\epsilon^{JMNZP} \rangle}{\langle \Psi_\epsilon^{JMNZP} | \Psi_\epsilon^{JMNZP} \rangle} = 0 \Rightarrow$$

Hill-Wheeler-Griffin equation
$f_{\epsilon,iK}^{JNZP}$ and E_ϵ^{JNZP}

- Grasp more correlations $\Rightarrow$ better description of nuclear structure
- Access to low-energy nuclear spectroscopy

Major challenges

Interaction

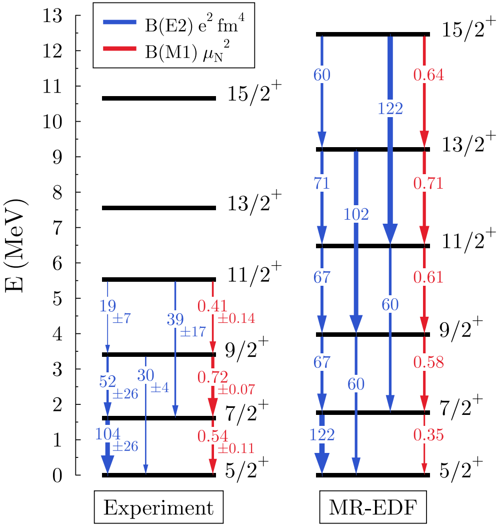
- Most problematic
- Simple Skyrme-type interaction (zero-range)
- Include all exchange and pairing terms in the functional!
  $\rightarrow$ mathematically safe concerning symmetry restoration

$\updownarrow$

CPU time

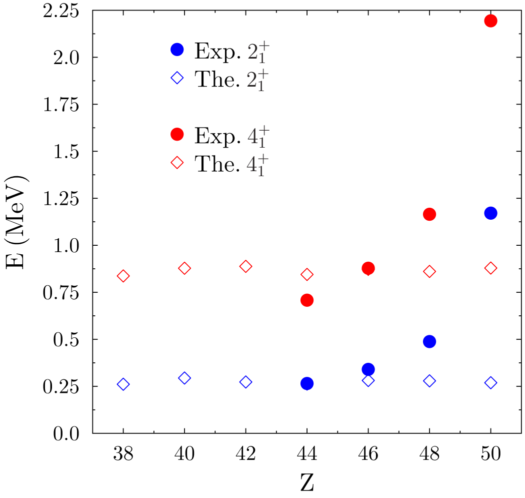
- Required $\left\{ \begin{array}{l} \text{MPI parallelization (embarrassingly parallel)} \\ \text{better algorithm} \end{array} \right.$
- Still can be improved a bit
- CPU time: not so cheap but still manageable (even heavy mass)

Application: ^{25}Mg with SLyMR0



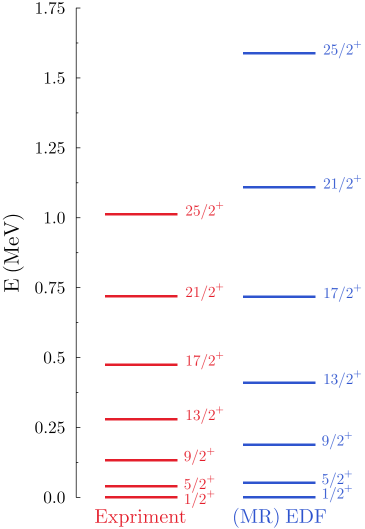
Bally *et al.*, PRL 113, 162501 (2014)

Application: some $N = 70$ isotones with SLyMR0



Paul *et al.*, in preparation

Toward heavy nuclei: ^{251}Md



Test calculation with SLyMR1 (R. Jodon, PhD Thesis at IPNL, 2014)

Conclusion

- Spectroscopy of even- and odd-mass nuclei possible!
- Even for heavy-mass nuclei (but quite intensive)
- Better effective interaction critically needed