Multi-Reference Energy Density Functional Theory: Status and perspectives

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Yukawa International Seminar
on Dynamics and Correlations in Exotic Nuclei (DCEN2011)
Kyoto, Japan, 26th September

UNIVERSITÉ DE BORDEAUX — CNRS — CENBG — SUPPORTED BY ANR

Sucesses so far

particle-number restoration operator

$$\hat{P}_{N_0} = \frac{1}{2\pi} \int_0^{2\pi} d\phi_N \underbrace{e^{-i\phi_N N_0}}_{\text{weight}} \quad \overbrace{e^{i\phi_N \hat{N}}}^{\text{rotation in gauge space}}$$

angular-momentum restoration operator

$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \, \sin(\beta) \int_0^{2\pi} d\gamma \, \underbrace{\mathcal{D}^{*J}_{MK}(\alpha, \beta, \gamma)}_{\text{Wigner function}} \quad \overbrace{\hat{R}(\alpha, \beta, \gamma)}^{\text{rotation in real space}}$$

K is the z component of angular momentum in the body-fixed frame.
Projected states are given by

$$|JM\kappa q\rangle = \sum_{K=-J}^{+J} f_{J,\kappa}(K) \, \hat{P}^J_{MK} \, \hat{P}^Z \, \hat{P}^N \, |q\rangle = \sum_{K=-J}^{+J} f_{J,\kappa}(K) \, |JMKq\rangle$$

$f_{J,\kappa}(K)$ is the weight of the component K and determined variationally

Axial symmetry (with the z axis as symmetry axis) allows to perform the α and γ integrations analytically, whereas the sum over K collapses, $f_{J,\kappa}(K) \sim \delta_{K0}$

Configuration Mixing via the Generator Coordinate Method

Superposition of angular-momentum projected SCMF states

$$|JM\nu\rangle = \sum_q \sum_{K=-J}^{+J} f_{J\nu}(q,K)\,|JMqK\rangle \quad \begin{cases} |JMqK\rangle & \text{projected mean-field state} \\ f_{J\nu}(q,K) & \text{weight function} \end{cases}$$

$$\frac{\delta}{\delta f^*_{J\nu}(q,K)} \frac{\langle JM\nu|\hat{H}|JM\nu\rangle}{\langle JM\nu|JM\nu\rangle} = 0 \quad \Rightarrow \quad \text{Hill-Wheeler-Griffin equation}$$

$$\sum_{q'} \sum_{K'=-J}^{+J} \left[\mathcal{H}_J(qK,q'K') - E_{J,\nu}\,\mathcal{I}_J(qK,q'K')\right] f_{J,\nu}(q'K') = 0$$

with

$$\begin{aligned} \mathcal{H}_J(qK,q'K') &= \langle JMqK|\hat{H}|JMq'K'\rangle \quad && \text{energy kernel} \\ \mathcal{I}_J(qK,q'K') &= \langle JMqK|JMq'K'\rangle && \text{norm kernel} \end{aligned}$$

Angular-momentum projected GCM gives the

- correlated ground state for each value of J
- spectrum of excited states for each J

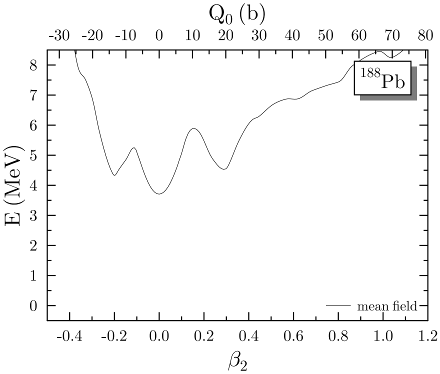
Semantics

- Single reference (SR) $\equiv$ "mean field" or "HFB"
- Multi reference (MR) $\equiv$ projection and Generator Coordinate Method

Our implementation(s)

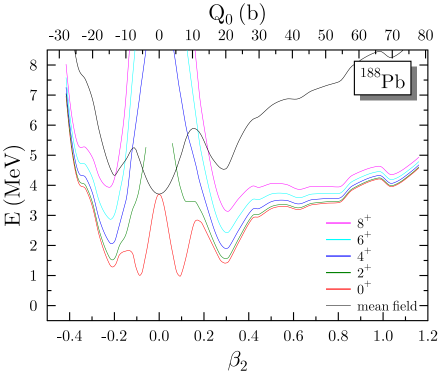
- Coordinate space representation on a 3d mesh using Lagrange-mesh techniques
- mean-field codes assume time-reversal invariance and good parity
- "HF+BCS" or "HFB" solved with two-basis method
- MR-EDF most often with states constrained to axial symmetry
- full space of occupied single-particle states
- Skyrme energy density functionals

Configuration mixing via the projected Generator Coordinate Method



M. B., P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.

Spectroscopy from MR EDF



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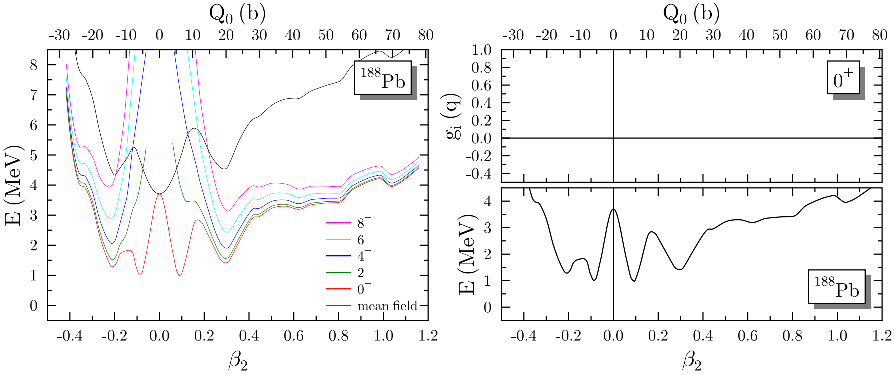

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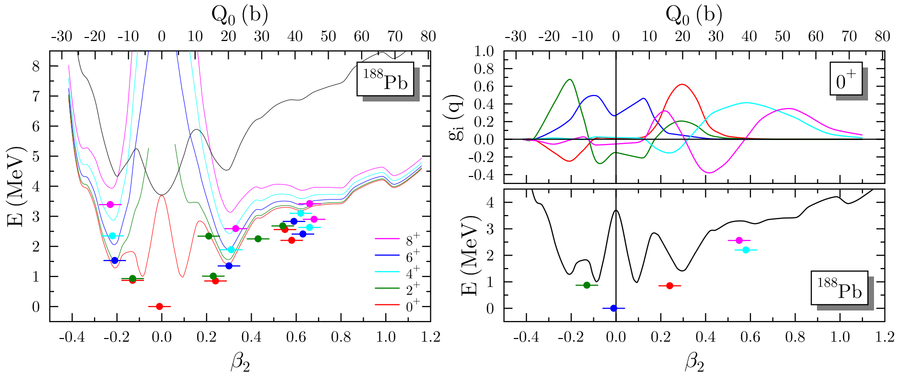

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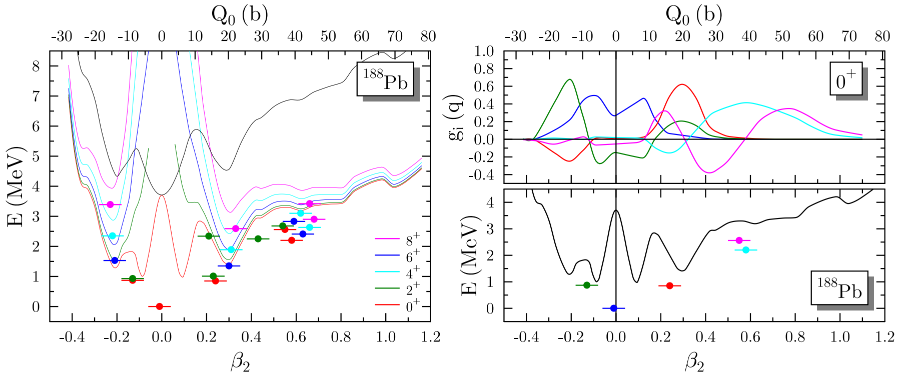
Attention: $g_i^2(q)$ is not the probability to find a mean-field state with intrinsic deformation q in the collective state



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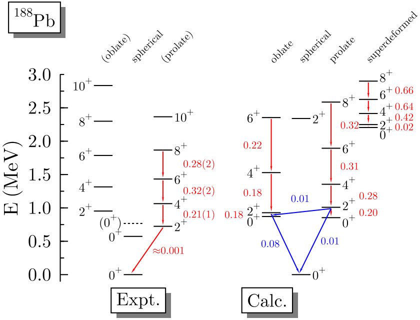
Spectroscopy from MR EDF: Transition moments

M. B., P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.
Experiment: T. Grahn *et al*, Phys. Rev. Lett. **97** (2006) 062501

