Towards microscopic optical potentials for symmetry breaking nuclei

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LUND UNIVERSITY

Outline

- Nuclear DFT provide masses with an error of 0.7 MeV [1].
- Good overal accuracy for groundstate spins and many more properties.
- Can they be generalized to provide accurate predictions of reactions ?
- We would like to solve for even and odd nuclei and directly use the spectra and wavefunctions to build optical potentials
- We would like to use the GCM method

[1] G. Scamps et al, Eur. Phys. J. A 57, 333 (2021)

Density functional theory

- Functionals globally fitted on masses, radii, fission barriers ...
- proper description of collective states, bulk properties (radii, stiffness,...)

HFB wave function:

$$|\phi\rangle = \prod_i \beta_i |0\rangle$$

$\beta_i, \beta_i^\dagger$ are quasi-particle destruction (creation) operators

- Beyond mean field trial wave function in the Generator Coordinate Method (GCM):

$$|\Psi\rangle = \int da\, f(a)\, |\phi(a)\rangle$$

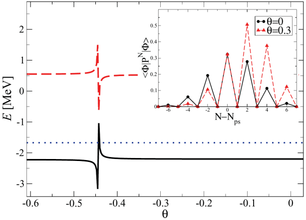
- symmetry restoration (fixed particle number, angular momentum) by projection techniques

Formal and technical issues arise if one uses functional in a beyond-mean field framework:

1. EDF's (Skyrme, Gogny) contain density dependence: not clear how to be used in the Projection+GCM
2. Approximate Hamiltonian with violation of Pauli principle leads to poles when restoring symmetries [1]
3. Ultraviolet divergencies [2]

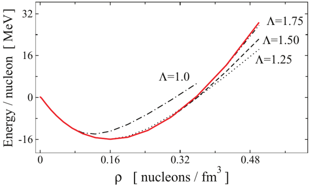
[1] T. Duguet, M. Bender, K. Bennaceur, D. Lacroix and T. Lesinski, PRC 79,044320 (2009) ; [2] B. G. Carlsson, J. Toivanen and U. von Barth, PRC 87, 054303 (2013).

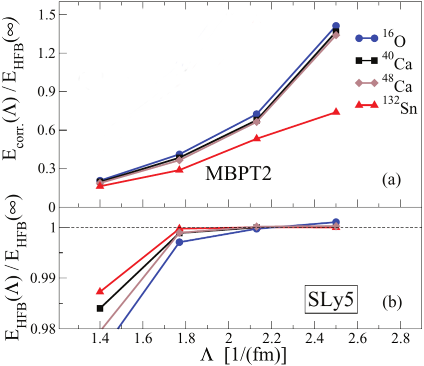
Poles in energy for a state in ^{142}Gd



B.G. Carlsson et. al., PRC 78, 034316 (2008)

Ultraviolet divergence





B.G. Carlsson et. al., PRC 87, 054303 (2013)

$\rightarrow$ Convenient to have a proper Hamiltonian for projection and GCM

Postulate an Effective Hamiltonian

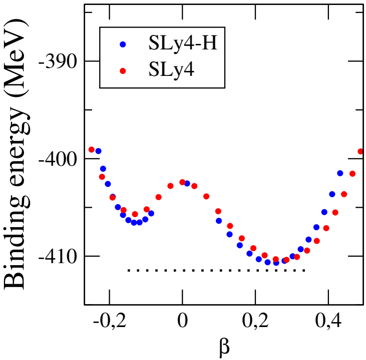
$$H^{eff} = \sum_i \epsilon_i a_i^\dagger a_i - \frac{1}{4}\chi \sum_{\mu ijkl} \left[Q_{ij}^{2\mu} Q_{kl}^{2\mu *} - Q_{ik}^{2\mu} Q_{jl}^{2\mu *} \right] a_i^\dagger a_j^\dagger a_k a_l$$
$$+ G \sum_{ijkl} P_{ij} P_{kl} a_i^\dagger a_j^\dagger a_k a_l$$

