Correction for spurious contributions to the Multi-Reference Energy Density Functional

Michael Bender

Université Bordeaux 1; CNRS/IN2P3; Centre d'Etudes Nucléaires de Bordeaux Gradignan, UMR5797
Chemin du Solarium, BP120, 33175 Gradignan, France

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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
PRC 79 (2009) 044320

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

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

- 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

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

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

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

$$\begin{pmatrix} \frac{\langle \mathrm{L}|\alpha\beta^\dagger|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} & \frac{\langle \mathrm{L}|\alpha\beta|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \\ \frac{\langle \mathrm{L}|\alpha^\dagger\beta^\dagger|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} & \frac{\langle \mathrm{L}|\alpha^\dagger\beta|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \end{pmatrix} = \begin{pmatrix} D^T & 0 \\ 0 & 0 \end{pmatrix} \qquad \left|\langle \mathrm{L}|\mathrm{R}\rangle\right| = \sqrt{\det D^{-1}}$$

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

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

- 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

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

and a functional depending on this density matrix

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

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:

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

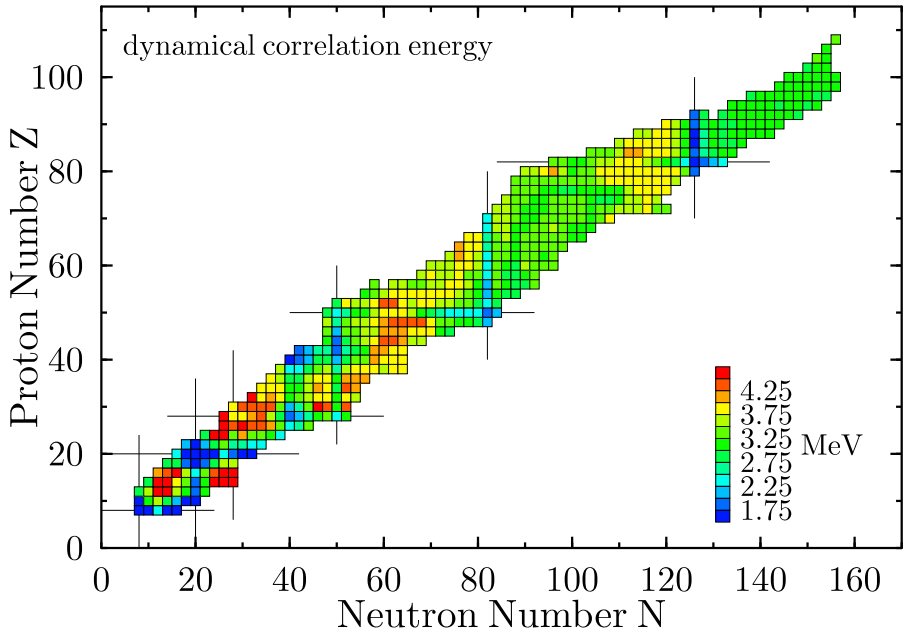
Coulomb interaction $\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$

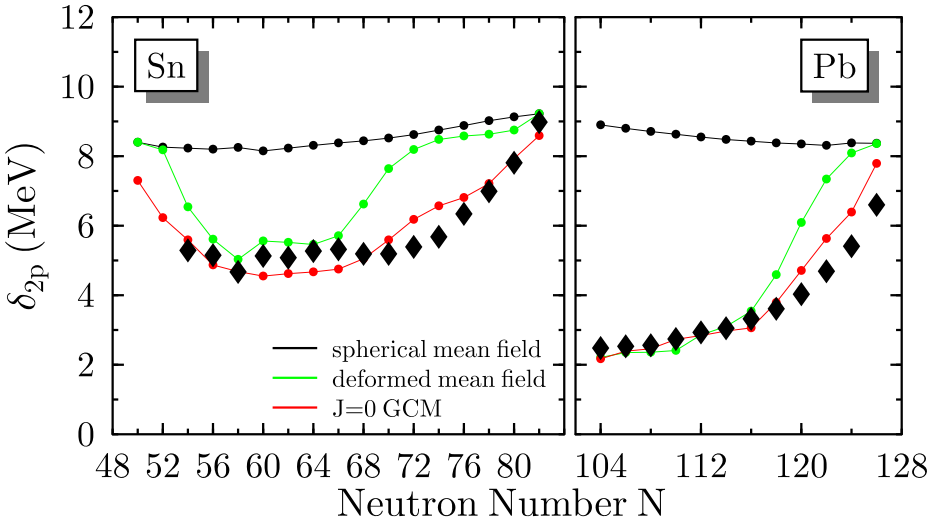
$$\mathcal{E} = \frac{1}{2}\iint d^3r\,d^3r'\,\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\Big[\rho_p(\mathbf{r})\rho_p(\mathbf{r}') - \rho_p(\mathbf{r},\mathbf{r}')\rho_p(\mathbf{r}',\mathbf{r}) + \kappa_p^*(\mathbf{r},\mathbf{r}')\kappa_p(\mathbf{r},\mathbf{r}')\Big]$$