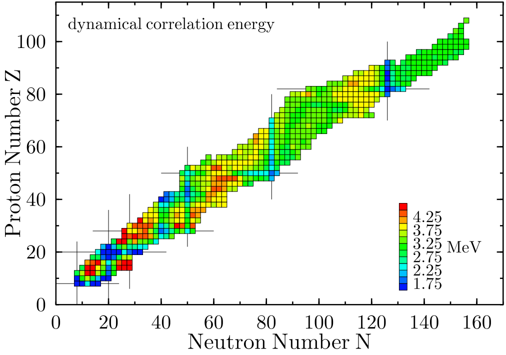


- in-band and out-of-band $E2$ transition moments directly in the laboratory frame with correct selection rules
- full model space of occupied particles
- only occupied single-particle states contribute to the kernels ("horizontal expansion")
- $\Rightarrow$ *no effective charges necessary*
- *no adjustable parameters*

$$B(E2; J'_{\nu'} \to J_\nu) = \frac{e^2}{2J'+1} \sum_{M=-J}^{+J} \sum_{M'=-J'}^{+J'} \sum_{\mu=-2}^{+2} |\langle JM\nu | \hat{Q}_{2\mu} | J' M' \nu' \rangle|^2$$

$$\beta_2^{(t)} = \frac{4\pi}{3R^2 A} \sqrt{\frac{B(E2; J \to J-2)}{(J\,0\,2\,0\,|(J-2)\,0)^2 e^2}} \quad \text{with} \quad R = 1.2\, A^{1/3}$$

Static and Dynamic Quadrupole Correlation Energies



M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

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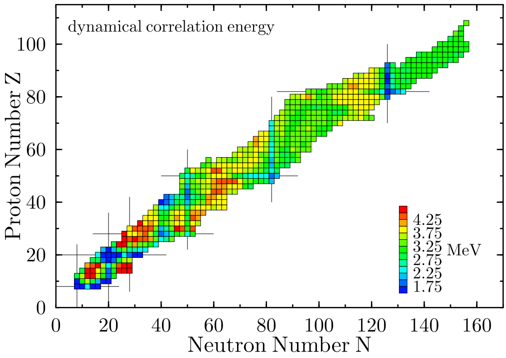

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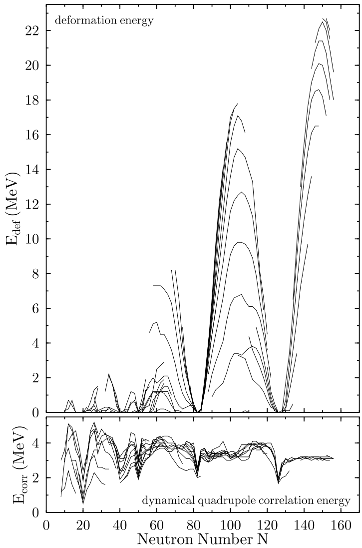
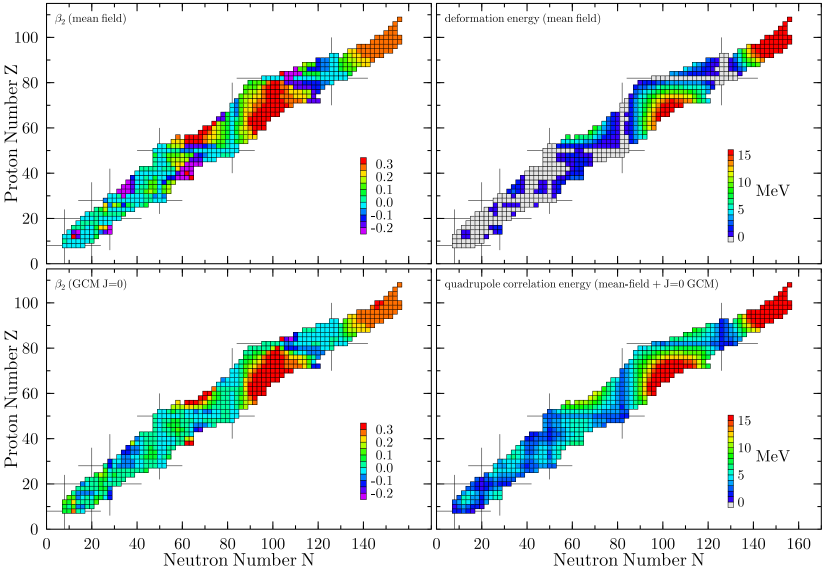


Intrinsic Deformation and Quadrupole Correlation Energy



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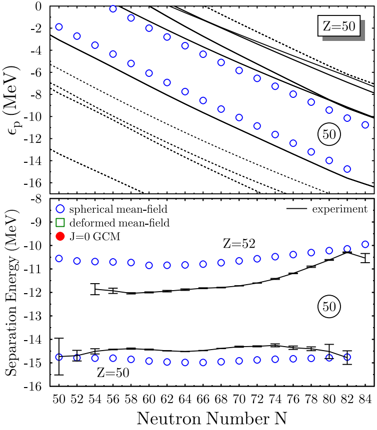
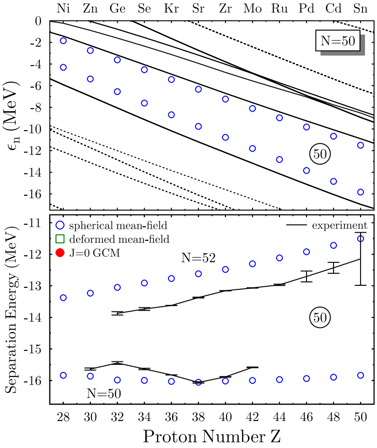
Eigenvalues of the single-particle Hamiltonian vs. S_{2q}



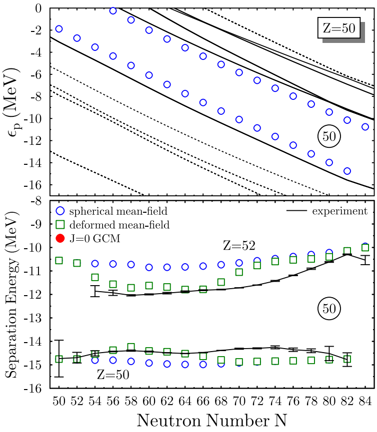


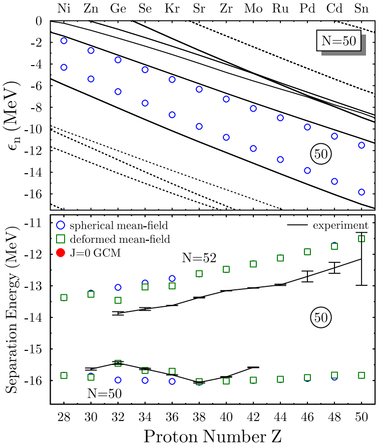
lower panel: $-S_{2p}(Z=50, N)/2$
The global linear trend is taken out subtracting
$\frac{N-82}{2}\,[S_{2p}(Z{=}50, N{=}50) - S_{2p}(Z{=}50, N{=}82)]$
using the spherical mean-field S_{2p}

M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

lower panel: $-S_{2n}(Z, N=50)/2$
The global linear trend is taken out subtracting
$\frac{N-50}{2}\,[S_{2n}(Z{=}28, N{=}50) - S_{2n}(Z{=}50, N{=}50)]$
using the spherical mean-field S_{2n}

Eigenvalues of the single-particle Hamiltonian vs. S_{2q}





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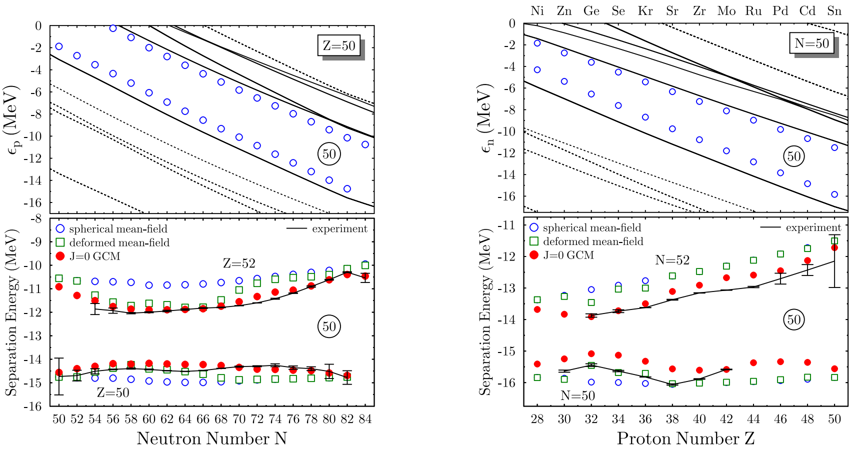

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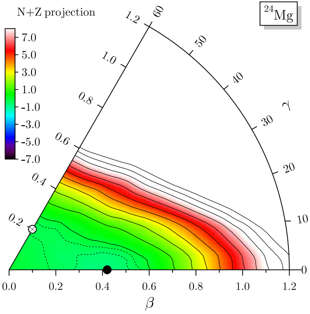
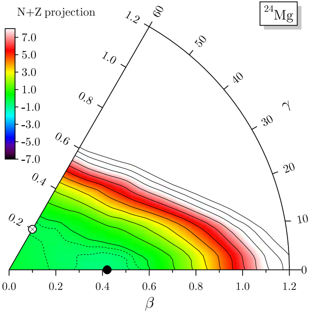
mean-field deformation energy surface

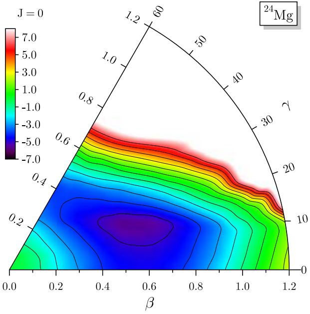


Angular momentum projection of triaxial states

mean-field deformation energy surface



$J = 0$ projected deformation energy surface



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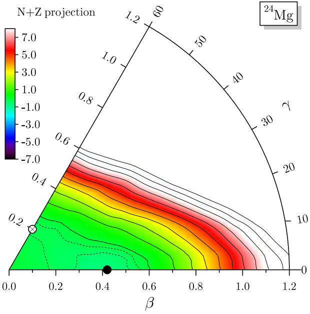