- spherical part computed from HF with EDF's (Skyrme,...)
- Quadrupole interaction with Woods-Saxon shape [1] with χ as strength parameter
- Pairing strength G fixed with the uniform method [2]

[1] K. Kumar and B. Sørensen, Nuclear Physics A 146, 1 (1970)
[2] Nilsson and Ragnarsson, shapes and shells in nuclear structure (1995)

Results of the fits of χ

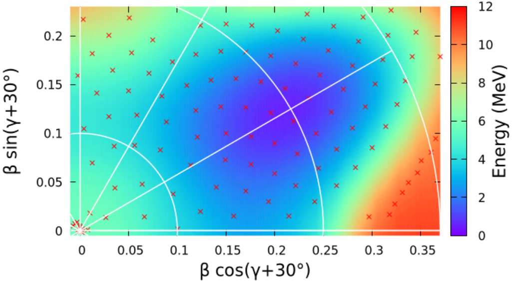
- HF energies for ^{48}Cr from Skyrme - SLy4
- Effective Hamiltonian denoted SLy4-H



HFB energy surface

- Solve the constrained-HFB equations with H^{eff}
- 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

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



β-quadrupole deformation
γ-degree of triaxiality

Need overlaps betweeen all the states

$$\mathcal{O} = \langle \phi_a | \phi_b \rangle$$

In this context, overlaps are notoriously challenging to compute accurately

N. Onishi et al, NP 80 (1966); K. Hara et al, NPA 385 (1982); K. Neergard et al, NPA 402 (1983); Q. Haider et al (1992); F. Donau, PRC 58 (1998), K. Schmid, PPN 565 (2004); M. Oi et al, PLB 606 (2005); M. Bender et al, PRC 78(2008); L. M. Robledo, PRC 79 (2009); T. R. Rodríguez et al, PRC 81 (2010); B. Avez et al, PRC 85 (2012); G. F. Bertsch and L. M. Robledo, PRL 108 (2012); B. Bally et al, PRC97 (2018);T. Mizusaki et al, PLP 779 (2018).......

PHYSICAL REVIEW LETTERS **126,** 172501 (2021)

New and Practical Formulation for Overlaps of Bogoliubov Vacua

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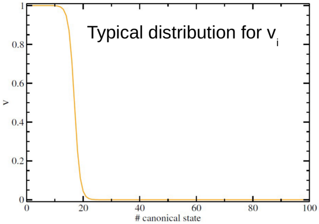
In this Letter, we present a new expression for the overlaps of wave functions in Hartree-Fock-Bogoliubov based theories. Starting from the Pfaffian formula by Bertsch *et al.* [1], an exact and computationally stable formula for overlaps is derived. We illustrate the convenience of this new formulation with a numerical application in the context of the particle-number projection method. This new formula allows for substantially increased precision and versatility in chemical, atomic, and nuclear physics applications, particularly for methods dealing with superfluidity, symmetry restoration, and uses of nonorthogonal many-body basis states.

DOI: 10.1103/PhysRevLett.126.172501

* we start with the formula by Bertsch and Robledo (2012)

$$\langle \Phi_a | \Phi_b \rangle = \frac{(-1)^\eta}{\prod_{i,i'} v_i v'_{i'}} \mathrm{pf} \begin{pmatrix} V^T U & V^T V'^* \\ -V'^\dagger V & U'^\dagger V'^* \end{pmatrix}$$

v^2_i is the occupation probability of the canonical basis state i



$$|\Phi_a\rangle = \prod_i \beta_i |0\rangle$$

$$|\Phi_b\rangle = \prod_i \beta'_i |0\rangle$$

U,V (U'V') are the matrices of the Bogoliubov transformation associated with Φ_a and Φ_b

