From nuclear DFT to spectra and reaction observables

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Outline

- Motivation and idea
- Hamiltonian
- Many-body formalism
- Results
- Next-generation model

Motivation and idea

- DFT (in-medium interactions) $\longrightarrow$ high accuracy masses, radii…

- Put into effective Hamiltonian form

  $\longrightarrow$ Correlation energies, restored symmetries, wavefunctions next-generation mass models

  $\longrightarrow$ Spectra, optical potentials, crossections, unified description of reaction observables

- Must be numerically efficient $\longrightarrow$ valid for entire nuclear chart
- Provide reaction observables for nuclear technology and nucleosynthesis
- Scientific goal: use symmetry-restored many-body wave functions to connect nuclear spectra, transition strengths, and neutron-scattering observables.

Hamiltonian, in-medium interaction

Two-body part: $V^{(2)}(\mathrm{r}_1'\mathrm{r}_2'\mathrm{r}_1\mathrm{r}_2) = v(\mathrm{r}',\mathrm{r})\delta(\mathrm{R}-\mathrm{R}')$

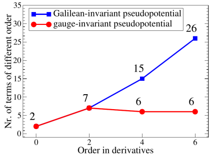
$$\begin{aligned}\bar{v}(\mathrm{k}',\mathrm{k}) &= \frac{1}{(2\pi)^3}\int\int e^{-i\mathrm{k}\cdot\mathrm{r}} v\left(\mathrm{r},\mathrm{r}'\right) e^{i\mathrm{k}'\cdot\mathrm{r}'} d\mathrm{r} d\mathrm{r}' \\ &= t_0\left(1+x_0P_\sigma\right)+\frac{1}{2}t_1\left(k^2+k'^2\right) \\ &+ t_2\mathrm{k}\cdot\mathrm{k}'+iW_0\left(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2\right)\cdot\mathrm{k}\times\mathrm{k}'+\ldots\end{aligned}$$

Many-body part:

$$V_\rho = v_\rho\left(\mathrm{r}',\mathrm{r}\right)\left[\rho\left(\mathrm{R}\right)\right]^\alpha\delta\left(\mathrm{R}-\mathrm{R}'\right)$$

$$\bar{v}_\rho(\mathrm{k}',\mathrm{k}) = \tfrac{t_3}{6}\left(1+x_3P^\sigma\right)$$

$$\begin{aligned}\rho^{2+\alpha} &\simeq a\rho^2 \;\; \text{(2-body)} \\ &+ b\rho^3 \;\; \text{(3-body)} \\ &+ c\rho^4 \;\; \text{(4-body)} \\ &+ \ldots\end{aligned}$$



Latest (N2LO) fitts to data:

RMS = 0.649 MeV (2457 masses):

RMS=0.0267 fm (810 charge radii)

RMS=0.43 MeV (45 fission barriers)

Original NLO; T. Skyrme., Nuc. Phys. 9, 615 (1959)
N3LO extension: B.G. Carlsson et. al., PRC 78, 044326 (2008)
Latest N2LO fitts: G. Grams et. al., arXiv:2601.05968 (2026)

Hamiltonian, fluctuations

In the global masstable calculations correlation effects are included as a separate part of the Hamiltonian and treated appriximately.

Here we aim for a microscopic description of the correlation effects.

Starting point, normal ordering around spherical state

$$H = E_0 + \Gamma + \tilde{V}^{(2)} + \tilde{V}^{(3)} + \ldots$$

Constant: E_0

One-body monopole field: Γ

Two- and three-body fluctuations: $\tilde{V}^{(2)}$, $\tilde{V}^{(3)}$

Hamiltonian, fluctuations expansion

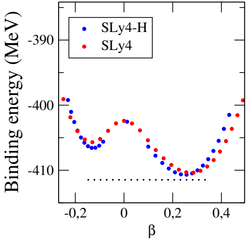
Zero-order approximation:

$$\Gamma = \sum_i \epsilon_i a_i^\dagger a_i$$

$$\tilde{V}^{(2)} = -\frac{1}{4}\chi \sum_{\mu ijkl} \left[Q_{ij}^{2\mu} Q_{kl}^{2\mu *} - Q_{ik}^{2\mu} Q_{jl}^{2\mu *} \right] a_i^\dagger a_j^\dagger a_k a_l + G \sum_{ijkl} P_{ij} P_{kl} a_i^\dagger a_j^\dagger a_k a_l$$

$$Q^{L\mu}(\mathrm{r}) = -r \frac{\partial f}{\partial r} Y_{L\mu} + \frac{v_{so}\lambda^2}{2} r \left(-\frac{1}{r^2}\frac{\partial f}{\partial r} + \frac{1}{r}\frac{\partial^2 f}{\partial r^2} \right) \frac{1}{2} \left(\mathrm{l}\cdot\mathrm{s} Y_{L\mu} + Y_{L\mu} \mathrm{l}\cdot\mathrm{s} \right)$$

Γ provides a spherical single-particle reference field; QQ-part captures quadrupole collectivity; PP-part captures proton/neutron pairing correlations.
$Q(\mathrm{r})$ gives a surface gaussian type of interaction that exactly reproduces the shape of the deformed mean-field



Full vs fluctuation expansion (^{48}Cr)

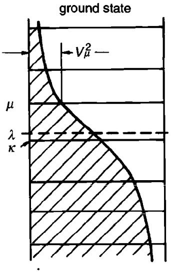
K. Kumar and B. Sørensen, Nuclear Physics A 146, 1 (1970)

Many-body formalism

- Next step, solve Hamiltonian in complete model spaces using the full nucleon degrees of freedom (microscopic approach)
- Use intuition built during the last 70 years to design optimal many-body basis states (pairing, deformation, centrifugal field)

$\longrightarrow$ non-orthogonal basis based on Bogoliubov many-body states

Many-body formalism, overlaps



$$\psi = \prod_\nu \left(U_\nu + V_\nu a_\nu^\dagger a_{\bar{\nu}}^\dagger \right) |0\rangle$$

- K. Neergård et al, NPA 402 (1983) - fails when U_ν become small
- G. F. Bertsch and L. M. Robledo, PRL 108 (2012) - fails when V_ν become small
- B. G. Carlsson and J. Rotureau, PRL 126 (2021) - First exact formula

$$\langle \psi | \psi' \rangle = \lim_{\epsilon \to 0} (-1)^{N/2} \frac{(\det C)^* \det C'}{\prod_{ii'} v_i v'_{i'}} \mathrm{pf} \left(\begin{bmatrix} V^T U & V^T V'^* \\ -V'^\dagger V & U'^\dagger V'^* \end{bmatrix} \right)$$
$$= (-1)^{N/2} \mathrm{pf} \left(\begin{bmatrix} -\bar{U}\sigma & \Lambda D^\dagger D' \Lambda' \\ -\Lambda' D'^T D'^* \Lambda & \sigma \bar{U}' \end{bmatrix} \right)$$

Many-body formalism, overlaps

Even number parity overlaps:

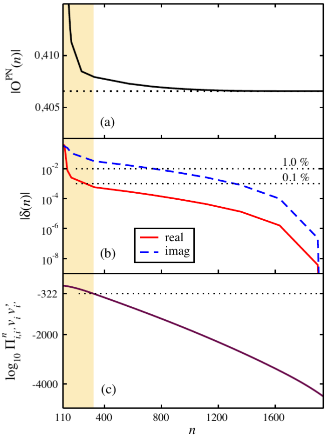
$$\langle \psi | \psi' \rangle = (-1)^{n/2} \mathrm{pf}\left(\mathcal{A}\right)$$

odd number parity overlaps:

$$\left\langle \psi | \beta_\gamma \beta_\delta^\dagger | \psi' \right\rangle = (-1)^{n/2} \mathrm{pf} \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ -\mathcal{B}^T & \mathcal{C} \end{pmatrix}$$

$$= (-1)^{n/2} \mathrm{pf}\left(\mathcal{A}\right) \mathrm{pf}\left(\mathcal{C} + \mathcal{B}^T \mathcal{A}^{-1} \mathcal{B}\right)$$

$$= (-1)^{n/2} \mathrm{pf}\left(\mathcal{A}\right) \left(\mathcal{C} + \mathcal{B}^T \mathcal{A}^{-1} \mathcal{B}\right)_{12}$$