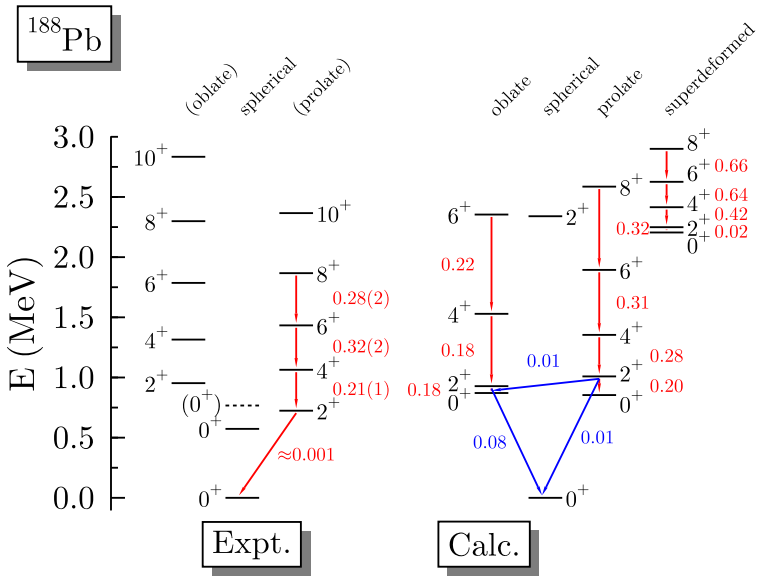
Approximate Coulomb functionals

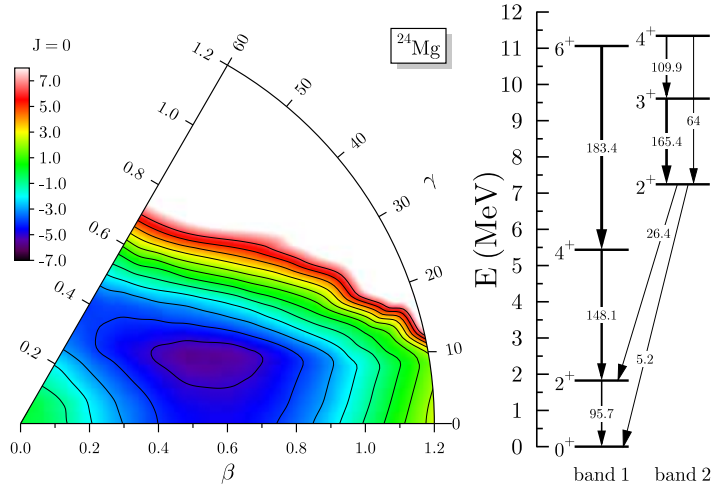
$$\mathcal{E} = \frac{e^2}{2}\iint d^3r\,d^3r'\,\frac{\rho_p(\mathbf{r})\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} - \frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}\int d^3r\,\rho_p^{4/3}(\mathbf{r})$$