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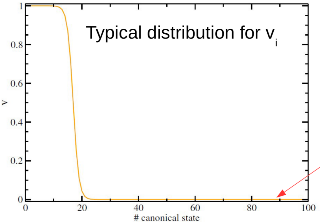


Numerical issue related to small values of v_i

Introducing the matrices Λ, Λ' : $\Lambda = \begin{pmatrix} \sqrt{v_0} & & \\ & \ddots & \\ & & \sqrt{v_{N-1}} \end{pmatrix}$ $\Lambda' = \begin{pmatrix} \sqrt{v'_0} & & \\ & \ddots & \\ & & \sqrt{v'_{N-1}} \end{pmatrix}$

$$\langle \Phi_a | \Phi_b \rangle = \frac{\Lambda\Lambda'}{\Lambda\Lambda'} \langle \Phi_a | \Phi_b \rangle$$

$$\vdots$$

$$= \boxed{(-1)^{N/2} \mathrm{pf} \begin{pmatrix} -\bar{U}\sigma & \Lambda D^{\dagger} D' \Lambda' \\ -\Lambda' D'^{T} D^{*} \Lambda & \sigma \bar{U}' \end{pmatrix}}$$

→ substantially increased precision vs previous formula and can be truncated in a systematic manner

B. G. Carlsson and J.R, PRL 126, 172501 (2021)

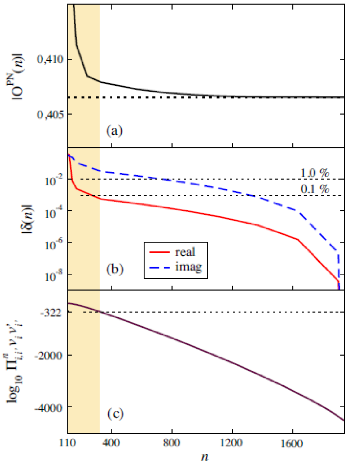


FIG. 1. Matrix element $\mathcal{O}^{PN}(n)$ as a function of the number of canonical basis states included in the computation n. Panel (a) shows the modulus of the matrix elements at $\phi = \pi/10$ as a function of n. The dotted line corresponds to the value in the full model space when $n = N$. Panel (b) shows the absolute value of the relative error $\delta(n)$ for both the real part (full line) and imaginary part (dashed line) of the matrix element (see text). The two horizontal dotted lines indicate the error at 1% and 0.1%. Panel (c) shows the decimal logarithm of the denominator of the prefactor in Eq. (1). The horizontal dotted line indicates the value 10^{-322}, which corresponds approximately to the smallest number that can be represented using the double-precision data type. The shaded area represents the range of validity of using Eq. (1) to compute the overlap at the double-precision level.

B. G. Carlsson and J.R, PRL 126, 172501 (2021)

Minimal canonical basis

Even number parity $|\Phi\rangle$:

$$\mathcal{O} = (-1)^{n/2} \mathrm{pf} \begin{pmatrix} [-\bar{U}\sigma]_{n\times n} & [\Lambda D^{\dagger} D' \Lambda']_{n\times n'} \\ -[\Lambda' D'^{T} D^{*} \Lambda]_{n'\times n} & [\sigma \bar{U}']_{n'\times n'} \end{pmatrix}$$

Odd number parity $\beta_a^{\dagger}|\Phi\rangle$:

$$\mathcal{O} = (-1)^{n/2} \mathrm{pf} \begin{pmatrix} -[\bar{U}\sigma]_{n\times n} & [\Lambda D^{\dagger} D' \Lambda']_{n\times n'} & [\Lambda D^{\dagger} \mathrm{V}^{(a)*}]_{n\times 1} & [\Lambda D^{\dagger} \mathrm{U}'^{(a')}]_{n\times 1} \\ & [\sigma \bar{U}']_{n'\times n'} & -[\Lambda' D'^{T} \mathrm{U}^{(a)*}]_{n'\times 1} & -[\Lambda' D'^{T} \mathrm{V}'^{(a')}]_{n'\times 1} \\ & & 0 & [\mathrm{U}^{(a)\dagger} \mathrm{U}'^{(a')}]_{1\times 1} \\ & & & 0 \end{pmatrix}$$

n and n' are number of v_i and v_i' in the respective canonical basis

Solves the problem to have exact and generaly applicable formulas for overlaps of Bogoliubov vacua