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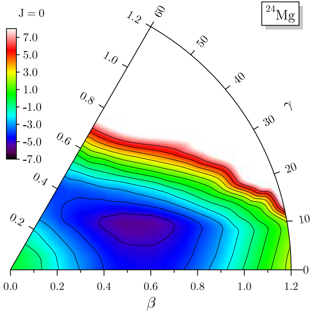
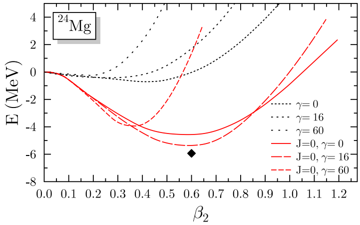
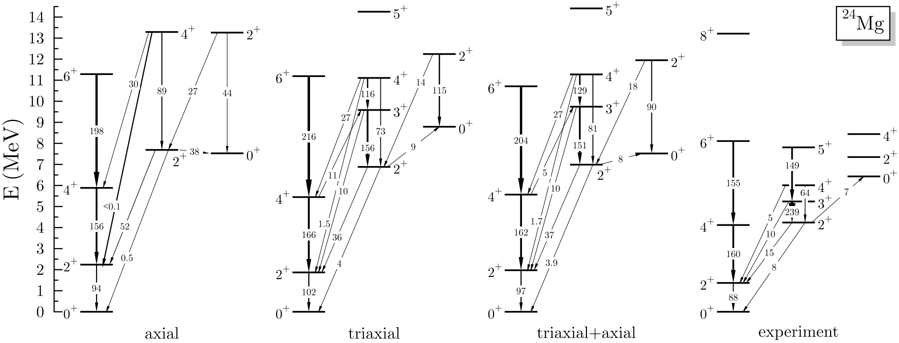




M. B. and P.-H. Heenen, Phys. Rev. C **78** (2008) 024309

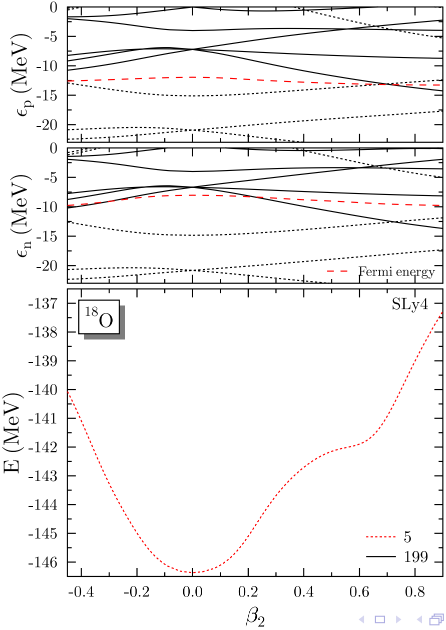
Mixing of angular-momentum projected triaxial states of different intrinsic deformation



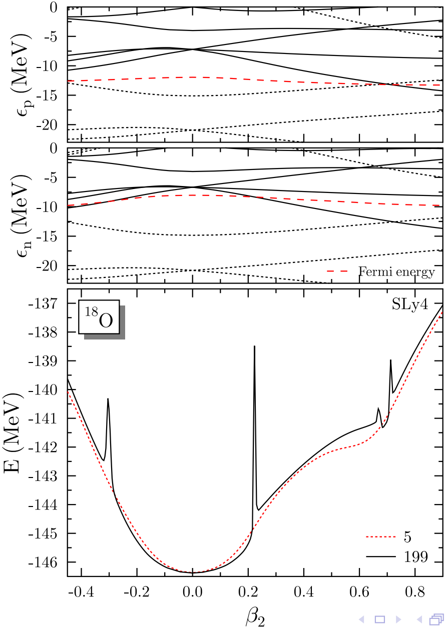
M. B. and P.-H. Heenen, Phys. Rev. C **78** (2008) 024309

Regularized MR EDF

Here is a problem . . .



Here is a problem . . .



The poles are a consequence of using the Generalized Wick theorem of Balian and Brézin

$$\frac{\langle \mathrm{L}|\hat{H}^{(2)}|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} = \frac{\langle \mathrm{L}|\sum_{ijmn}\hat{H}^{(2)}_{ijmn} a_i^\dagger a_j^\dagger a_n a_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle}$$

$$= \sum_{ijmn} \hat{H}^{(2)}_{ijmn} \Big[\frac{\langle \mathrm{L}|\hat{a}_i^\dagger \hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \frac{\langle \mathrm{L}|\hat{a}_j^\dagger \hat{a}_n|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} - \frac{\langle \mathrm{L}|\hat{a}_i^\dagger \hat{a}_n|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \frac{\langle \mathrm{L}|\hat{a}_j^\dagger \hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} + \frac{\langle \mathrm{L}|\hat{a}_i^\dagger \hat{a}_j^\dagger|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \frac{\langle \mathrm{L}|\hat{a}_n \hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \Big] \langle \mathrm{L}|\mathrm{R}\rangle$$

to *postulate* an MR EDF *that does not corespond to an operator*.

$$\begin{aligned} \mathcal{E} \quad = \quad & \Big[\sum_{ijmn} \hat{v}^{\rho\rho}_{ijmn} \frac{\langle \mathrm{L}|\hat{a}_i^\dagger \hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \frac{\langle \mathrm{L}|\hat{a}_j^\dagger \hat{a}_n|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} - \hat{v}'^{\rho\rho}_{ijmn} \frac{\langle \mathrm{L}|\hat{a}_i^\dagger \hat{a}_n|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \frac{\langle \mathrm{L}|\hat{a}_j^\dagger \hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \\ & + \hat{v}^{\kappa\kappa}_{ijmn} \frac{\langle \mathrm{L}|\hat{a}_i^\dagger \hat{a}_j^\dagger|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \frac{\langle \mathrm{L}|\hat{a}_n \hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \Big] \langle \mathrm{L}|\mathrm{R}\rangle \end{aligned}$$

as the $\frac{1}{\langle \mathrm{L}|\mathrm{R}\rangle}$ divergence for orthogonal states $\langle \mathrm{L}|\mathrm{R}\rangle \to 0$ does not cancel out anymore.

Translating to coordinate space representation

$$\int d^3r \, \rho^2(\mathbf{r}) = \int d^3r \left[\sum_{ik} \rho_{ki} \psi_i^\dagger(\mathbf{r}) \psi_k(\mathbf{r}) \right] \left[\sum_{lj} \rho_{lj} \psi_j^\dagger(\mathbf{r}) \psi_l(\mathbf{r}) \right]$$

$$= \sum_{ijkl} \underbrace{\int d^3r \, \psi_i^\dagger(\mathbf{r}) \psi_j^\dagger(\mathbf{r}) \psi_k(\mathbf{r}) \psi_l(\mathbf{r})}_{\bar{v}_{ijkl}^{\rho\rho}} \, \rho_{ki} \, \rho_{lj}$$

and similar for other terms.

True contact force $t_0\,(1 + x_0 \hat{P}^{\sigma})\,\delta(\mathbf{r} - \mathbf{r}')$

$$\begin{aligned}\mathcal{E} &= \int d^3r\,\Big\{ \tfrac{3}{8}\,t_0\,\rho_0^2(\mathbf{r}) - \tfrac{1}{8}\,t_0\,(1+2x_0)\,\rho_1^2(\mathbf{r}) - \tfrac{1}{8}\,t_0\,(1-2x_0)\,\mathbf{s}_0^2(\mathbf{r}) \\ &\quad -\tfrac{1}{8}\,t_0\,\mathbf{s}_1^2(\mathbf{r}) + \tfrac{1}{8}\,t_0\,(1+x_0)\,\breve{\mathbf{s}}_0(\mathbf{r})\cdot\breve{\mathbf{s}}_0^*(\mathbf{r}) + \tfrac{1}{8}\,t_0\,(1-x_0)\,\breve{\rho}_1(\mathbf{r})\,\breve{\rho}_1^*(\mathbf{r})\Big\}\end{aligned}$$

(see Perlinska *et al.* PRC 69 (2004) 014316 for definition of $\breve{\mathbf{s}}_0(\mathbf{r})$ and $\breve{\rho}_1(\mathbf{r})$)

Contact functional:

$$\begin{aligned}\mathcal{E} &= \int d^3r\,\Big\{ C_0^{\rho}[\rho_0,\ldots]\,\rho_0^2(\mathbf{r}) + C_1^{\rho}[\rho_0,\ldots]\,\rho_1^2(\mathbf{r}) + C_0^{s}[\rho_0,\ldots]\,\mathbf{s}_0^2(\mathbf{r}) \\ &\quad + C_1^{s}[\rho_0,\ldots]\,\mathbf{s}_1^2(\mathbf{r}) + C_0^{\breve{s}}[\rho_0,\ldots]\,\breve{\mathbf{s}}_0(\mathbf{r})\cdot\breve{\mathbf{s}}_0^*(\mathbf{r}) + C_1^{\breve{\rho}}[\rho_0,\ldots]\,\breve{\rho}_1(\mathbf{r})\,\breve{\rho}_1^*(\mathbf{r})\Big\}\end{aligned}$$

Functionals corresponding to "true Hamiltonians" vs. "true" functionals

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Coulomb interaction $\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$

$$\mathcal{E} = \frac{1}{2}\iint d^3r\,d^3r'\,\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\Big[\rho_p(\mathbf{r})\rho_p(\mathbf{r}') - \rho_p(\mathbf{r},\mathbf{r}')\rho_p(\mathbf{r}',\mathbf{r}) + \kappa_p^*(\mathbf{r},\mathbf{r}')\kappa_p(\mathbf{r},\mathbf{r}')\Big]$$