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



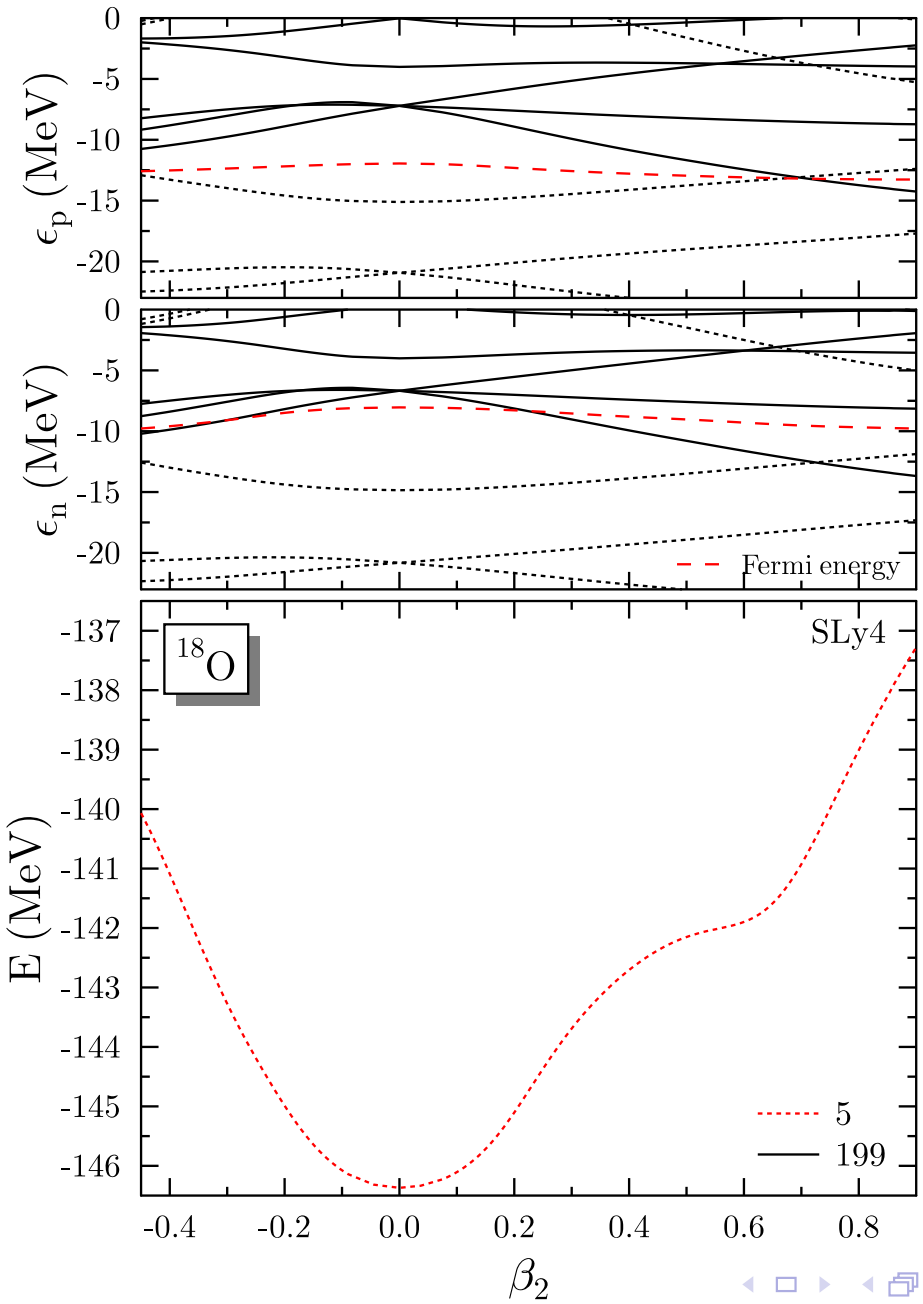






⇒ see my forthcoming talk at Niigata for details

Here is a problem . . .



