Regularization of Multi-Reference Energy Density Functional Calculations

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17th Nuclear Physics Workshop "Maria and Pierre Curie"
on "**Symmetry and symmetry breaking in nuclear physics**"
22 – 25 September 2010, Kazimierz Dolny

Essential reading

Particle-Number Projection and the Density Functional Theory
J. Dobaczewski, M. V. Stoitsov, W. Nazarewicz, P.-G. Reinhard
PRC 76 2007 054315

Configuration mixing within the Energy Density Functional formalism: correction for spurious processes
D. Lacroix, T. Duguet, and M. Bender
PRC 79 (2009) 044318

Particle-Number Restoration within the Energy Density Functional Formalism
M. Bender, T. Duguet, and D. Lacroix
PRC 79 (2009) 044319

Particle-number restoration within the energy density functional formalism: Non-viability of terms depending on non-integer powers of the density matrices
T. Duguet, M. Bender, K. Bennaceur, D. Lacroix, and T. Lesinski
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+ (at least) 2 further papers in preparation by
M. Bender, T. Duguet, P.-H. Heenen and D. Lacroix (et al.)

What are strict HFB and strict GCM?

- HF(B): basic ingredients are one independent-particle (product) state $|\mathrm{SR}_q\rangle$ of Slater determinant or HFB type and a Hamilton operator $\hat{H}$ and

$$E_q^{HF(B)} = \langle \mathrm{SR}_q|\hat{H}|\mathrm{SR}_q\rangle$$

Constrained variation leads to the HF(B) equations

$$\delta\Big[\langle \mathrm{SR}_q|\hat{H}|\mathrm{SR}_q\rangle - \lambda_N\langle \mathrm{SR}_q|\hat{N}|\mathrm{SR}_q\rangle - \lambda_q\langle \mathrm{SR}_q|\hat{Q}|\mathrm{SR}_q\rangle - \mathrm{Tr}\{\Lambda\big(\mathcal{R}^2-\mathcal{R}\big)\}\Big] = 0$$

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- GCM: coherent superposition of HF(B) states

$$|\mathrm{MR}_\mu\rangle = \sum_q f_\mu(q)\,|\mathrm{SR}_q\rangle$$

$$E_\mu = \langle \mathrm{MR}_\mu|\hat{H}|\mathrm{MR}_\mu\rangle = \frac{\sum_{q,q'} f_\mu^*(q)\,\langle \mathrm{SR}_q|\hat{H}|\mathrm{SR}_{q'}\rangle\, f_\mu(q')}{\sum_{q'',q'''} f_\mu^*(q'')\,\langle \mathrm{SR}_{q''}|\mathrm{SR}_{q'''}\rangle\, f_\mu(q''')}$$

weights $f_\mu(q)$ determined by variation

$$\frac{\delta E_\mu}{\delta f_\mu^*(q)} = 0 \qquad \sum_{q'}\Big[\langle \mathrm{SR}_q|\hat{H}|\mathrm{SR}_{q'}\rangle - E_\mu\langle \mathrm{SR}_q|\mathrm{SR}_{q'}\rangle\Big]\; f_\mu(q') = 0$$

Projection is a special case of GCM, where degenerate states that differ in orientation are mixed and the symmetry group determines (most of) the weight function.

How to calculate GCM kernels: Generalized Wick theorem

A matrix element of the operator $\hat{O}$ between two SR states

$$\begin{array}{lcl} |\mathrm{L}\rangle & : & \hat{\alpha}_I,\ \hat{\alpha}_I^\dagger \\ |\mathrm{R}\rangle & : & \hat{\beta}_r,\ \hat{\beta}_r^\dagger \end{array} \qquad \text{with} \qquad \begin{pmatrix} \hat{\alpha} \\ \hat{\alpha}^\dagger \end{pmatrix} = \begin{pmatrix} (D^{-1})^* & -E \\ -E^* & D^{-1} \end{pmatrix} \begin{pmatrix} \hat{\beta} \\ \hat{\beta}^\dagger \end{pmatrix}$$

is obtained for a one-body operator as

$$\langle \mathrm{L}| \sum_{ij} \hat{O}_{ij} a_i^\dagger a_j |\mathrm{R}\rangle = \sum_{ij} \hat{O}_{ij} \frac{\langle \mathrm{L}|\hat{a}_i^\dagger \hat{a}_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \langle \mathrm{L}|\mathrm{R}\rangle$$

for a two-body operator as

$$\langle \mathrm{L}| \sum_{ijmn} \hat{O}_{ijmn} a_i^\dagger a_j^\dagger a_n a_m |\mathrm{R}\rangle$$

$$= \sum_{ijmn} \hat{O}_{ijmn} \left[\frac{\langle \mathrm{L}|\hat{a}_i^\dagger \hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \frac{\langle \mathrm{L}|\hat{a}_j^\dagger \hat{a}_n|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} - \frac{\langle \mathrm{L}|\hat{a}_i^\dagger \hat{a}_n|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \frac{\langle \mathrm{L}|\hat{a}_j^\dagger \hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} + \frac{\langle \mathrm{L}|\hat{a}_i^\dagger \hat{a}_j^\dagger|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \frac{\langle \mathrm{L}|\hat{a}_n \hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \right] \langle \mathrm{L}|\mathrm{R}\rangle$$

etc. with

$$\begin{pmatrix} \frac{\langle \mathrm{L}|\alpha\alpha^\dagger|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} & \frac{\langle \mathrm{L}|\alpha\alpha|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \\ \frac{\langle \mathrm{L}|\alpha^\dagger\alpha^\dagger|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} & \frac{\langle \mathrm{L}|\alpha^\dagger\alpha|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \end{pmatrix} = \begin{pmatrix} 1 & ED \\ 0 & 0 \end{pmatrix} \qquad \begin{pmatrix} \frac{\langle \mathrm{L}|\beta\beta^\dagger|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} & \frac{\langle \mathrm{L}|\beta\beta|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \\ \frac{\langle \mathrm{L}|\beta^\dagger\beta^\dagger|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} & \frac{\langle \mathrm{L}|\beta^\dagger\beta|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ DE^* & 0 \end{pmatrix}$$

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What are SR EDF and MR EDF?

- SR EDF: basic ingredients are the density matrix corresponding to one independent-particle (product) state $|\mathrm{SR}_q\rangle$ of Slater determinant or HFB type

$$\mathcal{R}_{qq} = \begin{pmatrix} \rho_{qq} & \kappa_{qq} \\ -\kappa^*_{qq} & 1-\rho^*_{qq} \end{pmatrix} = \begin{pmatrix} \langle \mathrm{SR}_q|\hat{a}^\dagger\hat{a}|\ \mathrm{SR}_q\rangle & \langle \mathrm{SR}_q|\hat{a}\hat{a}|\ \mathrm{SR}_q\rangle \\ \langle \mathrm{SR}_q|\hat{a}^\dagger\hat{a}^\dagger|\ \mathrm{SR}_q\rangle & \langle \mathrm{SR}_q|\hat{a}\hat{a}^\dagger|\ \mathrm{SR}_q\rangle \end{pmatrix} = \mathcal{R}^2_{qq}$$

and a functional depending on this density matrix

$$\mathcal{E}^{\mathrm{SR}}_q \equiv \mathcal{E}^{\mathrm{SR}}_q[\rho_{qq}, \kappa_{qq}, \kappa^*_{qq}]\,,$$

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$$\mathcal{E}^{\mathrm{SR}}_q \equiv \mathcal{E}^{\mathrm{SR}}_q[\rho_{qq}, \kappa_{qq}, \kappa^*_{qq}]\,,$$

- MR EDF: basic ingredients are the *transition* density matrix between two independent-particle (product) states $|\mathrm{SR}_q\rangle$ and $|\mathrm{SR}_{q'}\rangle$ of Slater determinant or HFB type

$$\mathcal{R}_{qq'} = \begin{pmatrix} \rho_{qq'} & \kappa_{qq'} \\ -\kappa^*_{qq'} & 1-\rho^*_{qq'} \end{pmatrix} = \begin{pmatrix} \dfrac{\langle \mathrm{SR}_q|\hat{a}^\dagger\hat{a}|\ \mathrm{SR}_{q'}\rangle}{\langle \mathrm{SR}_q|\mathrm{SR}_{q'}\rangle} & \dfrac{\langle \mathrm{SR}_q|\hat{a}\hat{a}|\ \mathrm{SR}_{q'}\rangle}{\langle \mathrm{SR}_q|\mathrm{SR}_{q'}\rangle} \\ \dfrac{\langle \mathrm{SR}_q|\hat{a}^\dagger\hat{a}^\dagger|\ \mathrm{SR}_{q'}\rangle}{\langle \mathrm{SR}_q|\mathrm{SR}_{q'}\rangle} & \dfrac{\langle \mathrm{SR}_q|\hat{a}\hat{a}^\dagger|\ \mathrm{SR}_{q'}\rangle}{\langle \mathrm{SR}_q|\mathrm{SR}_{q'}\rangle} \end{pmatrix}$$

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$$\mathcal{E}^{\mathrm{MR}}_\mu = \frac{\sum_{q,q'} f^*_\mu(q)\,\mathcal{E}^{\mathrm{MR}}_{qq'}[\rho_{qq'}, \kappa_{qq'}, \kappa^*_{qq'}]\,f_\mu(q')}{\sum_{q'',q'''} f^*_\mu(q'')\,\langle \mathrm{SR}_{q''}|\mathrm{SR}_{q'''}\rangle\,f_\mu(q''')}$$

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

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

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

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

Contact functional:

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

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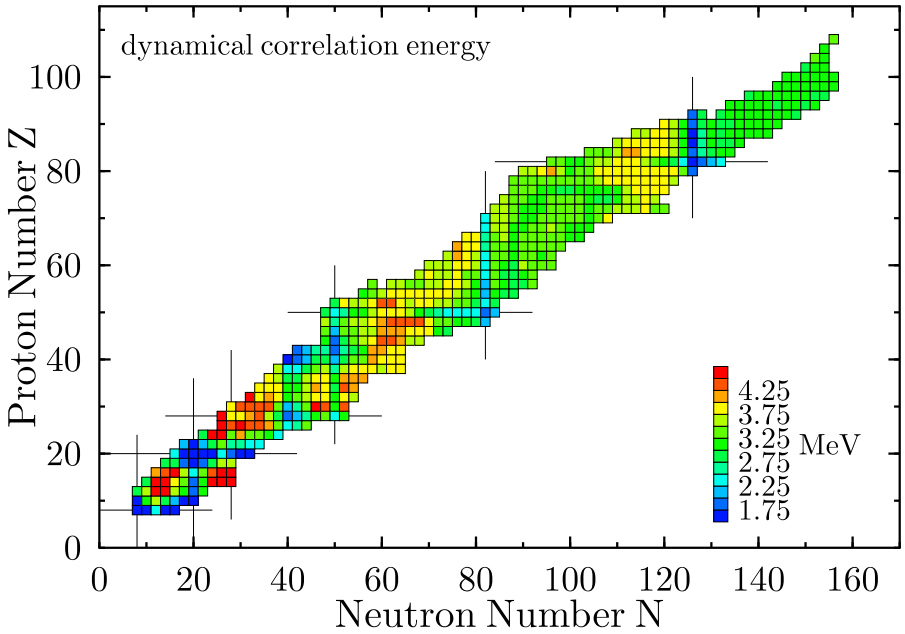
Coulomb interaction $\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$