Approximate Coulomb functionals

$$\mathcal{E} = \frac{e^2}{2}\iint d^3r\,d^3r'\,\frac{\rho_p(\mathbf{r})\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} - \frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}\int d^3r\,\rho_p^{4/3}(\mathbf{r})$$

$$
\begin{aligned}
&\int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, c_N^2} \, \mathcal{E}_{GWT}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0 \, *}] \, \langle \Phi_0 | \Phi_\varphi \rangle \\
&= \quad \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, c_N^2} \Bigg[\sum_\mu t_{\mu\mu} \, \frac{v_\mu^2 \, e^{2i\varphi}}{u_\mu^2 + v_\mu^2 \, e^{2i\varphi}} \\
&\qquad + \frac{1}{2} \sum_{\mu\nu} \bar{v}^{\rho\rho}_{\mu\nu\mu\nu} \, \frac{v_\mu^2 \, e^{2i\varphi}}{u_\mu^2 + v_\mu^2 \, e^{2i\varphi}} \, \frac{v_\nu^2 \, e^{2i\varphi}}{u_\nu^2 + v_\nu^2 \, e^{2i\varphi}} \\
&\qquad + \frac{1}{4} \sum_{\mu\nu} \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\nu\bar{\nu}} \, \frac{u_\mu \, v_\mu}{u_\mu^2 + v_\mu^2 \, e^{2i\varphi}} \, \frac{u_\nu \, v_\nu \, e^{2i\varphi}}{u_\nu^2 + v_\nu^2 \, e^{2i\varphi}} \Bigg] \prod_{\lambda>0} (u_\lambda^2 + v_\lambda^2 \, e^{2i\varphi})
\end{aligned}
$$

there are terms with $\mu = \nu$ which diverge for $u_\mu^2 = v_\mu^2 = 0.5 \Leftrightarrow \frac{|u_\mu|}{|v_\mu|} = 1$ and $\varphi = \pi/2$ [Anguiano, Egido, Robledo NPA696(2001)467]

Same divergence pointed out by Dönau, PRC 58 (1998) 872 in terms of approximations in a Hamiltonian-based framework.

First analysis of the homologue in a strict energy density functional framework and of EDF-specific consequences by Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315

Similar problem discussed by Tajima, Flocard, Bonche, Dobaczewski and Heenen, NPA542 (1992) 355 for EDF kernels between HFB vacua and two-quasiparticle states.

Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315
M. B., T. Duguet, and D. Lacroix, PRC 79 (2009) 044319

substitute $z = e^{i\varphi}$ $\Rightarrow$ contour integrals in the complex plane

Projected energy functional

$$\mathcal{E}_N = \oint_{C_1} \frac{dz}{2i\pi c_N^2} \frac{\mathcal{E}[z]}{z^{N+1}} \prod_{\mu>0} (u_\mu^2 + v_\mu^2 z^2)$$

norm

$$c_N^2 = \oint_{C_1} \frac{dz}{2i\pi} \frac{1}{z^{N+1}} \prod_{\mu>0} (u_\mu^2 + v_\mu^2 z^2),$$

transition density matrix and pairing tensor

$$\rho_{\mu\nu}^{0z} = \frac{v_\mu^2 z^2}{u_\mu^2 + v_\mu^2 z^2} \delta_{\nu\mu} \quad \kappa_{\mu\nu}^{0z} = \frac{u_\mu v_\mu}{u_\mu^2 + v_\mu^2 z^2} \delta_{\nu\bar{\mu}}\,, \quad \kappa_{\mu\nu}^{z0\,*} = \frac{u_\mu v_\mu z^2}{u_\mu^2 + v_\mu^2 z^2} \delta_{\nu\bar{\mu}}$$

Complex plane analysis II

- Contour integrals can be evaluated using Cauchy's residue theorem [Bayman, NP15 (1960) 33]
- the norm and all operator matrix elements have a pole at $z = 0$

$$c_N^2 = 2i\pi \, \mathcal{R}es(0) \left[\frac{1}{z^{N+1}} \prod_{\mu>0} \left(u_\mu^2 + v_\mu^2 \, z^2 \right) \right]$$

Complex plane analysis II

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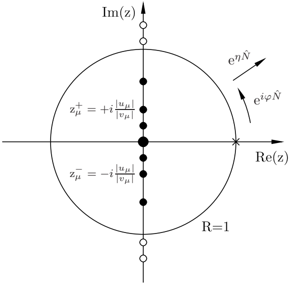
- the energy functional has poles at $z = 0$ and $z^{\pm} = \pm \frac{u_\mu}{v_\mu}$

$$\mathcal{E}_N = \sum_{\substack{z_i = 0 \\ |z_\mu^{\pm}| < 1}} \frac{2i\pi}{c_N^2} \, \mathcal{R}es(z_i) \left[\frac{\mathcal{E}[z]}{z^{N+1}} \prod_{\mu>0} \left(u_\mu^2 + v_\mu^2 z^2 \right) \right]$$

- poles entering or leaving the integration contour might generate divergences, steps, or discontinuities



- poles of the particle number restored EDF
- filled (open) circles: poles inside (outside) the standard integration contour at $R = 1$
- cross: SR energy functional at $\varphi = 0$.

- The poles are not directly caused by the breaking of the Pauli principle as such, but of the way how the EDF is constructed.
- This can be shown in a quasiparticle basis where the kernels can be constructed using a standard Wick theorem (SWT) or elementary operator algebra

$$\sum_{ijmn} \hat{H}^{(2)}_{ijmn} \langle \mathrm{L} | \hat{\alpha}^\dagger_i \hat{\alpha}^\dagger_j \hat{\alpha}_m \hat{\alpha}_n | \mathrm{R} \rangle$$

- This requires a particular quasiparticle basis where $|\mathrm{R}\rangle = \prod_i (A_{ii} + B_{i\bar{\imath}} \hat{\alpha}^\dagger_i \hat{\alpha}^\dagger_{\bar{\imath}}) \, |\mathrm{L}\rangle$, which is the canonical basis of the Bogoliubov transformation between the “left” and “right” quasiparticle bases.
- From this expression one can construct an MR EDF that does not contain divergent terms.

For technical details see
D. Lacroix, T. Duguet, and M. B., PRC 79 (2009) 044318
M. B., T. Duguet, and D. Lacroix, PRC 79 (2009) 044319
T. Duguet, M. B., K. Bennaceur, D. Lacroix, and T. Lesinski, PRC 79 (2009) 044320
+ papers in preparation by M. B., B. Avez, T. Duguet, P.-H. Heenen and D. Lacroix

The correction for a strictly bilinear functional (in a given nucleon species)

For particle-number restoration, the difference between both ways of constructing the functional is

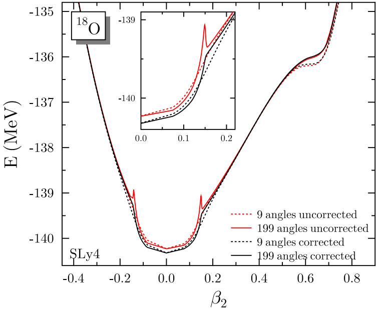
$$
\begin{aligned}
\mathcal{E}_{CG}^{N} &= \sum_{\mu>0} \left[\frac{1}{2} \left(\bar{v}^{\rho\rho}_{\mu\mu\mu\mu} + \bar{v}^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}} + \bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} + \bar{v}^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu} \right) - \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}} \right] \\
&\quad \times (u_\mu v_\mu)^4 \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, c_N^2} \, \frac{\left(e^{2i\varphi} - 1\right)^2}{u_\mu^2 + v_\mu^2 \, e^{2i\varphi}} \prod_{\substack{\nu>0 \\ \nu\neq\mu}} (u_\nu^2 + v_\nu^2 \, e^{2i\varphi}) \\
&= \sum_{\mu>0} \left[\tfrac{1}{2} \left(\bar{v}^{\rho\rho}_{\mu\mu\mu\mu} + \bar{v}^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}} + \bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} + \bar{v}^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu} \right) - \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}} \right] \\
&\quad \times \frac{(u_\mu v_\mu)^4}{2i\pi c_N^2} \oint_{C_1} \frac{dz}{z^{N+1}} \, \frac{\left(z^2 - 1\right)^2}{\left(u_\mu^2 + v_\mu^2 \, z^2\right)} \prod_{\substack{\nu>0 \\ \nu\neq\mu}} (u_\nu^2 + v_\nu^2 \, z^2)
\end{aligned}
$$

D. Lacroix, T. Duguet, and M. B., PRC 79 (2009) 044318, M. B., T. Duguet, and D. Lacroix, PRC 79 (2009) 044319

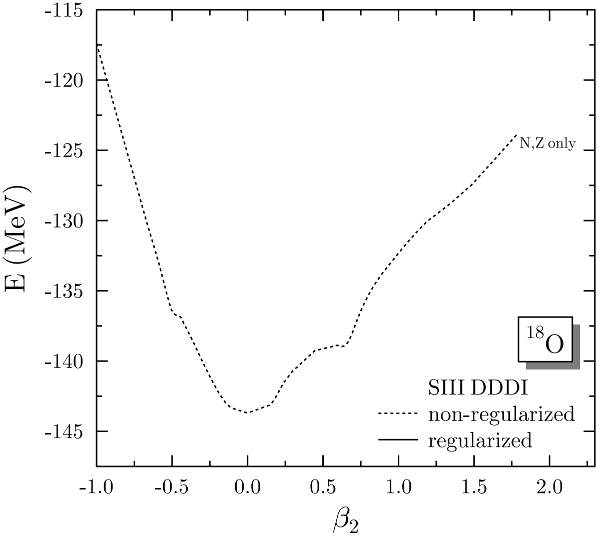
- The poles turn out to be a consequence of using the GWT to motivate the multi-reference energy functional
- They appear in terms that are spurious self-interactions or spurious self-pairing, the former known for long from condensed-matter DFT.
- self-interaction is related to broken antisymmetry of vertices in the functional (the interaction energy of a particle with itself should be zero)
- self-pairing comes from an incomplete combination of vertices (the energy from scattering a pair of particles onto themselves should be equal to the no-pairing value)
- The GWT adds a second level of spuriosity to these terms as it multiplies them with "unphysical" weight factors
- $\mathcal{E}^N_{CG}$ contains entirely the poles at $z^{\pm}_{\mu} = \pm \frac{|u_\mu|}{|v_\mu|}$ and a contribution from the pole at $z = 0$
- Subtracting $\mathcal{E}^N_{CG}$ as a correction from the energy functional removes the unphysical poles