Gives convergence in large
modelspaces needed for reactions

Many-body formalism, degrees of freedom

Method:

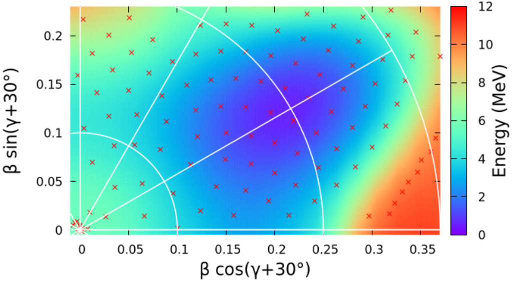
- Solve the constrained-HFB equations
- Sample the energy surface to get basis states
- The HFB-states form a non-orthogonal basis
- Application of projection techiques to restore symmetries
- Solve the Hill-Wheeler equations

Generator coordinates:

- Deformation (β, γ)
- Centrifugal field ω_x
- Pairing fields (g_p, g_n)

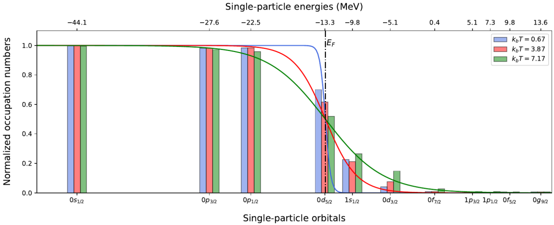
$\longrightarrow$ 5D-energy landscape

^{48}Cr (Z=24, N=24)



β-quadrupole deformation
γ-degree of triaxiality

Many-body formalism, degrees of freedom



For each vacua we include temperature excitation (couple-cluster singlet expansion):

$$|\Psi_1\rangle = \mathcal{N} e^{\sum_{k<k'} z_{k,k'} \beta_k^\dagger \beta_{k'}^\dagger} |\Psi_0\rangle$$

$$= \mathcal{N} \left(1 + \sum_{k<k'} z_{k,k'} \beta_k^\dagger \beta_{k'}^\dagger + \frac{1}{2} \sum_{k<k',k''<k'''} z_{k,k'} z_{k'',k'''} \beta_k^\dagger \beta_{k'}^\dagger \beta_{k''}^\dagger \beta_{k'''}^\dagger + .. \right) |\Psi_0\rangle$$

with a temperature weighting $z_{k,k'} = e^{-(E_k + E_{k'})/(k_B T)} p$

Temperature-like multi-quasiparticle excitations allows the basis to include noncollective particle-hole-like components.Turns GCM into an exact many-body method

Many-body formalism, Projection

Temparature excited 5D-grid gives a set of symmetry broken states $\{\phi_1, \phi_2, \phi_3, ...\}$.
Symmetry restored with projection operators: $\hat{P} = \hat{P}^I_{MK}\hat{P}^Z\hat{P}^N$.
Symmetry restoration and GCM require many overlaps between nonorthogonal HFB vacua, after rotations and gauge transformations.

From: $H_{iK',jK} = \left\langle \phi_i \middle| \hat{P}^\dagger \hat{H} \hat{P} \middle| \phi_j \right\rangle$ and $\mathcal{O}_{iK',jK} = \left\langle \phi_i \middle| \hat{P} \middle| \phi_j \right\rangle$