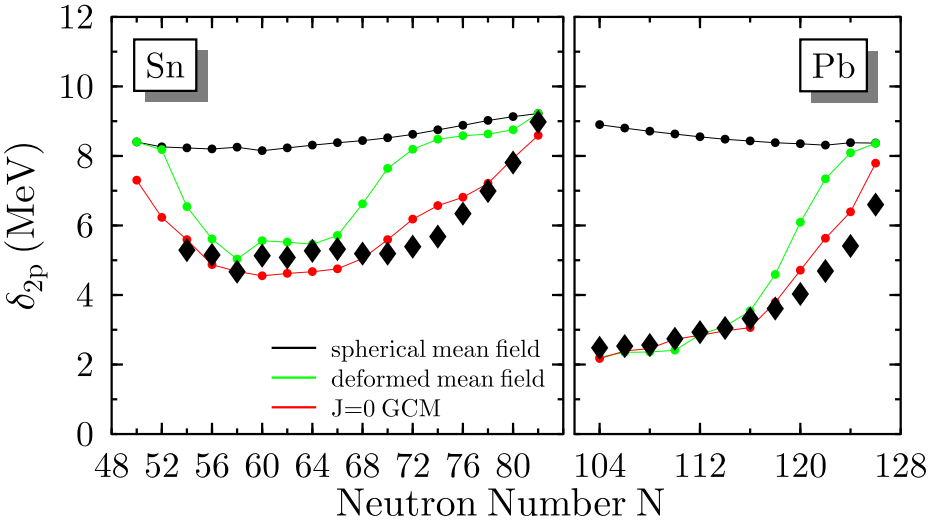
$$\mathcal{E} = \frac{1}{2}\iint d^3r\,d^3r'\,\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\Big[\rho_p(\mathbf{r})\rho_p(\mathbf{r}') - \rho_p(\mathbf{r},\mathbf{r}')\rho_p(\mathbf{r}',\mathbf{r}) + \kappa_p^*(\mathbf{r},\mathbf{r}')\kappa_p(\mathbf{r},\mathbf{r}')\Big]$$

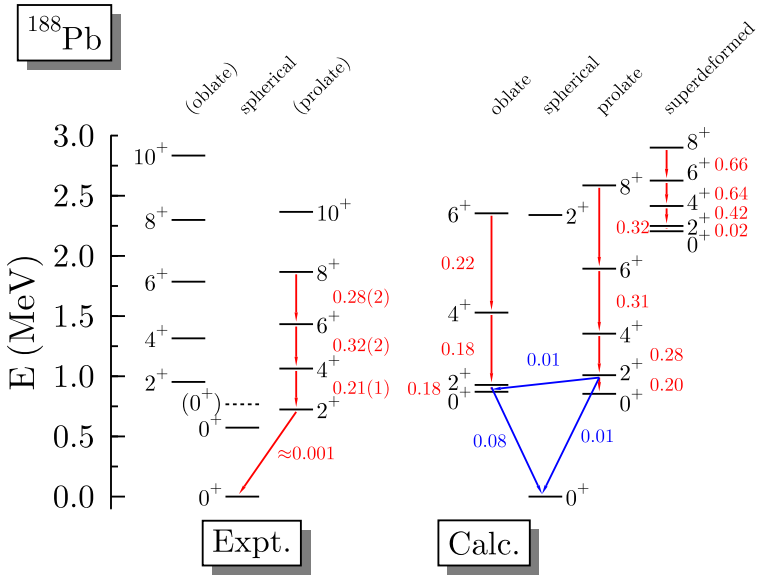
Approximate Coulomb functionals

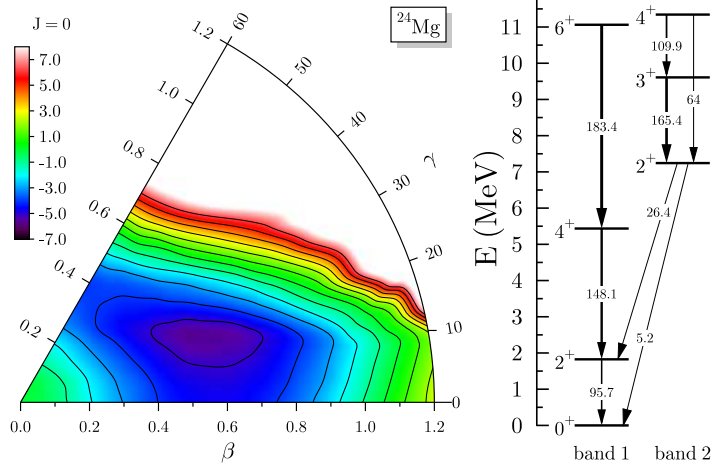
$$\mathcal{E} = \frac{e^2}{2}\iint d^3r\,d^3r'\,\frac{\rho_p(\mathbf{r})\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} - \frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}\int d^3r\,\rho_p^{4/3}(\mathbf{r})$$

Typical results obtained with MR EDF ("symmetry-restored GCM")

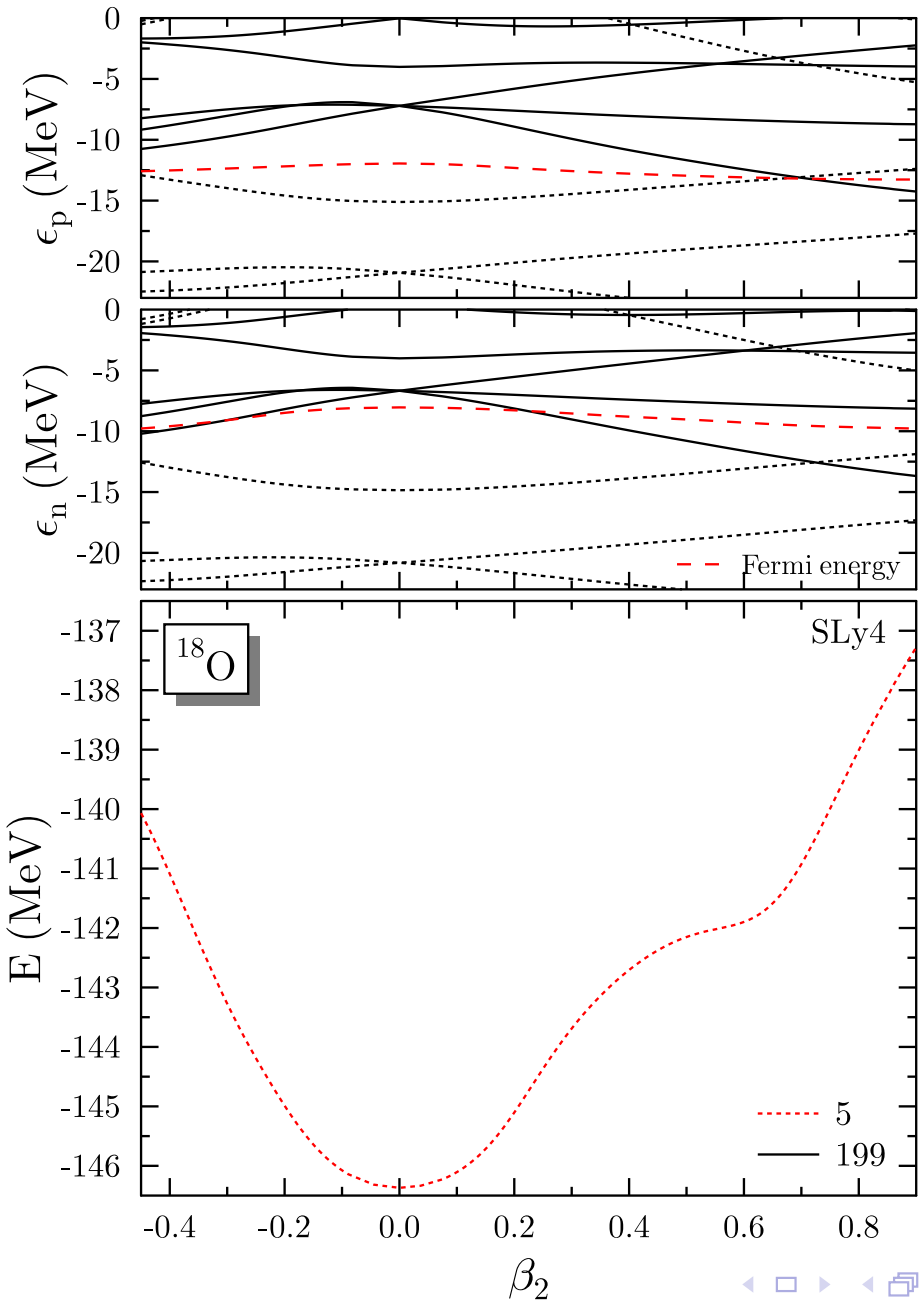








Here is a problem . . .



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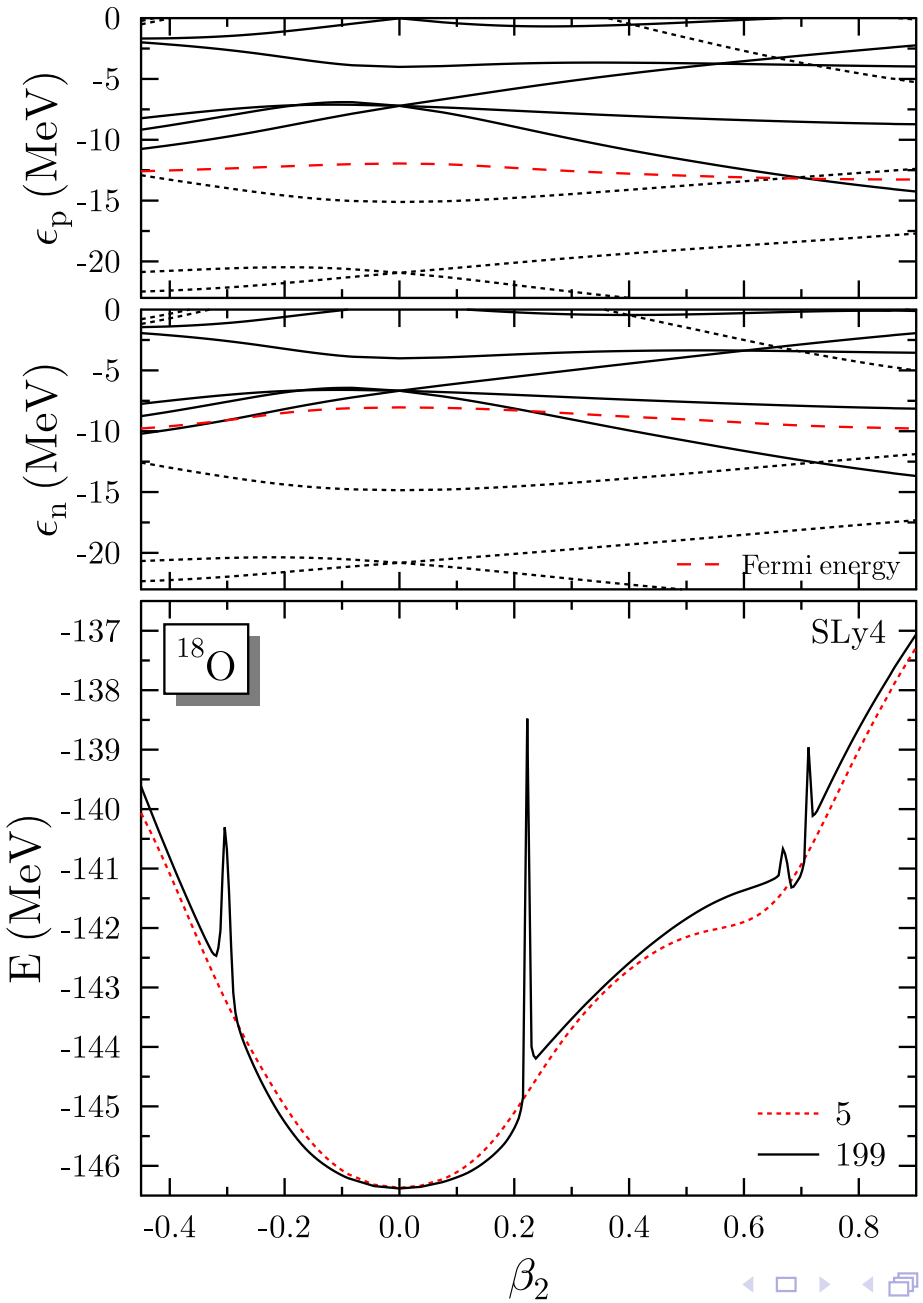