Non-viability of non-integer density dependencies

- we do not see a way to set up a regularization scheme for non-integer density dependencies
- we can simulate a "density-dependent Hamiltonian" regularizing the biliear part, leaving only the density dependence unregularized
- there remains a spurious contribution from branch cuts (see Duguet *et al.* PRC 79 (2009) 044320 for complex plane analysis)
- (partial) workaround: use projected densities for density dependence instead

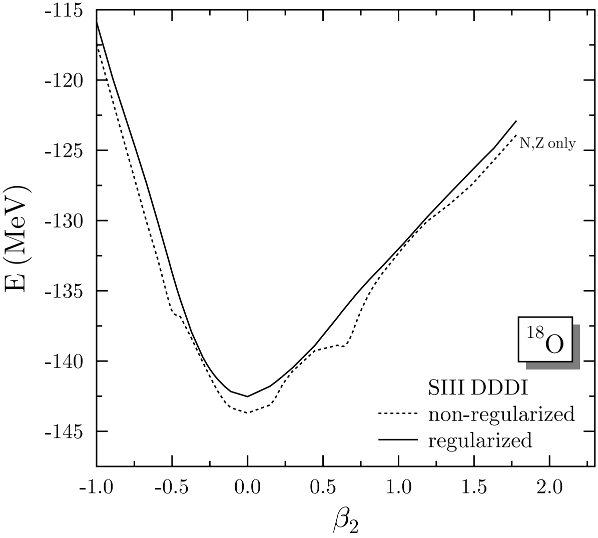


General configuration mixing: ^{18}O



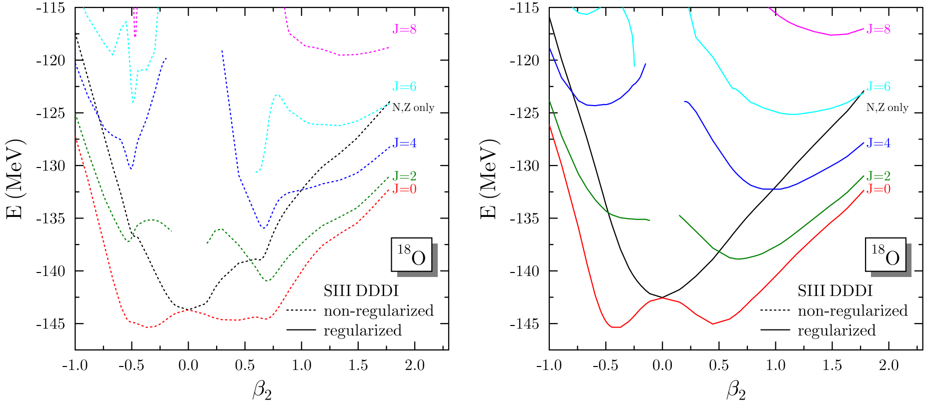
M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

General configuration mixing: ^{18}O



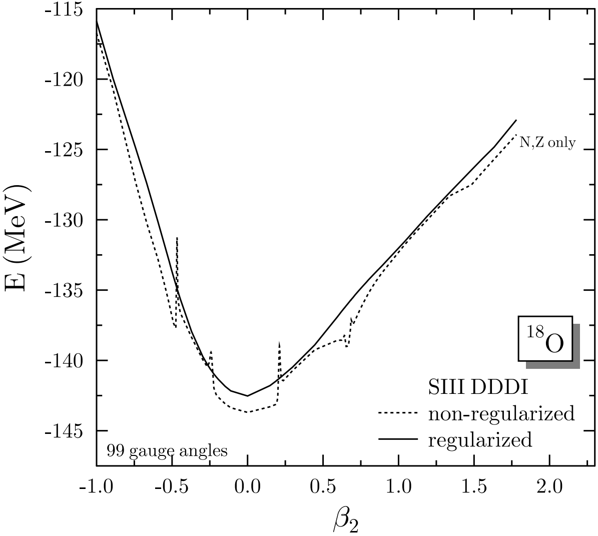
M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

General configuration mixing: ^{18}O



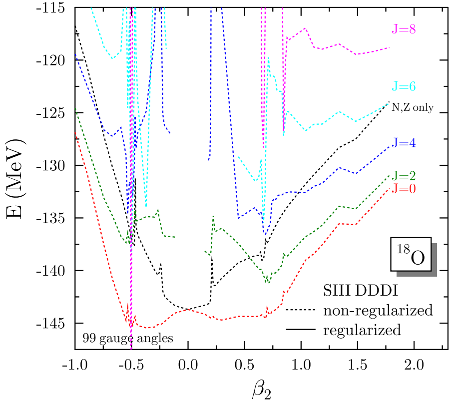
M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

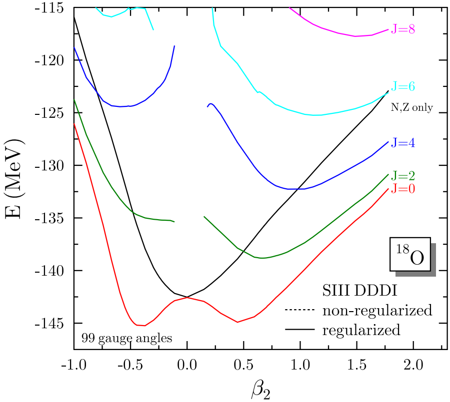
General configuration mixing: ^{18}O



M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

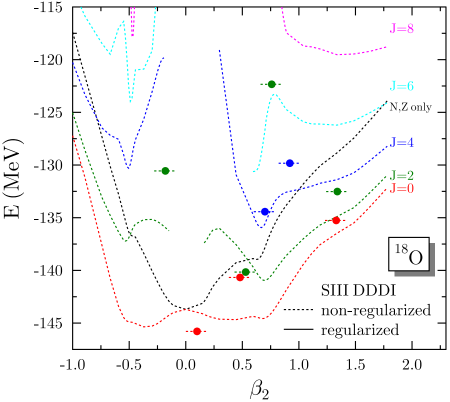
General configuration mixing: ^{18}O

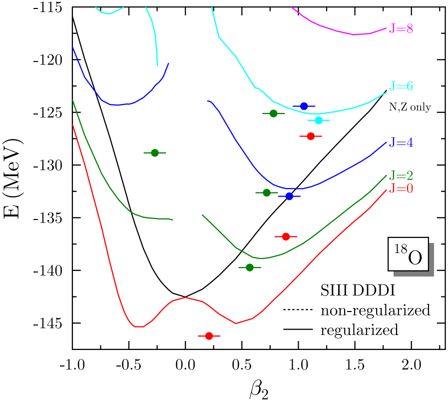




M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

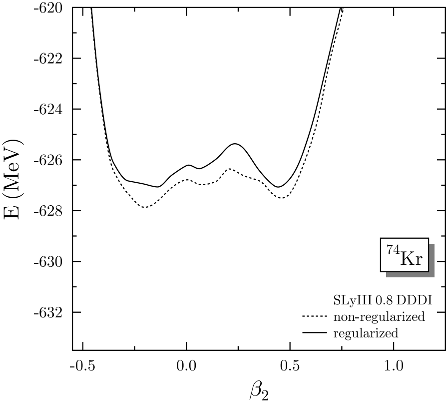
General configuration mixing: ^{18}O





M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

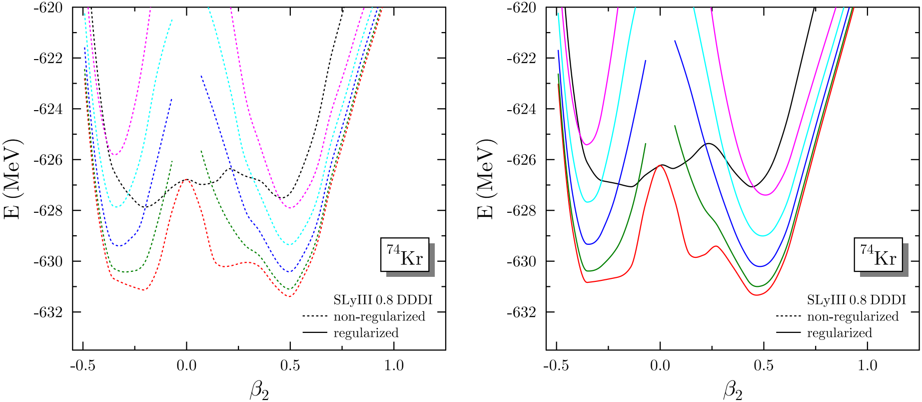
General configuration mixing: ^{74}Kr



- New bilinear + trilinear EDF fitted by K. Washiyama, K. Bennaceur, M. B., P.-H. Heenen, V. Hellemans (in preparation)