[1] B.G. Carlsson and J. Rutearou PRL 126 172501 (2021)

Projection and GCM

From: $H_{ij} = \left\langle \phi_i \left| \hat{H}^{eff} \hat{P}^I_{MK} \hat{P}^Z \hat{P}^N \right| \phi_j \right\rangle$

and $\mathcal{O}_{ij} = \left\langle \phi_i \left| \hat{P}^I_{MK} \hat{P}^Z \hat{P}^N \right| \phi_j \right\rangle$

One can set up the Hill-Wheeler equation:

$$\sum_j H_{ij} c^n_j = E_n \sum_j \mathcal{O}_{ij} c^n_j$$

Giving final states:

$$|IM, n\rangle = \sum_j c^n_j \, |\phi_j\rangle$$

and energies:

$$E^I_n$$

Minimal Canonical basis

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

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

$$
D^\dagger_b \rho D_a = \bar{\rho} = \begin{pmatrix} \bar{\rho}_{11} & 0 \\ 0 & 0 \end{pmatrix}
$$

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

$$
D^T_b \kappa^*_{01} D_a = \bar{\kappa}^*_{01} = \begin{pmatrix} (\bar{\kappa}^*_{01})_{11} & 0 \\ (\bar{\kappa}^*_{01})_{21} & 0 \end{pmatrix}
$$

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

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

Transitions directly from wave functions

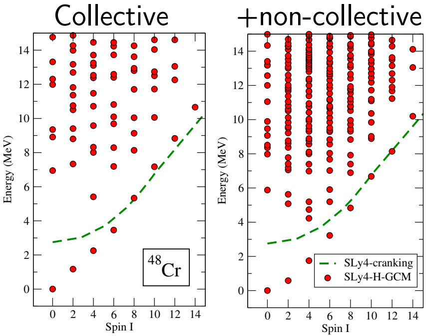
$$B\left(E2; I_i \rightarrow I_f\right) = \frac{1}{2I_i + 1} \sum_{M_f M_i \mu} \left| \left\langle I_f M_f | \hat{Q}_{2\mu} | I_i M_i \right\rangle \right|^2$$

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

GCM-basis

To sample the energy surface from H^{eff} we used:

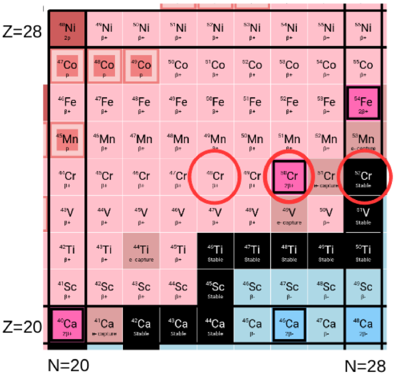
- Collective coordinates: $\beta, \gamma, \Delta, j_z$
- non-collective quasiparticle excitations $\rightarrow$ richer spectra



Cranking normalized to $I = 10$ state

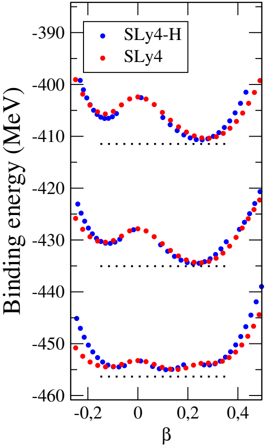
Lets test the new method with experiments