Particle-number projection

particle-number projector

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

normalized projected state discretized à la Fomenko, J. Phys. A3 (1970) 8 (for even particle number)

$$|\,\Psi_N\rangle \quad = \quad \frac{1}{c_N}\,\frac{1}{\pi} \int_0^{\pi} d\varphi\, e^{-i\varphi N_0}\, e^{i\varphi \hat{N}} \prod_{\mu>0} \left(u_\mu + v_\mu\, a_\mu^+\, a_{\bar{\mu}}^+\right) |0\rangle$$

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&= \frac{1}{c_N}\,\frac{1}{\pi}\int_0^{\pi} d\varphi\, e^{-i\varphi N_0} \prod_{\mu>0} \left(u_\mu + v_\mu\, e^{2i\varphi}\, a_\mu^+\, a_{\bar{\mu}}^+\right)|0\rangle \\
&= \frac{1}{c_N}\,\frac{1}{L}\sum_{\ell=1}^{L} e^{i\frac{\pi(\ell-1)}{L}} \prod_{\mu>0} \left(u_\mu + v_\mu\, e^{2i\frac{\pi(\ell-1)}{L}}\, a_\mu^+\, a_{\bar{\mu}}^+\right)|0\rangle
\end{aligned}$$

Bilinear toy energy density functional

Start with the single-reference energy density functional (all density matrices determined by the state $|q\rangle$)

$$\begin{aligned}\mathcal{E}[\rho^{qq},\kappa^{qq},\kappa^{qq\,*}] &= \mathcal{E}^{\rho}+\mathcal{E}^{\rho\rho}+\mathcal{E}^{\kappa\kappa} \\ &= \sum_{ij} t_{ij}\,\rho^{qq}_{ji}+\tfrac{1}{2}\sum_{ijkl}\bar{v}^{\rho\rho}_{ijkl}\,\rho^{qq}_{ki}\,\rho^{qq}_{lj}+\tfrac{1}{4}\sum_{ijkl}\bar{v}^{\kappa\kappa}_{ijkl}\,\kappa^{qq\,*}_{ij}\,\kappa^{qq}_{kl}\end{aligned}$$

for example

$$\begin{aligned}\int d^3r\;\rho^2(\mathbf{r}) &= \int d^3r\left[\sum_{ik}\rho_{ki}\psi^{\dagger}_i(\mathbf{r})\psi_k(\mathbf{r})\right]\left[\sum_{lj}\rho_{lj}\psi^{\dagger}_j(\mathbf{r})\psi_l(\mathbf{r})\right] \\ &= \sum_{ijkl}\underbrace{\int d^3r\;\psi^{\dagger}_i(\mathbf{r})\psi^{\dagger}_j(\mathbf{r})\psi_k(\mathbf{r})\psi_l(\mathbf{r})}_{\bar{v}^{\rho\rho}_{ijkl}}\;\rho_{ki}\;\rho_{lj}\end{aligned}$$

and similar for other terms.

- the vertices $\bar{v}^{\rho\rho}$ and $\bar{v}^{\kappa\kappa}$ might be different and not antisymmetrized.
- we assume that the vertices $\bar{v}^{\rho\rho}$ and $\bar{v}^{\kappa\kappa}$ are not density dependent
- generalization to higher-order polynomials in density matrices are straightforward, but not necesary for this discussion.

Particle-number projected energy functional

$$\int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi\, c_N^2} \, \mathcal{E}_{GWT}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}] \, \langle \Phi_0 | \Phi_\varphi \rangle$$

$$= \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi\, c_N^2} \Bigg[\sum_\mu t_{\mu\mu} \, \frac{v_\mu^2 \, e^{2i\varphi}}{u_\mu^2 + v_\mu^2 \, e^{2i\varphi}}$$

$$+ \frac{1}{2} \sum_{\mu\nu} \bar{v}^{\rho\rho}_{\mu\nu\mu\nu} \, \frac{v_\mu^2 \, e^{2i\varphi}}{u_\mu^2 + v_\mu^2 \, e^{2i\varphi}} \, \frac{v_\nu^2 \, e^{2i\varphi}}{u_\nu^2 + v_\nu^2 \, e^{2i\varphi}}$$

$$+ \frac{1}{4} \sum_{\mu\nu} \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\nu\bar{\nu}} \, \frac{u_\mu v_\mu}{u_\mu^2 + v_\mu^2 \, e^{2i\varphi}} \, \frac{u_\nu v_\nu \, e^{2i\varphi}}{u_\nu^2 + v_\nu^2 \, e^{2i\varphi}} \Bigg] \prod_{\lambda>0} (u_\lambda^2 + v_\lambda^2 \, e^{2i\varphi})$$

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.

Complex plane analysis I

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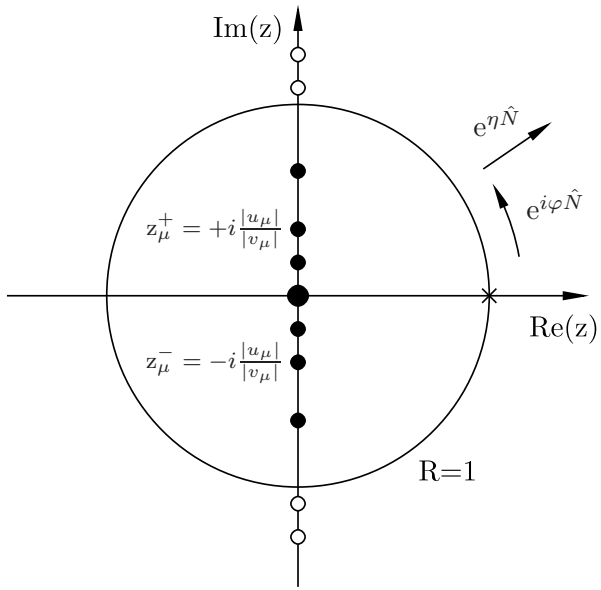
- the energy functional has poles at $z = 0$ and $z^\pm = \pm \frac{u_\mu}{v_\mu}$

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

- 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 origin of the poles I

- The poles are a consequence of using the GWT to motivate the MR EDF
- this can be shown constructing a basis where the kernels can be evaluated using a standard Wick theorem (SWT) or elementary operator algebra

Starting with two quasiparticle vacua

$$|\Phi_0\rangle = \mathcal{C}_0 \prod_\nu \alpha_\nu |0\rangle \qquad\qquad |\Phi_1\rangle = \mathcal{C}_1 \prod_\mu \beta_\mu |0\rangle$$

with quasiparticle operators constructed in their respective canonical basis

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} = \begin{pmatrix} \bar{U}^{\ell\dagger} & \bar{V}^{\ell\dagger} \\ \bar{V}^{\ell T} & \bar{U}^{\ell T} \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \qquad\qquad \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} \bar{U}^{r\dagger} & \bar{V}^{r\dagger} \\ \bar{V}^{rT} & \bar{U}^{rT} \end{pmatrix} \begin{pmatrix} b \\ b^\dagger \end{pmatrix}$$

which themselves are connected by a unitary transformation

$$\begin{pmatrix} a \\ a^\dagger \end{pmatrix} = \begin{pmatrix} R & 0 \\ 0 & R^* \end{pmatrix} \begin{pmatrix} b \\ b^\dagger \end{pmatrix}$$

The two sets of quasiparticle operators are connected by

$$\begin{aligned} \begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} &= \begin{pmatrix} \bar{U}^{\ell\dagger} & \bar{V}^{\ell\dagger} \\ \bar{V}^{\ell T} & \bar{U}^{\ell T} \end{pmatrix} \begin{pmatrix} R & 0 \\ 0 & R^* \end{pmatrix} \begin{pmatrix} \bar{U}^{r} & \bar{V}^{r*} \\ \bar{V}^{r} & \bar{U}^{r*} \end{pmatrix} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} \\ &= \begin{pmatrix} \bar{U}^{\ell\dagger} R \bar{U}^{r} + \bar{V}^{\ell\dagger} R^* \bar{V}^{r} & \bar{U}^{\ell\dagger} R \bar{V}^{r*} + \bar{V}^{\ell\dagger} R^* \bar{U}^{r*} \\ \bar{U}^{\ell T} R^* \bar{V}^{r} + \bar{V}^{\ell T} R \bar{U}^{r} & \bar{U}^{\ell T} R^* \bar{U}^{r*} + \bar{V}^{\ell T} R \bar{V}^{r*} \end{pmatrix} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} \end{aligned}$$

The origin of the poles II

This Bogoliubov transformation can be Bloch-Messiah-Zumino factorized

$$\begin{pmatrix} \alpha \\ \alpha^\dagger \end{pmatrix} \equiv \begin{pmatrix} A & B^* \\ B & A^* \end{pmatrix} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix}$$
$$\equiv \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix} \begin{pmatrix} \bar{A} & \bar{B}^* \\ \bar{B} & \bar{A}^* \end{pmatrix} \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix}$$

The two intermediate quasiparticle bases

$$\tilde{\alpha}^+ \equiv C^T \alpha^+ \qquad \tilde{\beta}^+ \equiv D^* \beta^+_\mu$$

whith $|\Phi_0\rangle$ still being vacuum of the $\tilde{\alpha}^+_\nu$, and $|\Phi_1\rangle$ still being vacuum of the $\tilde{\beta}^+_\nu$. $\{\tilde{\alpha}, \tilde{\alpha}^\dagger\}$ and $\{\tilde{\beta}, \tilde{\beta}^\dagger\}$ are connected through a BCS-like transformation

$$\tilde{\beta}^+_\nu = \bar{A}_{\nu\nu}\, \tilde{\alpha}^+_\nu + \bar{B}_{\bar{\nu}\nu}\, \tilde{\alpha}_{\bar{\nu}}$$

with 2×2 blocks of the structure

$$\begin{pmatrix} \bar{A}_{pp} & 0 \\ 0 & \bar{A}_{\bar{p}\bar{p}} \end{pmatrix} \qquad \begin{pmatrix} 0 & \bar{B}_{p\bar{p}} \\ -\bar{B}_{p\bar{p}} & 0 \end{pmatrix}$$

such that $|\Phi_1\rangle = \tilde{\mathcal{C}}_{01} \prod_{p>0} \left(\bar{A}^*_{pp} + \bar{B}^*_{p\bar{p}}\, \tilde{\alpha}^+_p \tilde{\alpha}^+_{\bar{p}}\right) |\Phi_0\rangle$
and $\langle\Phi_0|\Phi_1\rangle = \tilde{\mathcal{C}}_{01} \prod_{p>0} \bar{A}^*_{pp}$.

The origin of the poles III

Defining

$$\begin{aligned}
\langle\Phi_0|\Phi_1,p\rangle &= \tilde{\mathcal{C}}_{01}\prod_{\substack{p'>0\\p'\neq p,\bar{p}}}\bar{A}^*_{p'p'}\\
\langle\Phi_0|\Phi_1,p,q\rangle &= \tilde{\mathcal{C}}_{01}\prod_{\substack{p'>0\\p'\neq p,q,\bar{p},\bar{q}}}\bar{A}^*_{p'p'} \qquad \text{for } p\neq q
\end{aligned}$$

and $\langle\Phi_0|\Phi_1,\nu,\nu\rangle = \langle\Phi_0|\Phi_1,\nu,\bar{\nu}\rangle = 0$ one obtains for basic contractions

$$\begin{aligned}
\langle\Phi_0|\tilde{\alpha}^+_\nu\tilde{\alpha}_\mu|\Phi_1\rangle &= \langle\Phi_0|\tilde{\alpha}^+_\nu\tilde{\alpha}^+_\mu|\Phi_1\rangle = 0\\
\langle\Phi_0|\tilde{\alpha}_\nu\tilde{\alpha}^+_\mu|\Phi_1\rangle &= \delta_{\nu\mu}\langle\Phi_0|\Phi_1\rangle\\
\langle\Phi_0|\tilde{\alpha}_\nu\tilde{\alpha}_\mu|\Phi_1\rangle &= \delta_{\bar{\nu}\mu}\,\bar{B}^*_{\bar{\nu}\nu}\,\langle\Phi_0|\Phi_1,\nu\rangle
\end{aligned}$$

Quasiparticle wave functions associated with $\{\tilde{\alpha}_\nu,\tilde{\alpha}^+_\nu\}$

$$\begin{pmatrix}|\phi_\nu\rangle\\|\varphi_{\bar{\nu}}\rangle\end{pmatrix} = \begin{pmatrix}\bar{\alpha}^\dagger_\nu\\\bar{\alpha}_\nu\end{pmatrix}|-\rangle = \begin{pmatrix}\tilde{U}^{\ell\,T}a^\dagger\\\tilde{V}^{\ell\dagger}a^\dagger\end{pmatrix}|-\rangle\,,$$

with $\tilde{U}^0 = U^0C$ and $\tilde{V}^0 = V^0C$.