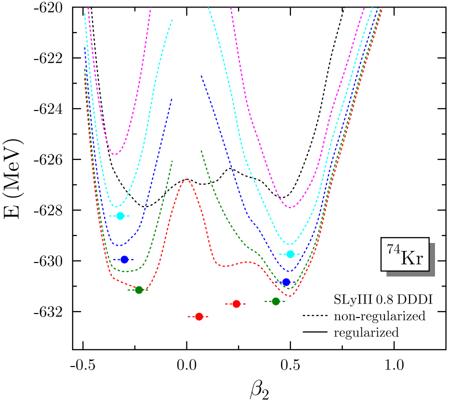
M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

General configuration mixing: ^{74}Kr

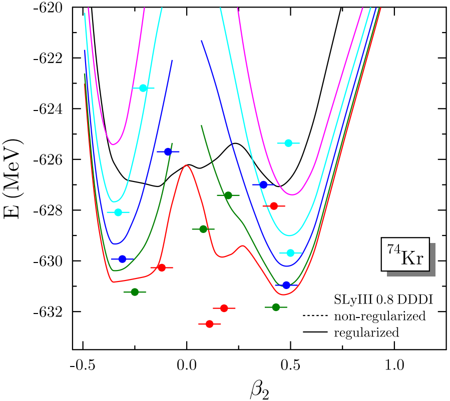


M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

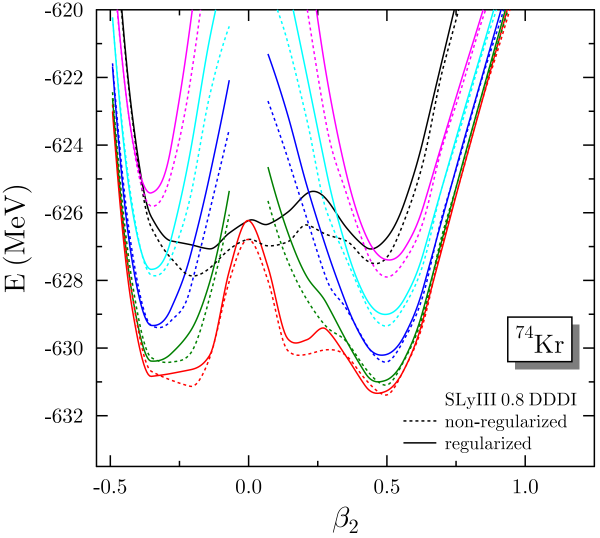
General configuration mixing: ^{74}Kr



M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

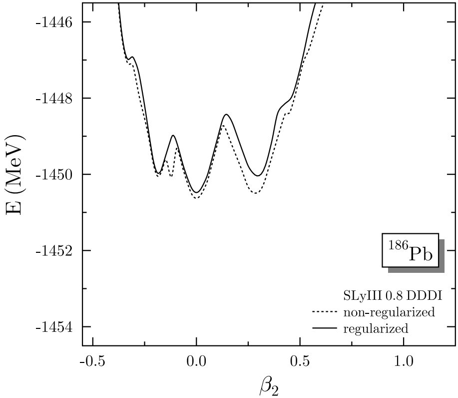


General configuration mixing: ^{74}Kr



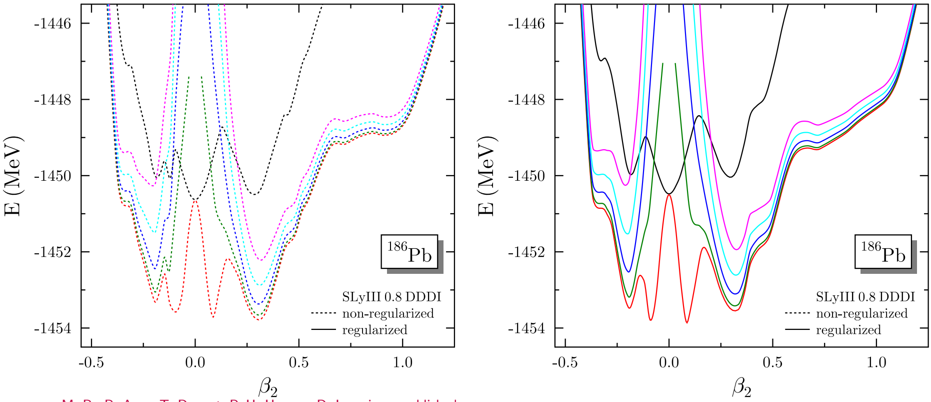
M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

General configuration mixing: ^{186}Pb



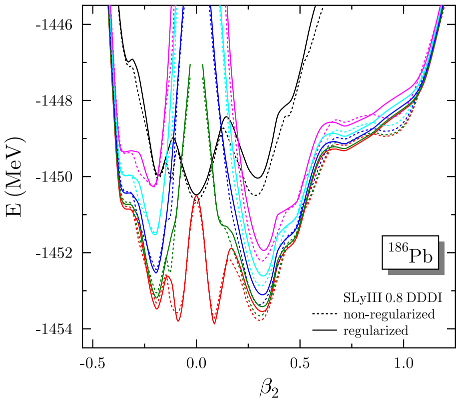
M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

General configuration mixing: ^{186}Pb



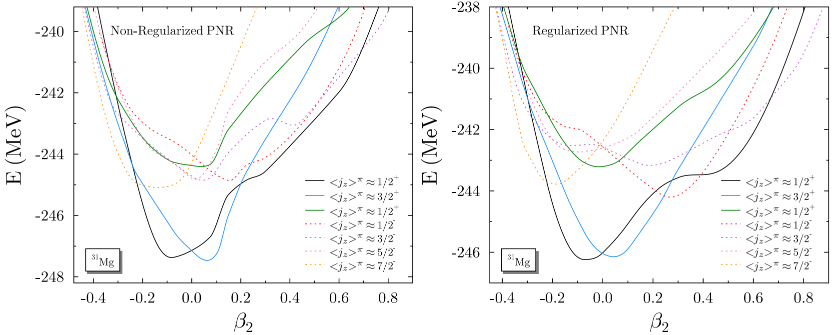
M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

General configuration mixing: ^{186}Pb



M. B., B. Avez, T. Duguet, P.-H. Heenen, D. Lacroix, unpublished

Particle-number restoration of ^{31}Mg



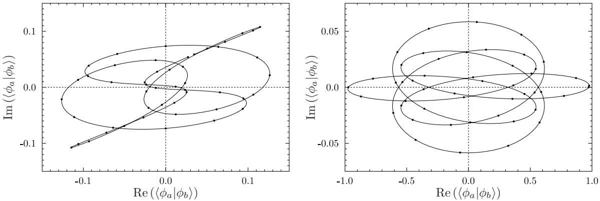
Benjamin Bally, Benoît Avez, M. B., P.-H. Heenen (unpublished)

Work in progress

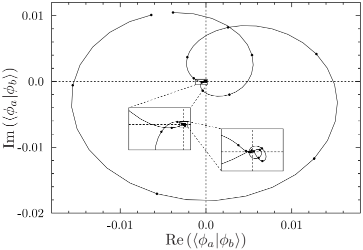
Overlap from Pfaffian formula, Benoît Avez & M. B., arXiv:1109.2078v1

α, β held fixed at some values, γ varied

lowest blocked one-quasiparticle state in ^{25}Mg

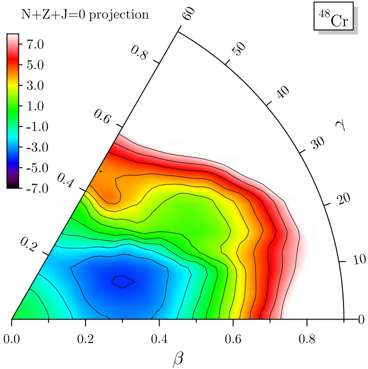


^{24}Mg cranked to $I = 8\hbar$

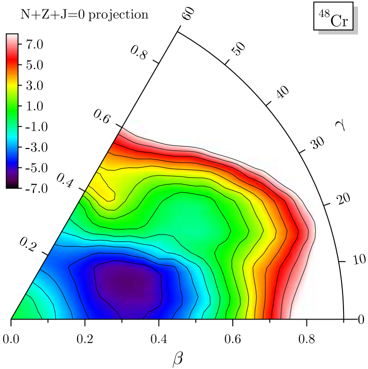


General configuration mixing: ^{48}Cr

non-regularized $N = Z = 24$, $J = 0$ projection



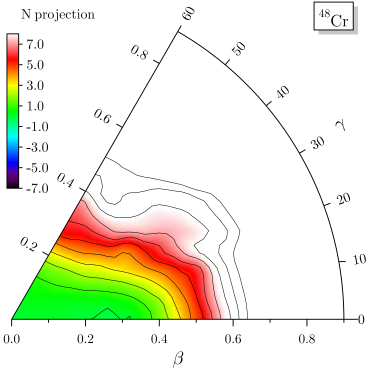
regularized $N = Z = 24$, $J = 0$ projection