Test cases: ^{48}Cr, ^{50}Cr, ^{52}Cr



Effective Hamiltonians

In all three cases we obtain good reproductions of the energy surfaces



Parameters for the calculations

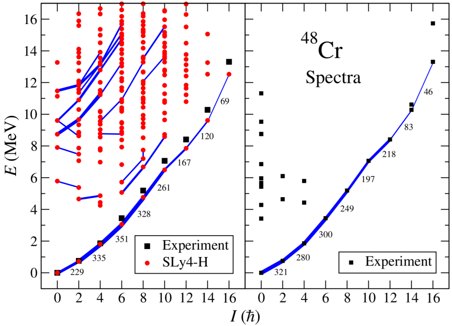
- Single-particle basis
  - Number of shells: 11 $\Rightarrow$ 728 states
- HFB-states
  - $\approx$ 200 within 12 MeV
- Projections
  - Particle number: $(Z, N) = (10, 10)$
  - Angular momentum: $(\alpha, \beta, \gamma) = (9, 18, 36)$
  - In total 116640 rotations per HFB-state
- Computational time: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

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

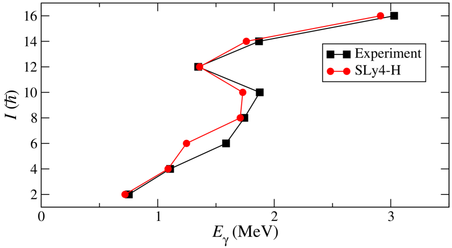
Half-full $f_{7/2}$ shell for both protons and neutrons

Terminating state at: $I = 16$

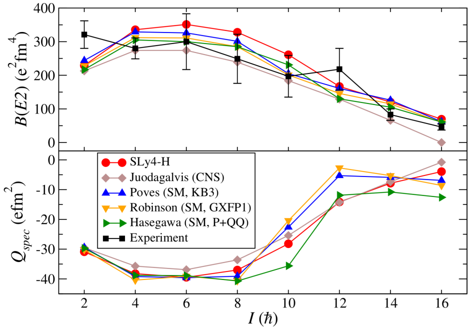
Spectra for ^{48}Cr



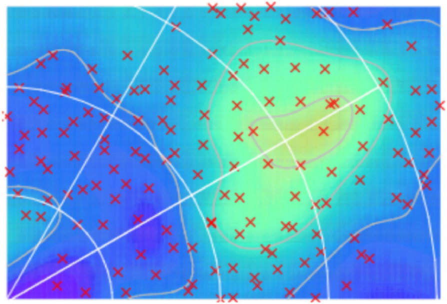
Backbending for ^{48}Cr



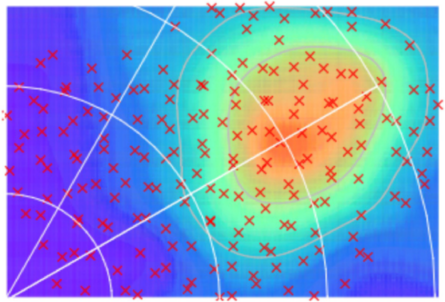
Transitions and quadrupole moments for ^{48}Cr



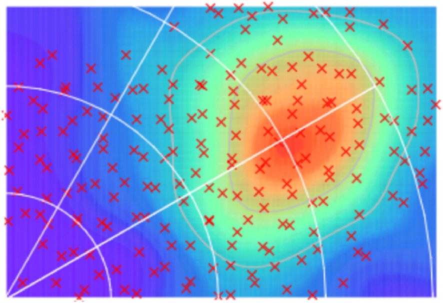
Amplitudes of HFB-states for ^{48}Cr; $I = 0$



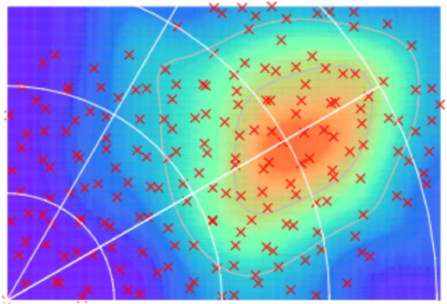
Amplitudes of HFB-states for ^{48}Cr; $I = 2$