Energy functional motivated with standard Wick theorem

$$\mathcal{E}_{SWT}[0,1] = \tfrac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\varphi_\nu\varphi_\mu} + \frac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\nu\phi_{\bar{\nu}}\varphi_\mu\phi_{\bar{\mu}}}$$
$$+\tfrac{1}{2}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\nu\varphi_\mu\phi_\nu\varphi_\mu}\bar{B}^*_{\nu\bar{\nu}}\frac{\langle\Phi_0|\Phi_{1,\nu}\rangle}{\langle\Phi_0|\Phi_1\rangle} + \tfrac{1}{4}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\nu\varphi_{\bar{\nu}}\varphi_\mu\phi_{\bar{\mu}}}\bar{B}^*_{\nu\bar{\nu}}\frac{\langle\Phi_0|\Phi_{1,\nu}\rangle}{\langle\Phi_0|\Phi_1\rangle}$$
$$+\tfrac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\mu\varphi_\nu\varphi_\mu\phi_\nu}\bar{B}^*_{\nu\bar{\nu}}\frac{\langle\Phi_0|\Phi_{1,\mu}\rangle}{\langle\Phi_0|\Phi_1\rangle} + \tfrac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\mu\phi_{\bar{\mu}}\phi_\nu\phi_{\bar{\nu}}}\bar{B}^*_{\nu\bar{\nu}}\frac{\langle\Phi_0|\Phi_{1,\nu}\rangle}{\langle\Phi_0|\Phi_1\rangle}$$
$$+\tfrac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\phi_\nu\phi_\mu}\bar{B}^*_{\nu\bar{\nu}}\bar{B}^*_{\mu\bar{\mu}}\frac{\langle\Phi_0|\Phi_{1,\nu,\mu}\rangle}{\langle\Phi_0|\Phi_1\rangle} + \tfrac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\nu\varphi_{\bar{\nu}}\phi_\mu\phi_{\bar{\mu}}}\bar{B}^*_{\nu\bar{\nu}}\bar{B}^*_{\mu\bar{\mu}}\frac{\langle\Phi_0|\Phi_{1,\nu,\mu}\rangle}{\langle\Phi_0|\Phi_1\rangle}$$

Energy functional motivated with generalized Wick theorem

$$\mathcal{E}_{GWT}[0,1] = \tfrac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\varphi_\nu\varphi_\mu} + \tfrac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\nu\phi_{\bar{\nu}}\varphi_\mu\phi_{\bar{\mu}}}$$
$$+\tfrac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\phi_\nu\varphi_\mu}\bar{B}^*_{\nu\bar{\nu}}\frac{\langle\Phi_0|\Phi_1,\nu\rangle}{\langle\Phi_0|\Phi_1\rangle} + \tfrac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\nu\varphi_{\bar{\nu}}\varphi_\mu\phi_{\bar{\mu}}}\bar{B}^*_{\nu\bar{\nu}}\frac{\langle\Phi_0|\Phi_1,\nu\rangle}{\langle\Phi_0|\Phi_1\rangle}$$
$$+\tfrac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\mu\varphi_\nu\varphi_\mu\phi_\nu}\bar{B}^*_{\nu\bar{\nu}}\frac{\langle\Phi_0|\Phi_1,\mu\rangle}{\langle\Phi_0|\Phi_1\rangle} + \tfrac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\mu\phi_{\bar{\mu}}\phi_\nu\phi_{\bar{\nu}}}\bar{B}^*_{\nu\bar{\nu}}\frac{\langle\Phi_0|\Phi_1,\nu\rangle}{\langle\Phi_0|\Phi_1\rangle}$$
$$+\tfrac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\phi_\nu\phi_\mu}\bar{B}^*_{\nu\bar{\nu}}\bar{B}^*_{\mu\bar{\mu}}\frac{\langle\Phi_0|\Phi_1,\nu\rangle}{\langle\Phi_0|\Phi_1\rangle}\frac{\langle\Phi_0|\Phi_1,\mu\rangle}{\langle\Phi_0|\Phi_1\rangle} + \tfrac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\nu\varphi_{\bar{\nu}}\phi_\mu\phi_{\bar{\mu}}}\bar{B}^*_{\nu\bar{\nu}}\bar{B}^*_{\mu\bar{\mu}}\frac{\langle\Phi_0|\Phi_1,\nu\rangle}{\langle\Phi_0|\Phi_1\rangle}\frac{\langle\Phi_0|\Phi_1,\mu\rangle}{\langle\Phi_0|\Phi_1\rangle}$$

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

Both are not equal as

$$\frac{\langle\Phi_0|\Phi_1,\nu,\mu\rangle}{\langle\Phi_0|\Phi_1\rangle} = \begin{cases} \dfrac{\langle\Phi_0|\Phi_1,\nu\rangle}{\langle\Phi_0|\Phi_1\rangle}\dfrac{\langle\Phi_0|\Phi_1,\mu\rangle}{\langle\Phi_0|\Phi_1\rangle} & \text{for } \nu\neq\mu,\ \bar{\mu} \\ 0 & \text{for } \nu=\mu,\ \bar{\mu} \end{cases}$$

The difference between the SWT and GWT expressions are the $\frac{\langle\Phi_0|\Phi_1,\mu\rangle}{\langle\Phi_0|\Phi_1\rangle}\frac{\langle\Phi_0|\Phi_1,\mu\rangle}{\langle\Phi_0|\Phi_1\rangle}$ and $\frac{\langle\Phi_0|\Phi_1,\mu\rangle}{\langle\Phi_0|\Phi_1\rangle}\frac{\langle\Phi_0|\Phi_1,\bar{\mu}\rangle}{\langle\Phi_0|\Phi_1\rangle}$ terms in the GWT expression. In a Hamiltonian-based theory with $\bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\phi_\nu\phi_\mu} = \bar{v}^{\kappa\kappa}_{\varphi_\nu\varphi_\mu\phi_\nu\phi_\mu}$ they are multiplied with a combination of matrix elements that is zero. In a EDF framework they multiply a matrix element that in general is non-zero. For particle-number restoration one obtains analytically

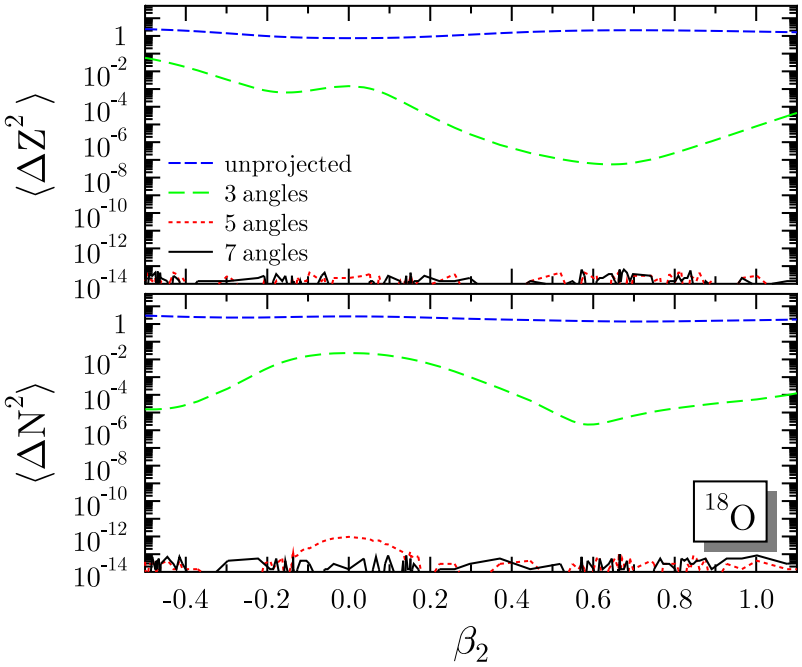
$$\begin{aligned}
\mathcal{E}^N_{CG} &= \sum_{\mu>0}\left[\frac{1}{2}\left(\bar{v}^{\rho\rho}_{\mu\mu\mu\mu}+\bar{v}^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}}+\bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}}+\bar{v}^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu}\right)-\bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}}\right]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

The origin of the poles VI

- 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

Does it remove all anomalies from particle-number projection?

Corrected PNP: ^{18}O I



- calculations with SIII (bilinear in density of given isospin, no divergence)
- projected wave function and all operator matrix elements are converged with $L = 5$ discretization points of the gauge space integral
- the projected energy functional does *not* converge with $L = 199$ points

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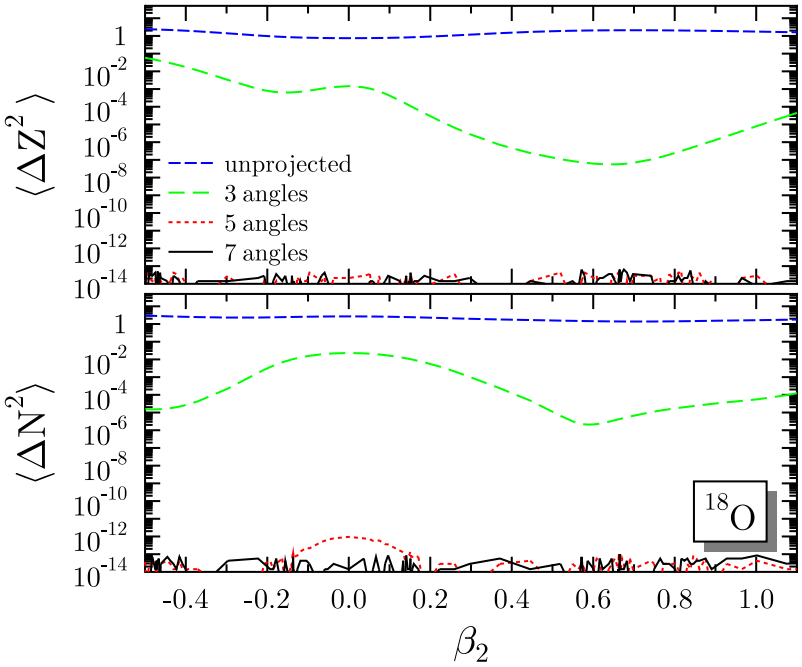