B. Avez, M. B., P.-H. Heenen, unpublished

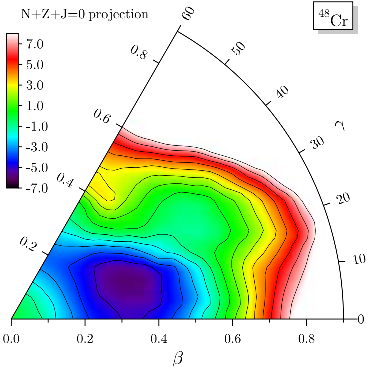
General configuration mixing: ^{48}Cr

regularized $N = Z = 24$ projection

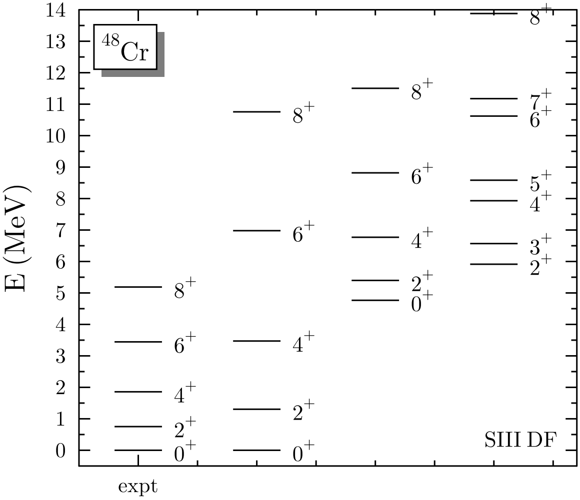


B. Avez, M. B., P.-H. Heenen, unpublished

regularized $N = Z = 24$, $J = 0$ projection



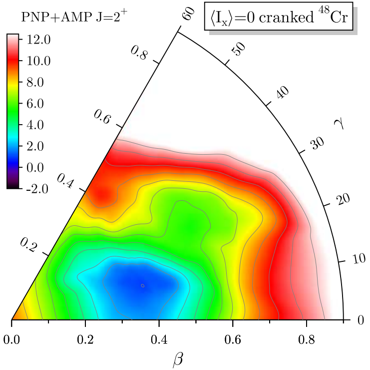
Preliminary: GCM of ^{48}Cr



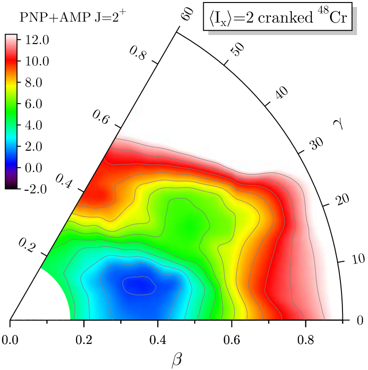
B. Avez, M. B., P.-H. Heenen, unpublished

Projection of cranked states: effect on energy surface for $J^\pi = 2^+$

$J^\pi = 2^+$ from HFB ground state

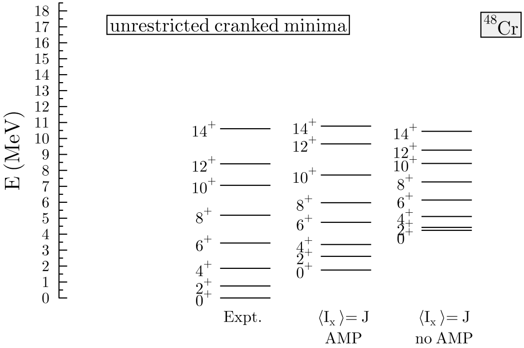


$J^\pi = 2^+$ from $\langle I_x \rangle = 2$ cranked state



B. Avez, M. B., P.-H. Heenen, unpublished

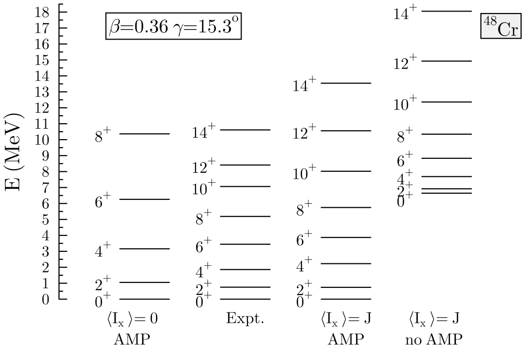
Projection of the rotational band from cranked HFB



- excitation spectra now too much compressed (at low spin)

B. Avez, M. B., P.-H. Heenen, unpublished

Deformation-constrained band build on the projected 0^+ minimum

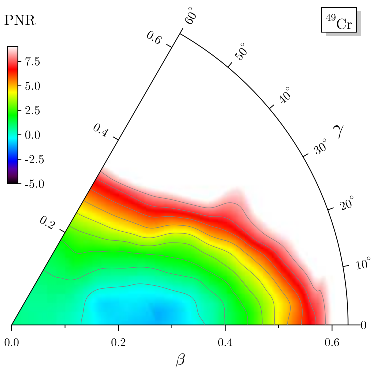


- improved moment of inertia at low spin
- for $J > 8$, the projected states from the cranked minima (previous slide) are lower in absolute energy
- backbending cannot be reproduced at fixed deformation

B. Avez, M. B., P.-H. Heenen, unpublished

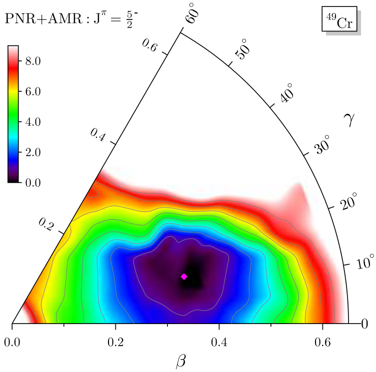
Particle-number and angular-momentum projection of ^{49}Cr

blocked states with $\langle j_x \rangle \approx \frac{5}{2}^-$

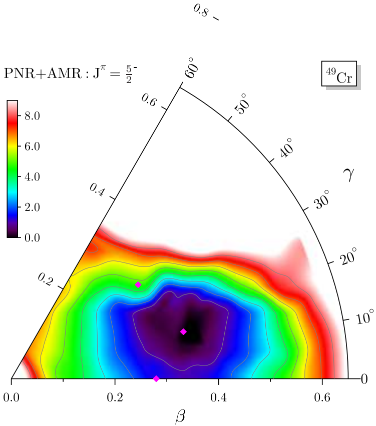


B. Bally, B. Avez, M. B., P.-H. Heenen, unpublished

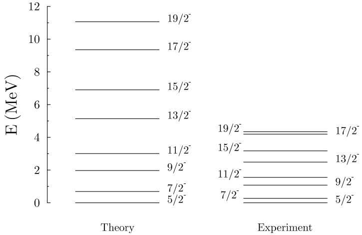
$J^\pi = \frac{5}{2}^-$ from blocked states with $\langle j_x \rangle \approx \frac{5}{2}^-$



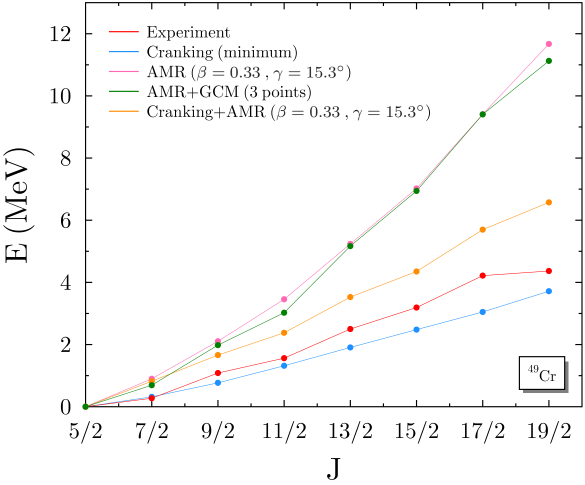
Incomplete GCM (3 points) ^{49}Cr



B. Bally, B. Avez, M. B., P.-H. Heenen, unpublished



EFfect of cranking on the yrast states of ^{49}Cr



B. Bally, B. Avez, M. B., P.-H. Heenen, unpublished

Remaining (and new) problems of regularized MR EDF

Regularization is *asymmetric* under exchange of left and right states

nondiagonal N and J projected matrix element between axial states in ^{48}Cr

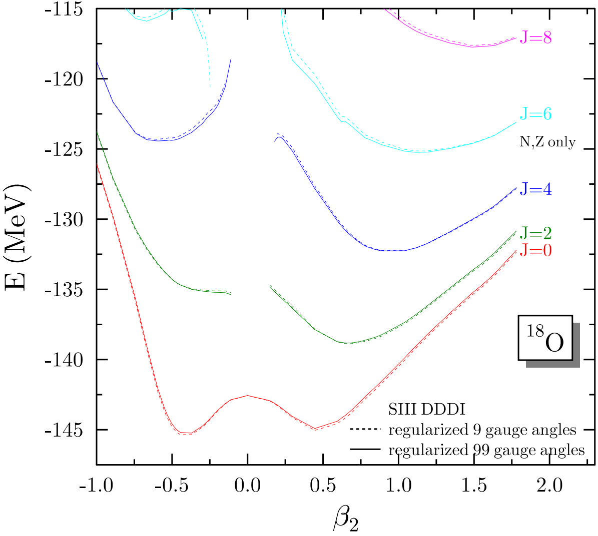
J	K_1	K_2	overlap	E^{LR}	E^{LR}_{reg}	E^{RL}	E^{RL}_{reg}
0	0	0	0.010439	−407.871	−408.782	−407.871	−409.057
2	0	0	0.042743	−407.031	−407.868	−407.031	−408.064
4	0	0	0.048782	−405.163	−405.844	−405.163	−405.886
6	0	0	0.035154	−402.322	−402.786	−402.322	−402.631

Similar in N-projected K decomposition of triaxial states

J	K_1	K_2	overlap	E	E_{reg}
2	0	0	0.07092697	−404.091	−404.653
2	0	2	-0.00180980	−404.327	−404.932
2	2	0	-0.00180982	−404.326	−405.538
2	2	2	0.00806622	−397.064	−397.147