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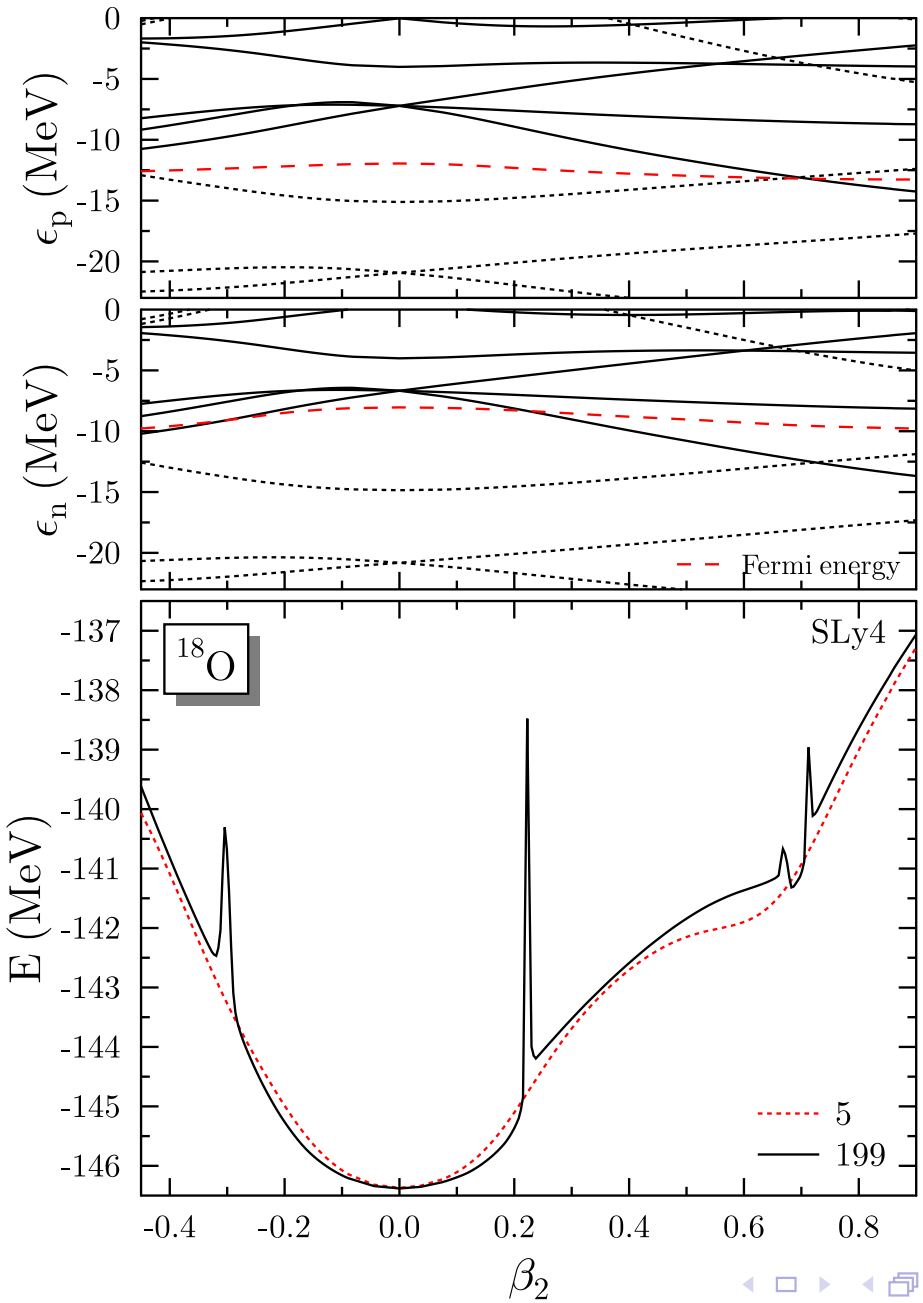


Single-reference description of pairing correlations

- Independent quasiparticle state (quasiparticle vacuum, HFB state)

$$|\Phi_\varphi\rangle = \mathcal{C}_\varphi \prod_\nu \alpha_\nu |0\rangle$$

- has BCS form in its canonical basis (u_μ, v_μ real)

$$|\Phi_\varphi\rangle = \prod_{\mu>0} \left(u_\mu + v_\mu\, e^{2i\varphi}\, a_\mu^+\, a_{\bar{\mu}}^+\right) |0\rangle$$

- static pairing correlations through spontaneous symmetry breaking of the $U(1)$ gauge symmetry $\Rightarrow$ orientation in gauge space φ
- $|\Phi_\varphi\rangle$ is not an eigenstate of $\hat{N}$
- intrinsic one-body fields depend on the orientation, observables still gauge invariant. $\Rightarrow$ orientation in gauge space can be set to convenient direction $\varphi = 0$ (similar to major axis system for deformed nuclei)

$$|\Phi_0\rangle = \prod_{\mu>0} \left(u_\mu + v_\mu\, a_\mu^+\, a_{\bar{\mu}}^+\right) |0\rangle$$

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)

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

removes components up to $N_0 \pm 2M$ from a state projected on N_0.