One can set up the Hill-Wheeler equation:

$$\sum_J H_{iK',jK} c^n_{jK} = E_n \sum_J \mathcal{O}_{iK',jK} c^n_{jK}$$

Giving final states:

$$\left|\psi^{I,M}_i\right\rangle = \sum_{j,K} C^n_{jK} \hat{P}^I_{MK} \hat{P}^N \hat{P}^Z \left|\phi_j\right\rangle$$

and energies:

$$E^{I,M}_i$$

Minimal Canonical basis

$$H_{IK,JK'} = \left\langle \phi_I \left| \hat{P}^{I\dagger}_{MK} \hat{H} \hat{P}^{I}_{MK'} \hat{P}_Z \hat{P}_N \right| \phi_J \right\rangle$$
$$= \left\langle \phi_I \left| \hat{H} \hat{P}^{I}_{KK'} \hat{P}_Z \hat{P}_N \right| \phi_J \right\rangle$$
$$= \sum_i w_i \left\langle \phi_I \left| \hat{H} \hat{R}_i \right| \phi_J \right\rangle$$

$$\left\langle a \left| \hat{H} \right| b \right\rangle = \langle a | b \rangle \, \frac{1}{2} \left(\mathrm{Tr}\left(\rho\Gamma\right) - \mathrm{Tr}\left(\Delta\kappa^*_{01}\right)\right)$$

$$D^\dagger_b \rho D_a = \bar{\rho} = \begin{pmatrix} \bar{\rho}_{11} & 0 \\ 0 & 0 \end{pmatrix}$$
$$D^\dagger_b \kappa_{10} D^*_a = \bar{\kappa}_{10} = \begin{pmatrix} (\bar{\kappa}_{10})_{11} & (\bar{\kappa}_{10})_{12} \\ 0 & 0 \end{pmatrix}$$
$$D^T_b \kappa^*_{01} D_a = \bar{\kappa}^*_{01} = \begin{pmatrix} (\bar{\kappa}^*_{01})_{11} & 0 \\ (\bar{\kappa}^*_{01})_{21} & 0 \end{pmatrix}$$

$$\left\langle a \left| \hat{H}_Q + \hat{H}_P \right| b \right\rangle = -\langle a|b\rangle \frac{\chi}{2} \sum_{\mu q q'} (-1)^\mu \, \mathrm{Tr}\left(\bar{\rho}^q_{11} \bar{Q}^{2\mu,q}\right) \times \mathrm{Tr}\left(\bar{\rho}^{q'}_{11} \bar{Q}^{2(-\mu),q'}\right)$$
$$+ \langle a|b\rangle \frac{\chi}{2} \sum_{q\mu} (-1)^\mu \, \mathrm{Tr}\left(\bar{\rho}^q_{11} \bar{Q}^{2\mu,q} \bar{\rho}^q_{11} \bar{Q}^{2(-\mu),q}\right)$$
$$+ \langle a|b\rangle \frac{1}{2} \sum_{q} G^q \mathrm{Tr}\left(\bar{\rho}^q_{11} \bar{P}_{q,1} \left(\bar{\rho}^q_{11}\right)^T \bar{P}^*_{q,2}\right)$$
$$- \langle a|b\rangle \frac{1}{4} \sum_{q} G^q \mathrm{Tr}\left(\left[(\bar{\kappa}^q_{10})_{11}, (\bar{\kappa}^q_{10})_{12}\right] \begin{bmatrix} \bar{P}^*_{q,11} \\ \bar{P}^*_{q,21} \end{bmatrix}\right) \times \mathrm{Tr}\left(\left[\bar{P}_{q,11}, \bar{P}_{q,12}\right] \begin{bmatrix} (\bar{\kappa}^{*q}_{01})_{11} \\ (\bar{\kappa}^{*q}_{01})_{21} \end{bmatrix}\right)$$
$$+ \langle a|b\rangle \frac{\chi}{2} \sum_{\mu q} \mathrm{Tr}\left(\bar{Q}^{2\mu,q} \left[(\bar{\kappa}^q_{10})_{11}, (\bar{\kappa}^q_{10})_{12}\right] \left(D^\dagger_a Q^{2\mu,q} D_b\right)^* \begin{bmatrix} (\bar{\kappa}^{*q}_{01})_{11} \\ (\bar{\kappa}^{*q}_{01})_{21} \end{bmatrix}\right)$$