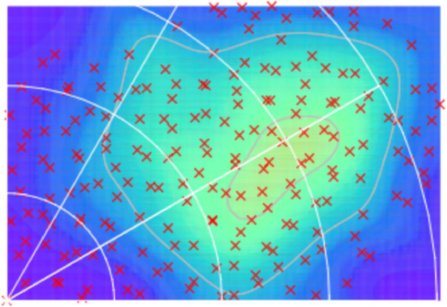
Amplitudes of HFB-states for ^{48}Cr; $I = 4$



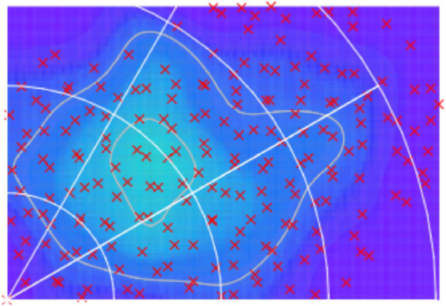
Amplitudes of HFB-states for ^{48}Cr; $I = 6$



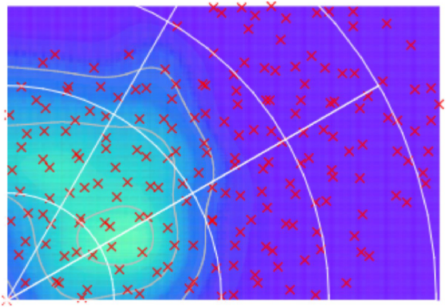
Amplitudes of HFB-states for ^{48}Cr; $I = 8$



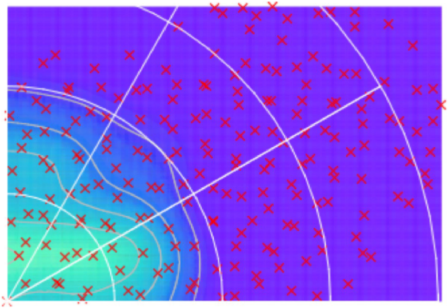
Amplitudes of HFB-states for ^{48}Cr; $I = 10$



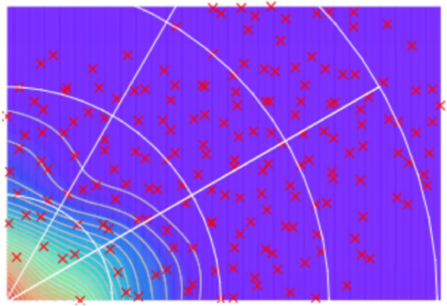
Amplitudes of HFB-states for ^{48}Cr; $I = 12$



Amplitudes of HFB-states for ^{48}Cr; $I = 14$



Amplitudes of HFB-states for ^{48}Cr; $I = 16$

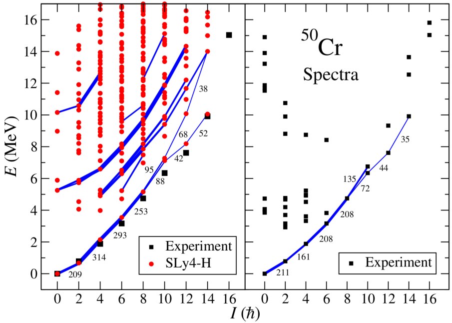


^{50}Cr, Z=24, N=26

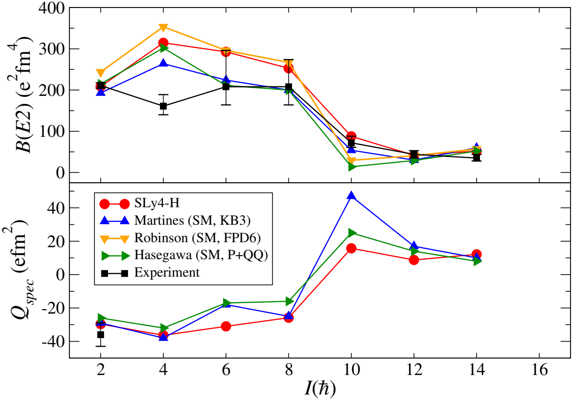
$f_{7/2}$ shell for both protons and neutrons