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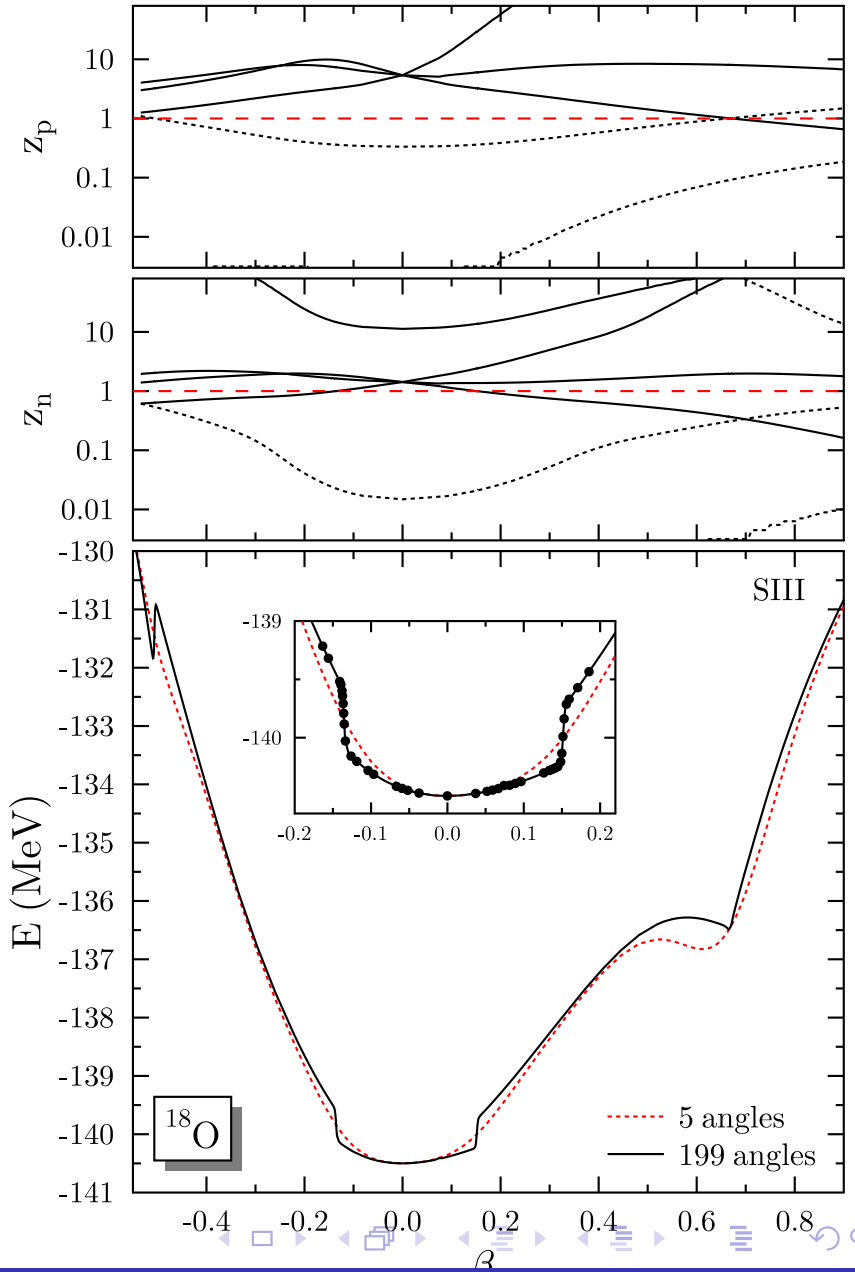
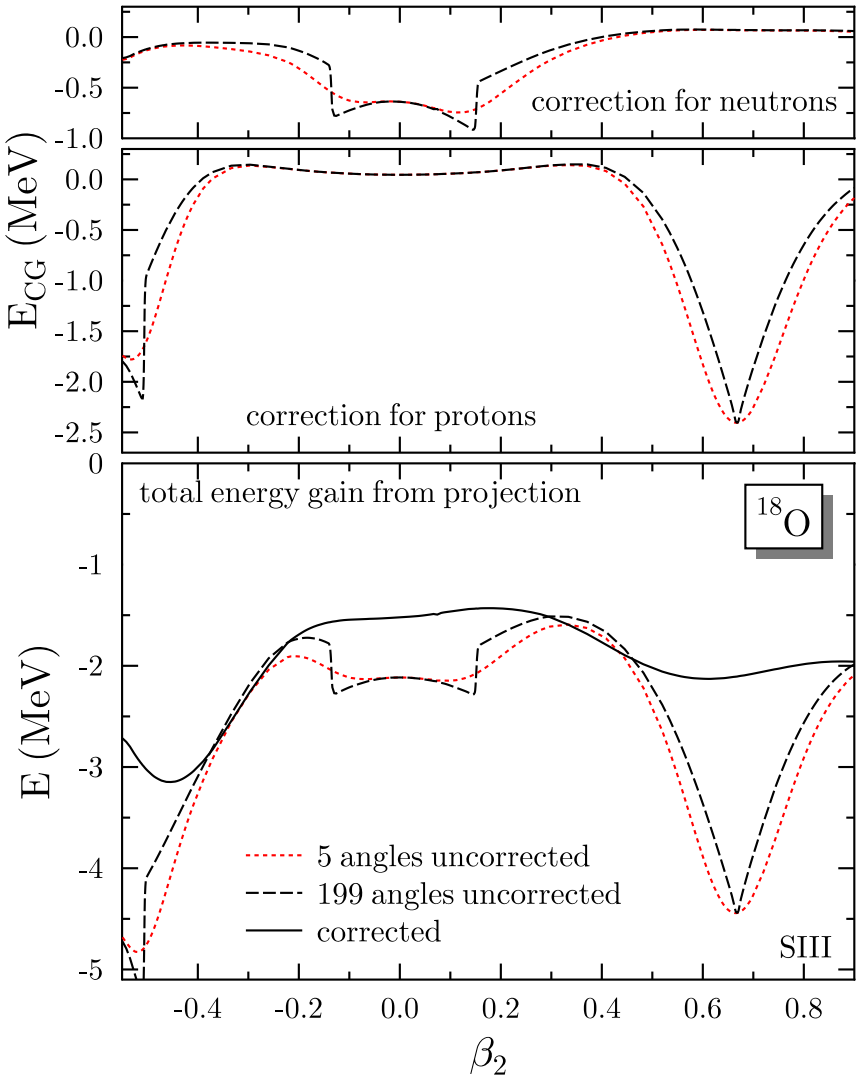
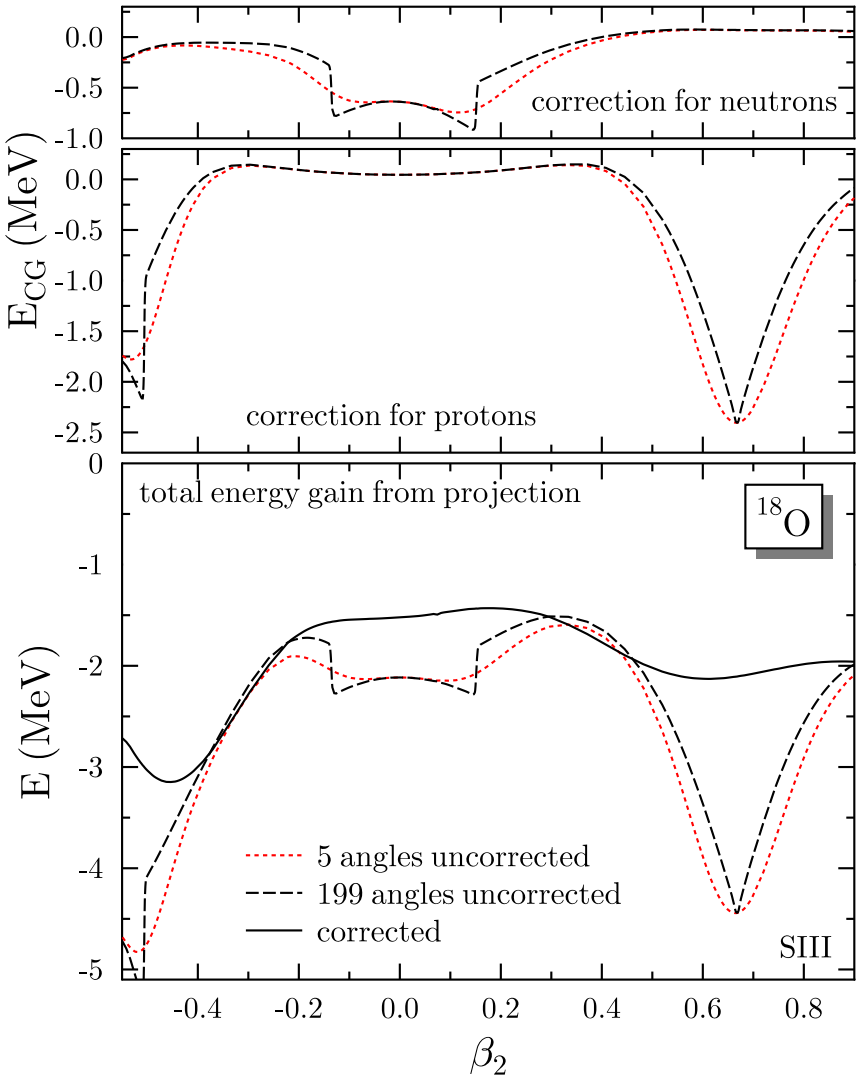
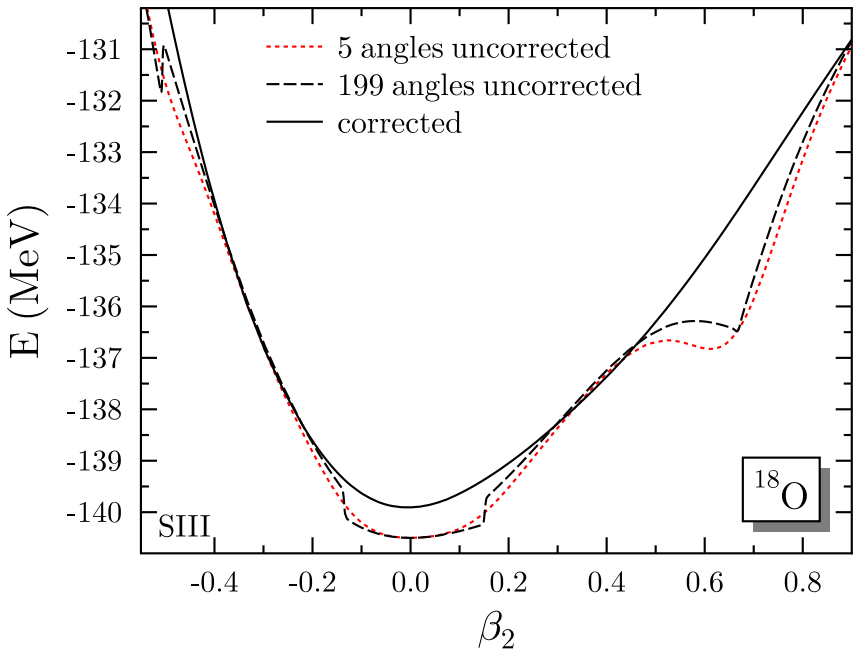