P. Bonche et. al. NPA 510, 466 (1990)

Transitions directly from wave functions

$$B\left(E2; I_i \to I_f\right) = \frac{1}{2I_i + 1} \sum_{M_f M_i \mu} \left| \left\langle I_f M_f | \hat{Q}_{2\mu} | I_i M_i \right\rangle \right|^2$$

Quadrupole operator: $\hat{Q}_{2\mu} \sim er^2 Y_{2\mu}$
No effective charges

Parameters for the calculations

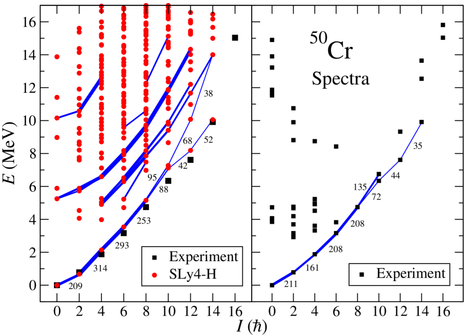
- Single-particle basis
  - Number of shells: 11 $\Rightarrow$ 728 states
- HFB-states
  - $\approx$ 200 within 12 MeV
- Projections
  - Particle number: $(Z, N) = (10, 10)$
  - Angular momentum: $(\alpha, \beta, \gamma) = (9, 18, 36)$
  - In total 116640 rotations per HFB-state
- Computational time: $\sim$1 week on $\sim$400 cpu:s for each nucleus

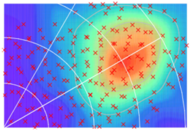
Results, spectra

^{50}Cr, Z=24, N=26

Fermi-level in $f_{7/2}$ shell for both protons and neutrons

Terminating state at:
$I = 14$





Sampling of deformation surface I=6

J. Ljungberg et al. PRC 106, 014314 (2022)

Results, optical potentials

By calculating full spectra of ^{49,50,51}Cr we can set up the Greens function in the Källén-Lehman representation:

$$G_{\alpha,\beta}(E) = \lim_{\eta \to 0^+} \sum_i \frac{\left\langle \Psi_0 \left| a_\alpha \right| \Psi_i^+ \right\rangle \left\langle \Psi_i^+ \left| a_\beta^\dagger \right| \Psi_0 \right\rangle}{E - \left(E_i^+ - E_0 - i\eta\right)} + \sum_i \frac{\left\langle \Psi_i^- \left| a_\alpha \right| \Psi_0 \right\rangle \left\langle \Psi_0 \left| a_\beta^\dagger \right| \Psi_i^- \right\rangle}{E + \left(E_i^- - E_0 - i\eta\right)}$$

By first constructing the unperturbed Greens function $G_0(E)$ from U^0 we can solve the Dyson equation $G(E) = G_0(E) + G_0(E)\Sigma(E)G(E)$obtaining the self-energy $\Sigma(E)$ from which we can construct the otical potential: $V(E) = U^0 + \Sigma(E)$ This allows for microscopic calculations of neutron scattering crossections.

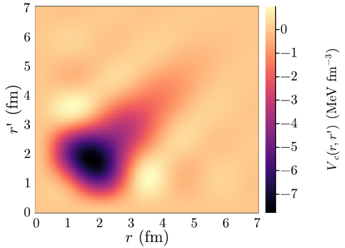
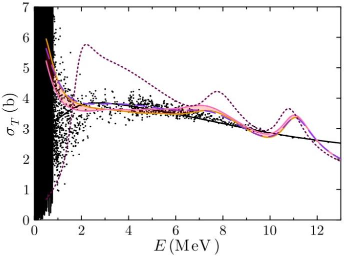


FIG. 11. Real part of the central d-wave optical potential of ^{50}Cr for an incoming neutron energy of 3.25 MeV.

Results, neutron crossections

- ^{50}Cr as a structural-material isotope of interest for evaluated data.
- Microscopic crossections for deformed nuclei
- The current strongest window is roughly the few-MeV to 10-MeV regime; below it, resolved resonances and continuum coupling are demanding.
- Above 10 MeV basis looses accuracy
- GCM correlations supply absorption channels missing from a mean-field-only potential.