Terminating state at: $I = 14$

Spectra for ^{50}Cr



Transitions and quadrupole moments for ^{50}Cr

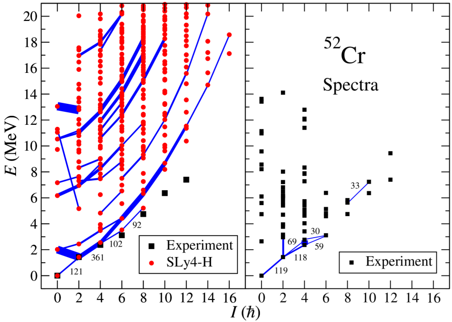


^{52}Cr, Z=24, N=28

Filled $f_{7/2}$ shell for neutrons

Terminating state at: $I = 8$

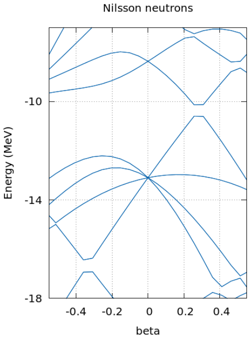
Spectra for ^{52}Cr

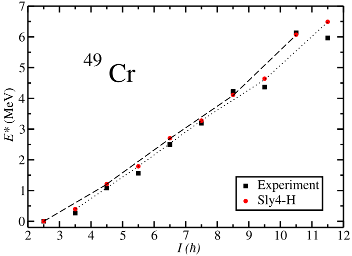


^{49}Cr, Z=24, N=25

Odd neutron in $f_{7/2}$ shell

odd nuclei: ${}^{49}_{24}Cr_{25}$





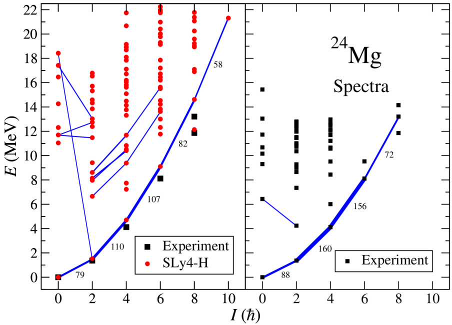
Standard test case for GCM

^{24}Mg, Z=12, N=12

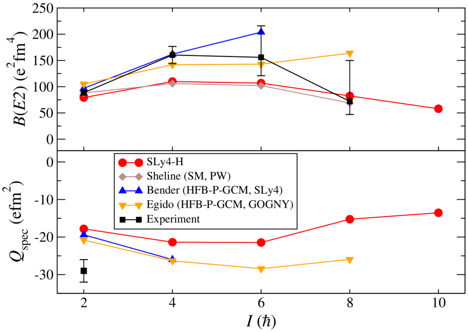
half-full $d_{5/2}$ shell

Terminating state at: $I = 8$

Spectra for ^{24}Mg



Transitions and quadrupole moments for ^{24}Mg



Summary/Outlook

- The simple effective Hamiltonian works surprisingly well.
- Allowed for fully symmetry restored descriptions in the full space following the bands to termination
- Next: more formal expansion of H^{eff} and computation of optical potential for nucleon-nucleus scatttering in progress

J. Ljungberg, B. G. Carlsson, J. Rotureau, A. Idini and I. Ragnarsson, arXiv:2204.10709 (2022), A. Såmark-Roth et al. PRL. 126, 032503 (2021), B.G. Carlsson and J. Rutearou PRL 126 172501 (2021)

Thank you for your attention!