Remedy: average "left" and "right" regularization

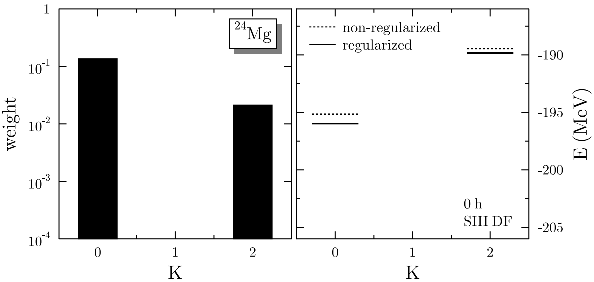
Non-convergence of combined N and J projection



Sum rules

- non-diagonal regularized MR EDF kernels can be decomposed on unphysical particle numbers (i.e. components that have strictly zero norm), including *negative* particle numbers
- Violation of physical sum rules in particle-number projection of non-diagonal regularized MR EDF kernels

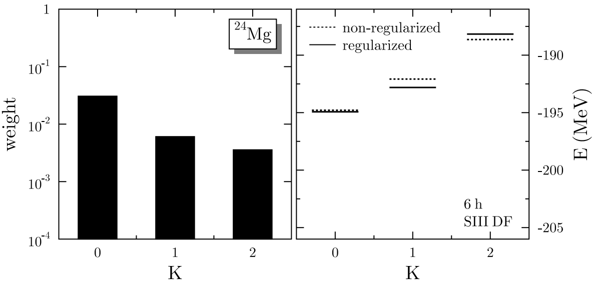
combined N, Z, $J = 2$ projection of triaxial ^{24}Mg



K decomposition, no K mixing yet

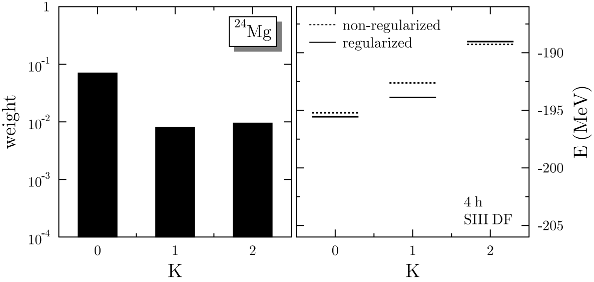
Small components

combined N, Z, $J = 2$ projection of a *cranked* triaxial ^{24}Mg



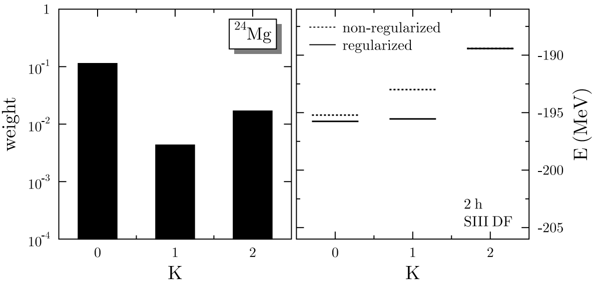
K decomposition, no K mixing yet

combined N, Z, $J = 2$ projection of a *cranked* triaxial ^{24}Mg



K decomposition, no K mixing yet

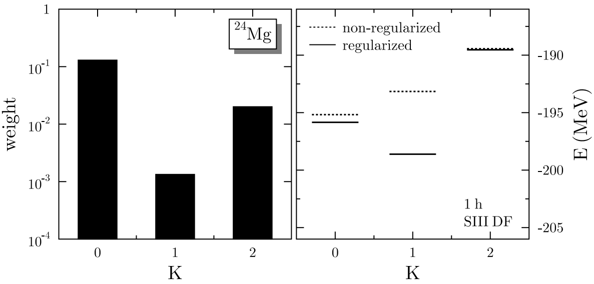
combined N, Z, $J = 2$ projection of a *cranked* triaxial ^{24}Mg



K decomposition, no K mixing yet

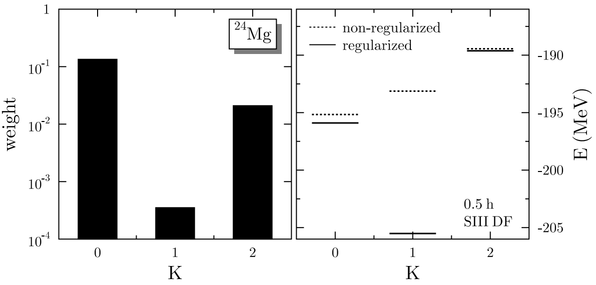
Small components

combined N, Z, $J = 2$ projection of a *cranked* triaxial ^{24}Mg



K decomposition, no K mixing yet

combined N, Z, $J = 2$ projection of a *cranked* triaxial ^{24}Mg



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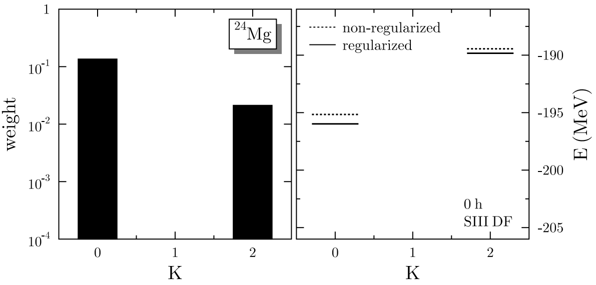

K decomposition, no K mixing yet

Outlook: Questions to be addressed and answered

- problems with collective states in MR-EDF calculations suggest that there is an urgent need for improved parameterizations of the nuclear energy density functional that give better single-particle spectra. Which are the relevant terms in the functional, how to adjust them to which observables? (the tensor interaction is *not* an important missing piece)
- How to define a suitable and exhaustive collective space for MR-EDF calculations? Which symmetries to break, which to restore, how many collective degrees of freedom to take into account, how to optimize the collective path/surface, how to take single-particle degrees of freedom into account, without sacrificing the applicability of the method to all nuclei (with computers available at the time this has been worked out)?
- A formal framework for MR-EDF calculations has be be established to avoid surprises from spurious contributions to the energy density functional, even when using clever tricks originally invented for operators. Do we have to go back to effective Hamiltonians?

The work presented here would have been impossible without my collaborators

on code development (in alphabetical order)

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on formal aspects of the regularization (in chronological order)

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Denis Lacroix	GANIL, Caen
Karim Bennaceur	IPN Lyon
Thomas Lesinski	IPN Lyon
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on development and benchmarking of new functionals (in alphabetical order)

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back-up slides

- related to broken antisymmetry of vertices in the functional
- The presence of self-interaction in the functionals used in DFT has been pointed out by J. P. Perdew and A. Zunger, Phys. Rev. B23, 5048 (1981).
- violation of the exchange symmetry in nuclear effective interactions has also been discussed from a different perspective and using different vocabulary by S. Stringari and D. M. Brink, *Constraints on effective interactions imposed by antisymmetry and charge independence*, Nucl. Phys. A304, 307 (1978).
- the interaction energy of a particle with itself should be zero
- One-particle limit of the interaction energy divided by the probability to occupy this state

$$\frac{\mathcal{E}_\mu - t_{\mu\mu}}{v_\mu^2} = \tfrac{1}{2}\, \bar{v}^{\rho\rho}_{\mu\mu\mu\mu}\, v_\mu^2 \, .$$

  In a composite system, the particle-number of other particle species is left untouched.
- complete correction for self-interaction requires so-called orbital-dependent energy functional; approximate corrections have been proposed for DFT

Self-pairing

- self-pairing comes from an incomplete combination of vertices
- Direct interaction energy: remove self-interaction and divide by the probability $P^{\Phi}_{\mu\bar{\mu}}$ to occupy the pair

$$\frac{\mathcal{E}_{\mu\bar{\mu}} - \mathcal{E}_{\mu} - \mathcal{E}_{\bar{\mu}}}{P^{\Phi}_{\mu\bar{\mu}}} = \tfrac{1}{2}\left(\bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} + \bar{v}^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu}\right) v^2_{\mu} + \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}} u^2_{\mu} \,.$$

Probability $P^{\Phi}_{\mu\bar{\mu}}$ to occupy the pair $P^{\Phi}_{\mu\bar{\mu}} = \dfrac{\langle \Phi_{\varphi} | a^{\dagger}_{\mu} a^{\dagger}_{\bar{\mu}} a_{\bar{\mu}} a_{\mu} | \Phi_{\varphi} \rangle}{\langle \Phi_{\varphi} | \Phi_{\varphi} \rangle} = v^2_{\mu}$

For a Hamiltonian $\bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} = \bar{v}^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu} = \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}} \equiv \bar{v}_{\mu\bar{\mu}\mu\bar{\mu}}$, the terms recombine

$$\frac{E_{\mu\bar{\mu}} - E_{\mu} - E_{\bar{\mu}}}{P^{\Phi}_{\mu\bar{\mu}}} = \bar{v}_{\mu\bar{\mu}\mu\bar{\mu}} \,,$$

into the HF interaction energy without pairing.

- The energy from scattering a pair of particles onto themselves should be equal to the no-pairing value
- To the best of our knowledge, self-pairing was never considered in the published literature so far.

Conceptual remarks

- a Hamiltonian + wave function framework does not show these pathologies, but at present there are no useful/sucessful strict Hamiltonian-based approaches using the full model space in sight.
- DME and LDA of the in-medium interaction motivates the use of functionals
- self-interaction and self-pairing are the price to pay for the enormous simplification of the many-body problem brought by an EDF approach
- there are higher-order self-interactions in higher-order functionals
- Restoring the effect of violations of Pauli's principle has to be scrutinized
- remember that violations of the Pauli principle are hard-wired into many many-body techniques even when using a Hamiltonian, for example into (Q)RPA through the quasi-boson approximation