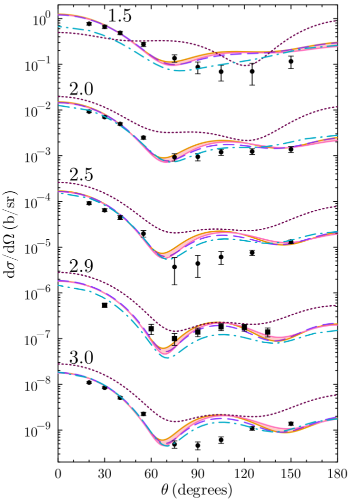


Total neutron scattering cross section calculated for ^{50}Cr

J. Boström, et al PRC 112, L051602 (2025).
J. Boström, et al, arXiv:2604.01033v1 (2026).

Results, differential crossections

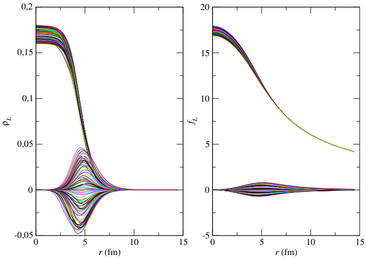
- Diffraction minima positions well reproduced → nuclear radii correctly captured
- Discrepancy between experimental datasets resolved: GCM agrees with Fedorov et al., consistent with ENDF evaluation



More on thursday (A. Idini)

J. Boström, et al PRC 112, L051602 (2025).
J. Boström, et al, arXiv:2604.01033v1 (2026).

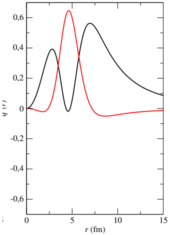
Next-generation models



For the next-generation models we have formalized the interaction expansion, e.g.

$$\frac{e_0^2}{|\mathrm{r}-\mathrm{r}'|} = \sum_{Lk\mu} Q^{k,L\mu}\left(\mathrm{r}'\right) Q^{k,L\mu}\left(\mathrm{r}\right)^* .$$

expanding in collective subspace $\{\rho_1 ... \rho_N, \Gamma\left(\rho_1\right), ..\Gamma\left(\rho_N\right)\}$. Three-body case: HOSVD/Tucker decomposition.



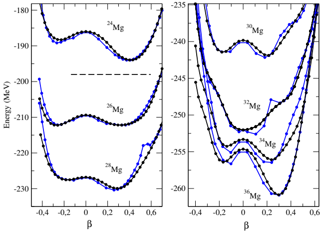
J. Johansen, LSP (2023), B.G. Carlsson, in preparation

Next-generation models

The repulsive three-body interaction gives a contribution that goes like: $E \sim 0.048 A^2 \beta^3$
For heavy nuclei it must be explictly included to generate full deformation landscapes.
We have recently finished using same tensor decomposition avoiding full cubic storage

$$V^{(3)} = \sum_{Lk} \left[\left[Q^{k,L}(\mathrm{r}_1)\, Q^{k,L}(\mathrm{r}_2) \right]_I Q^{k,L}(\mathrm{r}_3) \right]_0$$

First test of replacing phenomenological correlation energy with microscopic correlation gives some overbinding, 3 and 5 MeV for ^{24}Mg and ^{56}Fe (BSKG2)



Mg isotopes with explicit 3-body. HF-contribution.

B.G. Carlsson, in preparation

Summary/outlook

Summary:

- Nuclear DFT/in-medium interactions have been generalized to provide spectra and reaction observables
- Systematic predictions of scattering for nuclear technology
- Detailed predictions for deexcitation of fission fragments
- The program is moving from a spectroscopy method toward a scalable, nuclear-chart-wide structure–reaction framework.

Outlook:

- Cross sections converge more slowly than spectra; reaction-tailored bases.
- Master student: radii and densities
- PhD student j-matrix formalism for (n, γ) reactions
- Explicit 3-body contributions and effect on spectra

Thank you for your attention!

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  Master's thesis, Lund University (2025).