Corrected PNP: ^{18}O II



Corrected PNP: ^{18}O II





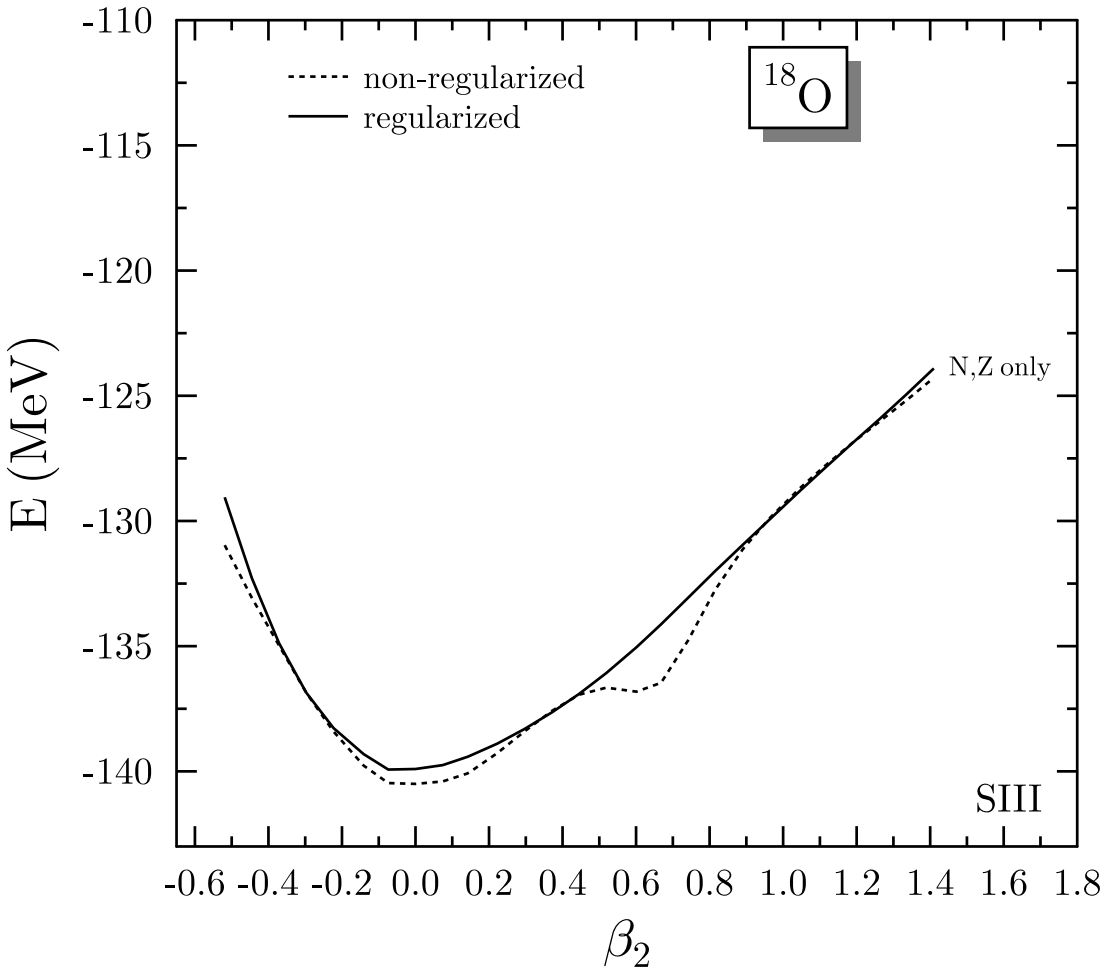
Further arguments pro regularization

Further arguments why regularization of the EDF by removal of the contribution defined above are provided by the analysis of

- shift invariance (change of integration radius) of observables
- radius-weighted sum rules
- non-radius-weighted sum rules
- analysis of the contribution of single poles to the energy

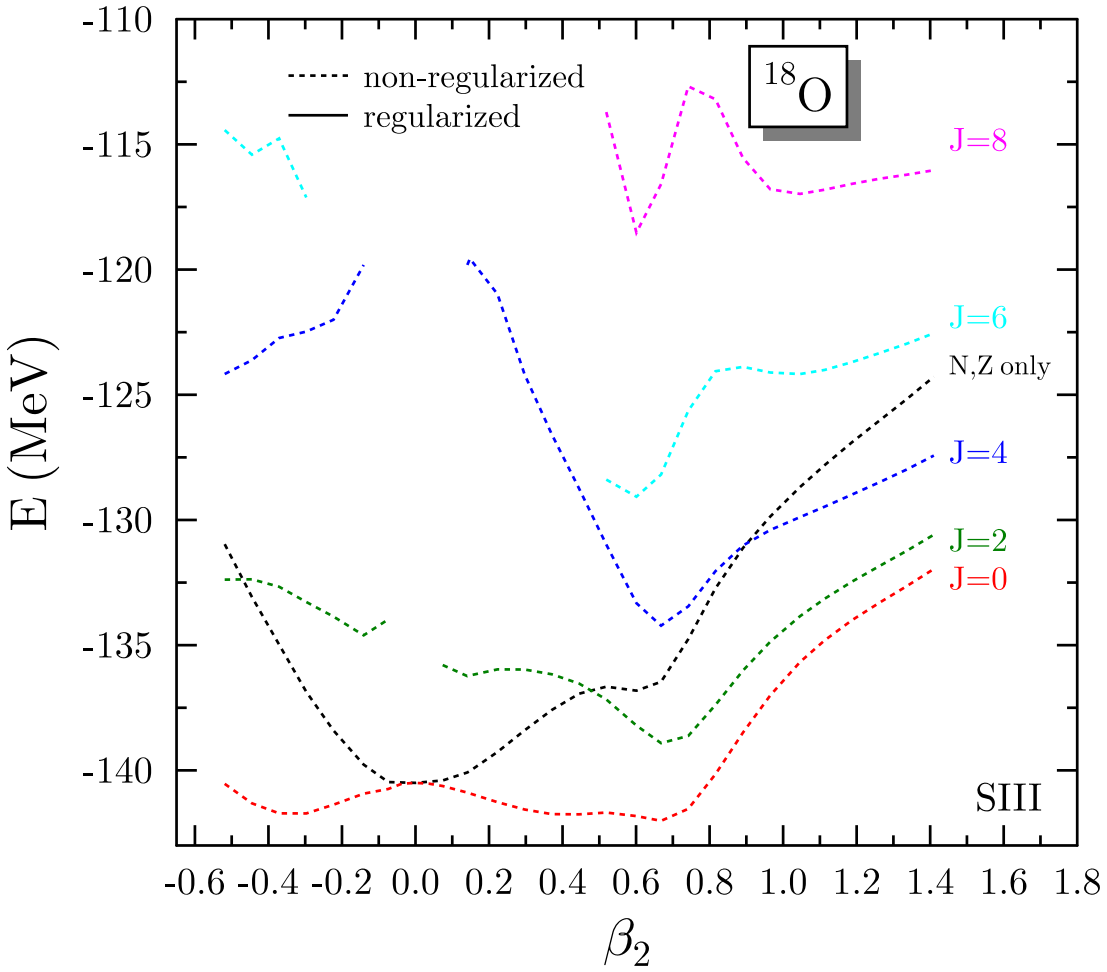
. . . see Bender, Duguet, Lacroix, PRC 79 (2009) 044319.

General configuration mixing



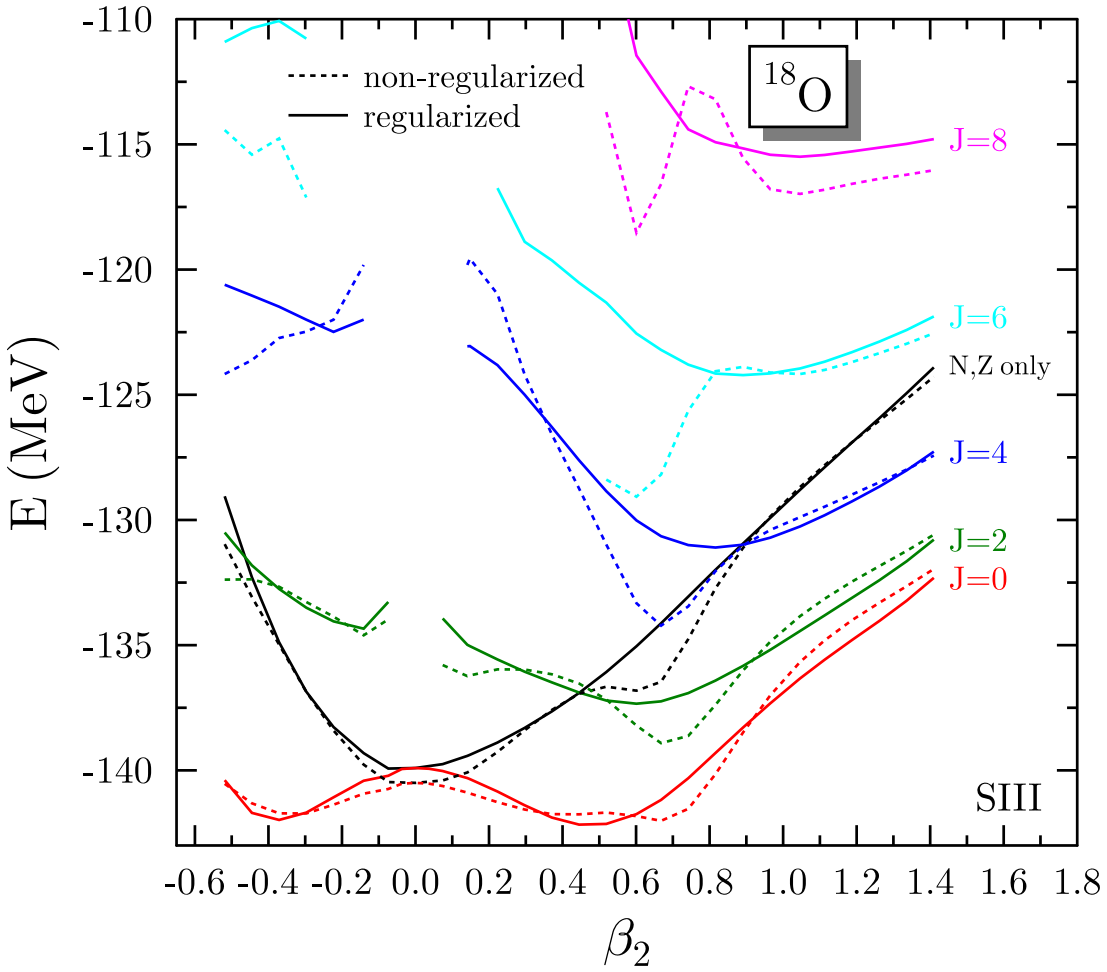
- The same as before: projection on N and Z discretized with 5 gauge angles . . .
- . . . but now calculated from a general algorithm that can handle *any* mixing

General configuration mixing



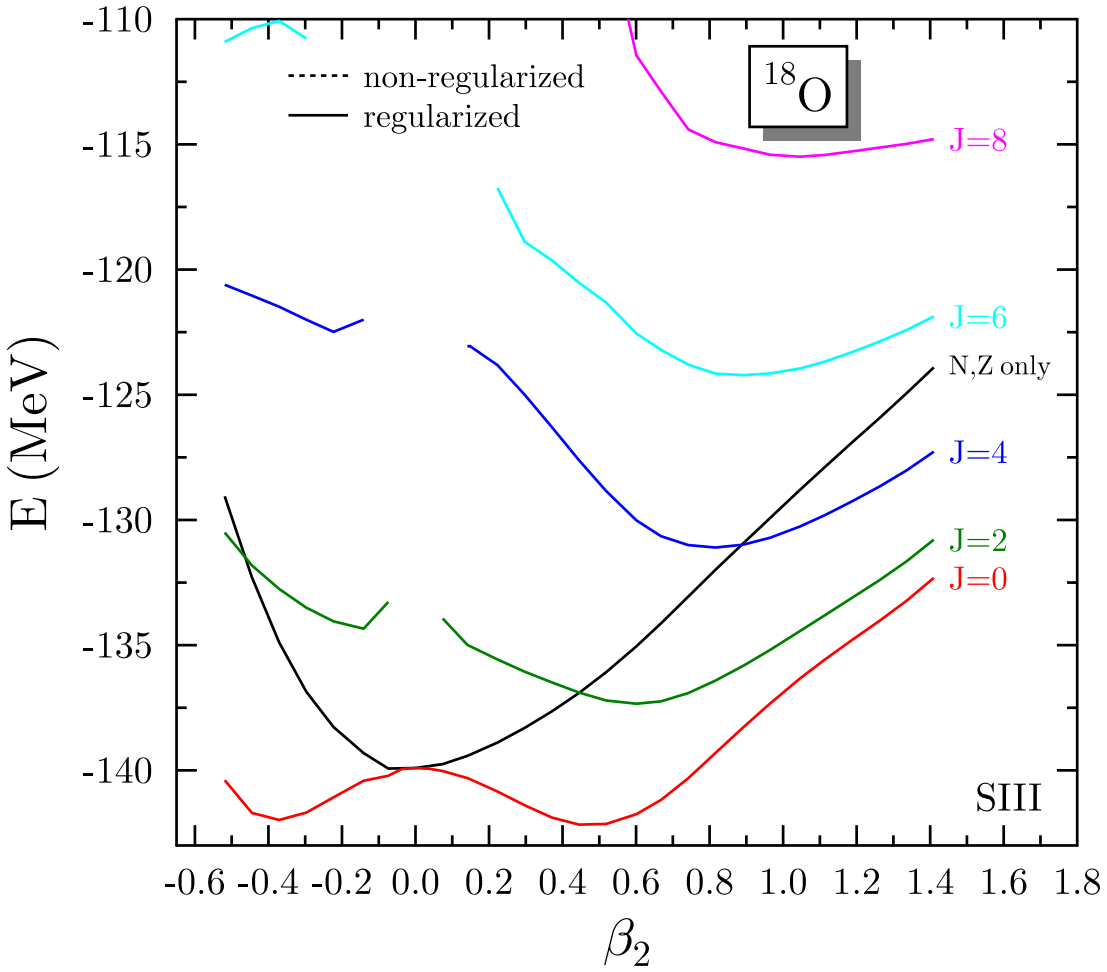
- Combined particle-number and angular-momentum restoration of the non-regularized EDF

General configuration mixing



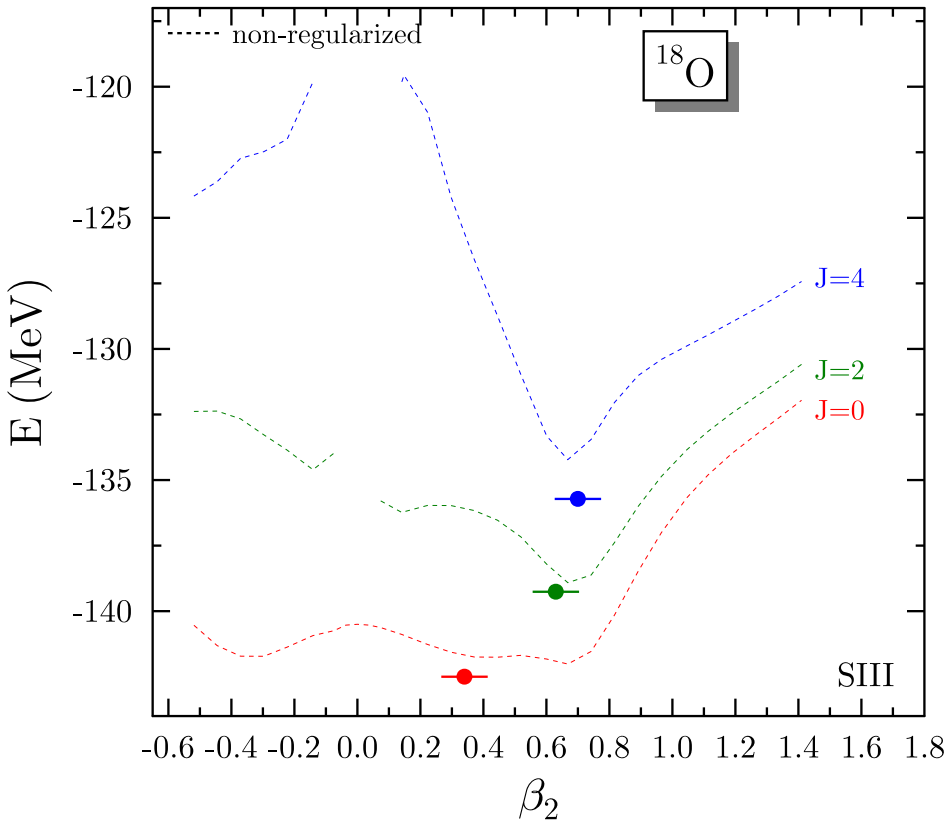
- Combined particle-number and angular-momentum restoration with regularization of the EDF

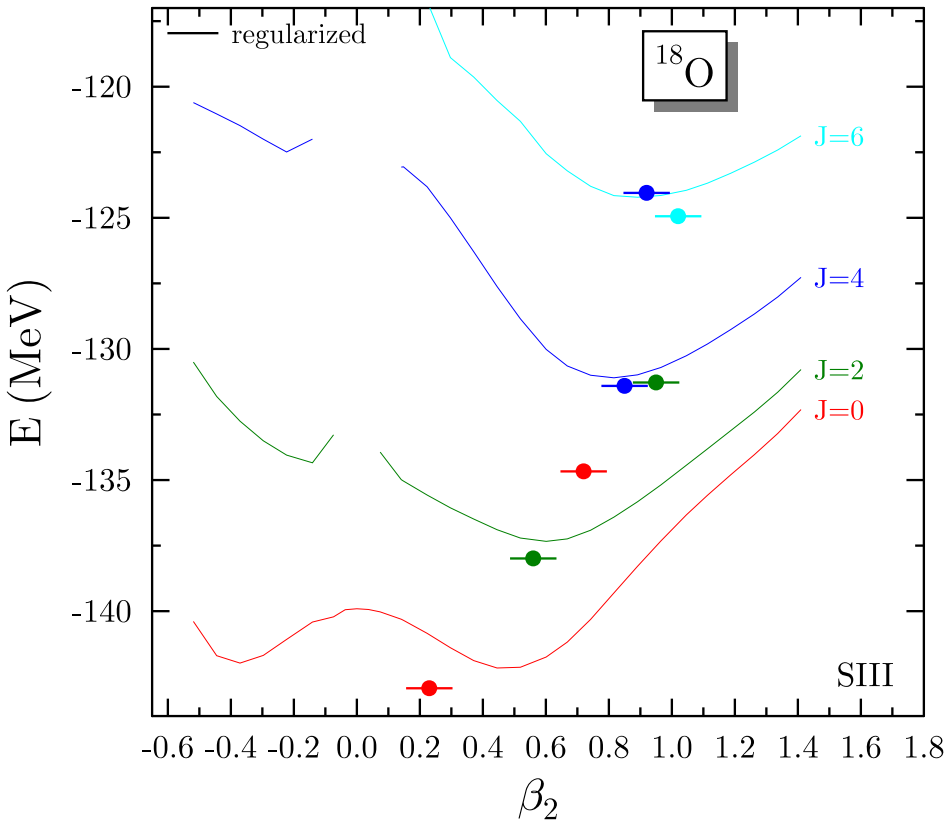
General configuration mixing



- Combined particle-number and angular-momentum restoration with regularization of the EDF

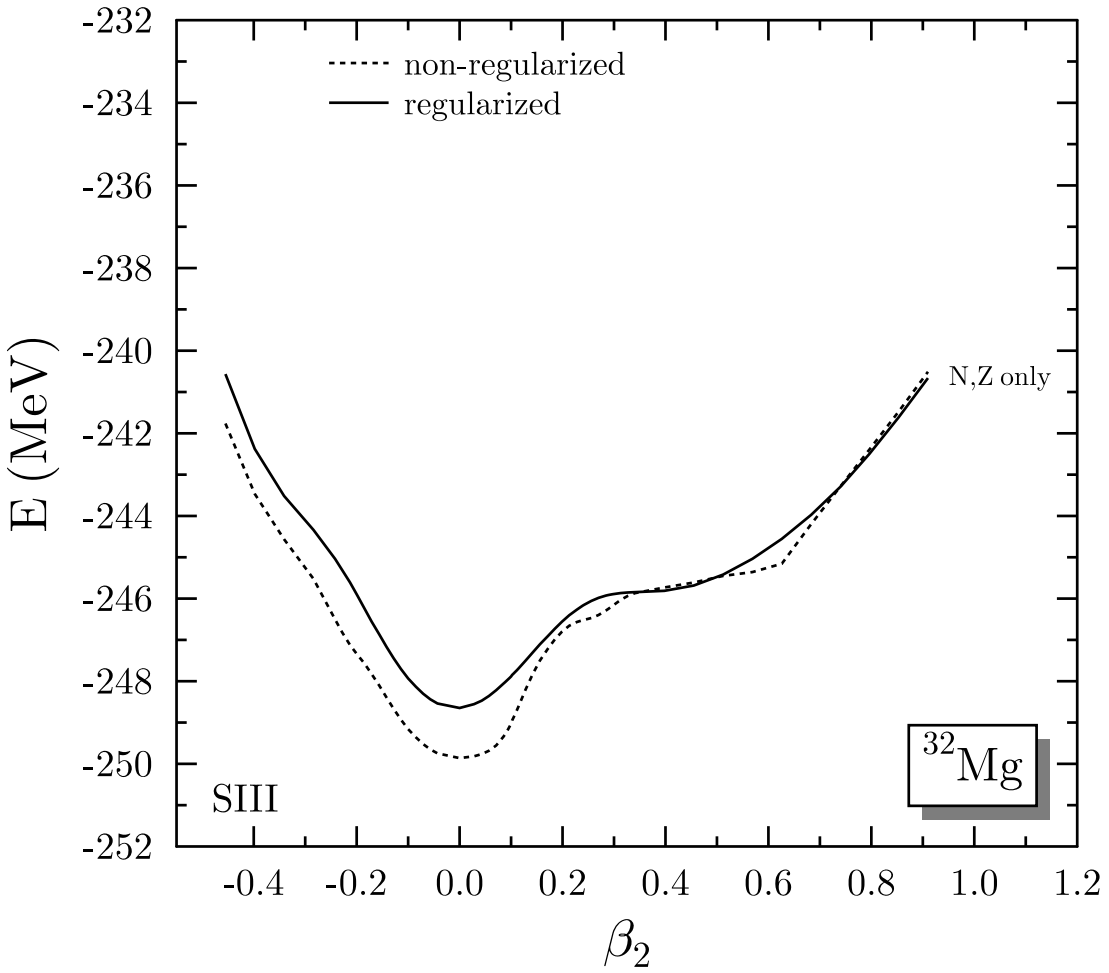
General configuration mixing



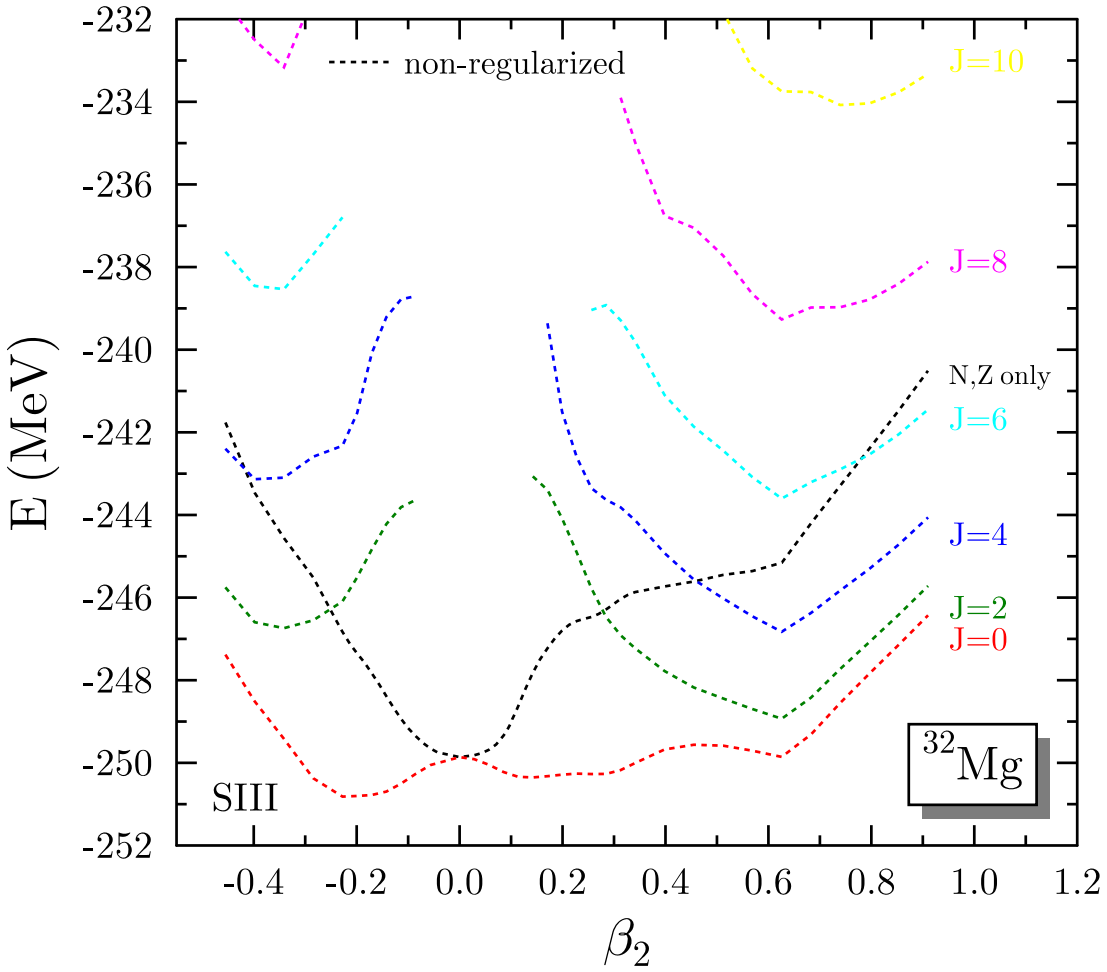


- Particle-number and angular-momentum restoration combined with mixing of different axial deformations without/with regularization of the EDF

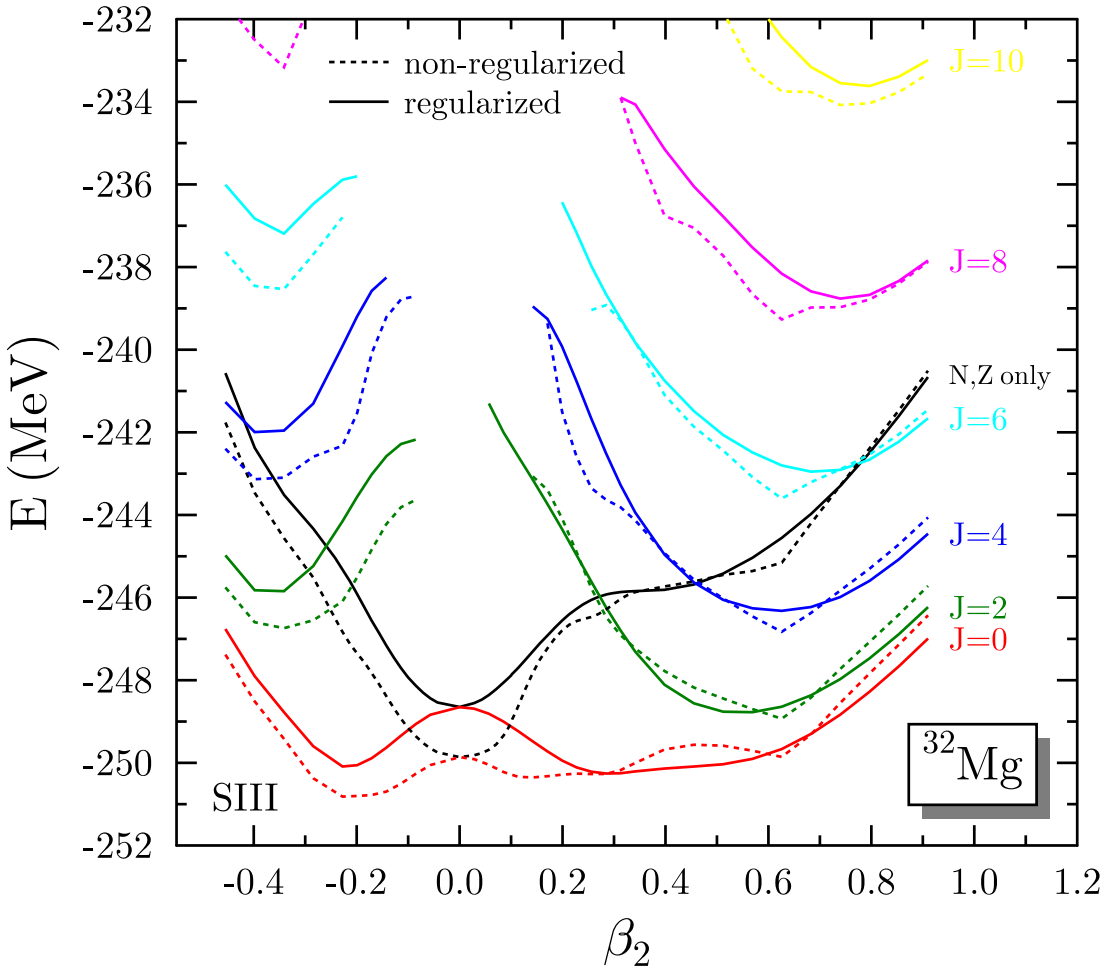
General configuration mixing: ^{32}Mg



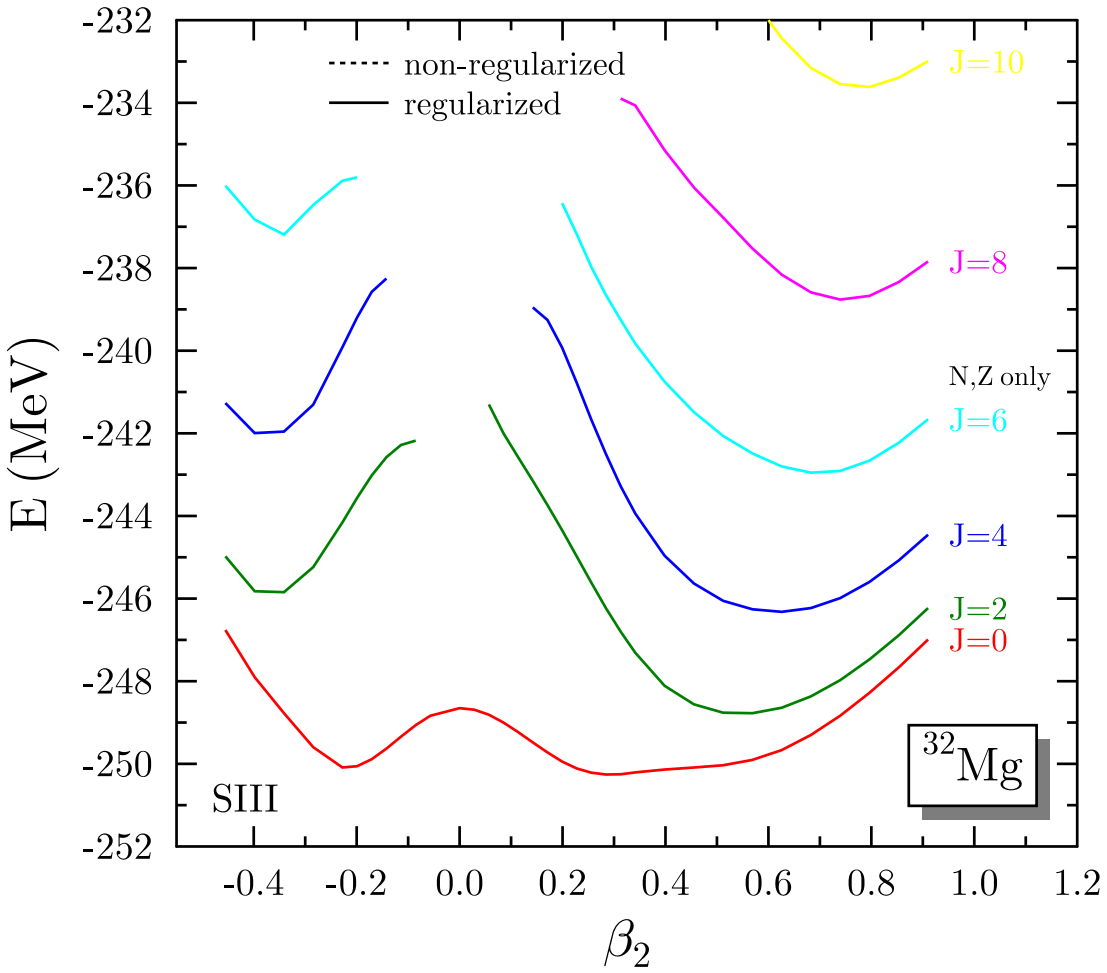
General configuration mixing: ^{32}Mg



General configuration mixing: ^{32}Mg

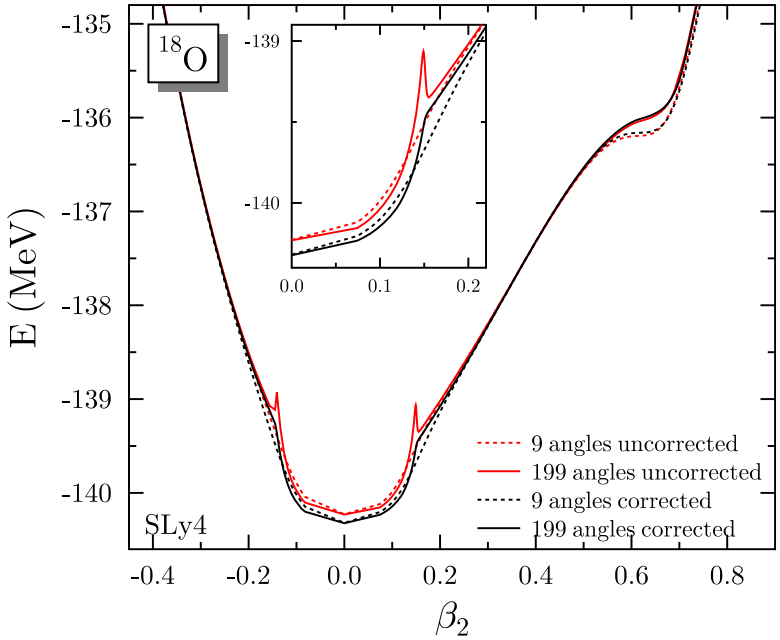


General configuration mixing: ^{32}Mg



Non-viability of non-integer density dependencies

- there is no way (we do not see a way) to set up a regularization scheme for non-integer density dependencies
- some "density-dependent Hamiltonians" are of this kind (Gogny force)
- same problem with standard Skyrme interactions ($\alpha \sim 1/3$) and Slater approximation for Coulomb exchange
- 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)



Conclusions

Summary

- all standard energy functionals contain small spurious self-interactions (and potentially self-pairing for Bogoliubov type auxiliary states)
- using the generalized Wick theorem to motivate a multi-reference energy functional gives these terms an unphysical weight *for any type of mixing*, including that of Slater determinants, which might lead to
- divergences for terms of order > 2 in density matrices of the same isospin
- . . . and always to steps or discontinutities when in particle number restoration a pole crosses the integration contour
- spurious energy can be isolated constructing a basis that permits to use the standard Wick theorem to evaluate the kernels.
- We are now able to do this for *any* mixing
- only energy density functionals with density dependencies of integer power are regularizable. "density dependent Hamiltonians" are *not* a priori free of anomalies

Outlook

- new energy density functionals necessary (what about Coulomb exchange?)

Acknowledgements

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Denis Lacroix	GANIL, Caen
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Karim Bennaceur	IPN Lyon
Thomas Lesinski	IPN Lyon

. . . thank you for your patience.

back-up slides

Reminder: Self-interaction

- 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

How to avoid or to remove these problems?

- Branch cuts are a consequence of using a non-analytical functional.
- Poles and steps are related to unphysical poles in the complex plane (they are unphysical as (i) they break so-called "shift invariance" [Dobaczewski *et al.* PRC 76 2007 054315] of the energy functional and (ii) they give a contribution to sum rules for states with zero norm, for example with $N \leq 0$).

Remedy:

- use density-dependent Hamiltonian without approximations and use particle-number projected density for the density dependence. As long as certain symmetries are not broken (that could lead to zero overlap), the pole problem is completely suppressed and one rests on the same step (Madrid)

Removing the problem: When you want to work with more general functionals or break more symmetries than usual:

- We do not see how to remove branch cuts other than using analyical functionals.
  $\Rightarrow$ use functionals depending on integer powers of the density matrix only
- to get rid of poles and steps: use correctable energy density functionals and work out the correction scheme proposed in Lacroix, Duguet, Bender, PRC 79 (2009) 044318 for arbitrary mixing.