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

Guided by the generalized Wick theorem (GWT) [Balian and Brézin, Il Nuovo Cimento, Vol. LXIV B, (1969) 37] for operator matrix elements it was postulated that the particle-number projected EDF is given by

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

transition density matrices in the canonical basis shared by both states

$$\rho^{0\varphi}_{\mu\nu} = \frac{v_\mu^2\, e^{2i\varphi}}{u_\mu^2 + v_\mu^2\, e^{2i\varphi}}\, \delta_{\nu\mu}\,, \quad \kappa^{0\varphi}_{\mu\nu} = \frac{u_\mu v_\mu e^{2i\varphi}}{u_\mu^2 + v_\mu^2\, e^{2i\varphi}}\, \delta_{\nu\bar{\mu}}\,, \quad \kappa^{\varphi 0\,*}_{\mu\nu} = \frac{u_\mu v_\mu}{u_\mu^2 + v_\mu^2\, e^{2i\varphi}}\, \delta_{\nu\bar{\mu}}$$

overlap

$$\langle\Phi_0|\Phi_\varphi\rangle = \prod_{\mu>0}\left(u_\mu^2 + v_\mu^2\, e^{2i\varphi}\right)$$

. . . but where is the problem?

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

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

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

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

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]

earlier warnings by Dönau, PRC 58 (1998) 872; Almehed, Frauendorf, Dönau, PRC 63 (2001) 044311.

similar problem discussed by Tajima, Flocard, Bonche, Dobaczewski and Heenen, NPA542 (1992) 355

rediscovered by Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315

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

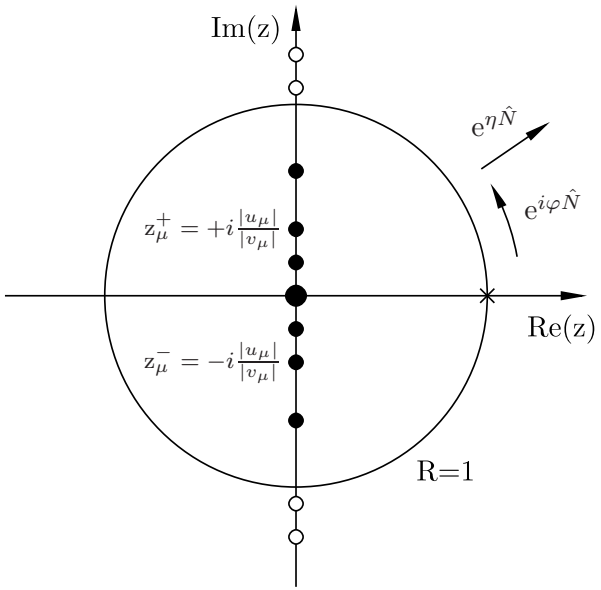
- Contour integrals can be evaluated using Cauchy's residue theorem [Bayman, NP15 (1960) 33]
- the norm and all operator matrix elements have a pole at $z = 0$

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

- 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 turn out to be a consequence of using the GWT to motivate the multi-reference energy functional
- this can be shown constructing a basis where the kernels can be evaluated using a standard Wick theorem (SWT) or elementary operator algebra

Idea: Starting with two quasiparticle vacua

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

and the respective quasiparticle operators given by

$$\alpha_\nu^+ = \sum_i \left(U_{i\nu}^0 \, a_i^+ + V_{i\nu}^0 \, a_i \right) \qquad \beta_\nu^+ = \sum_i \left(U_{i\nu}^1 \, a_i^+ + V_{i\nu}^1 \, a_i \right)$$

The two sets of quasiparticle operators are connected by a Bogoliubov transformation

$$\beta_\mu^+ = \sum_\nu \left(A_{\nu\mu} \, \alpha_\nu^+ + B_{\nu\mu} \, \alpha_\nu \right)$$

with $A = U^{0^+} U^1 + V^{0^+} V^1$ and $B = V^{0^T} U^1 + U^{0^T} V^1$

The origin of the poles II

Bloch-Messiah-Zumino decomposition of the transformation

$$\beta^+_\mu = \sum_\nu \left(A_{\nu\mu}\, \alpha^+_\nu + B_{\nu\mu}\, \alpha_\nu \right)$$

gives two intermediate quasiparticle bases

$$\tilde{\alpha}^+_\nu \equiv \sum_\mu \alpha^+_\mu\, D_{\mu\nu} \qquad\qquad \tilde{\beta}^+_\nu \equiv \sum_\mu \beta^+_\mu\, C_{\mu\nu}$$

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

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

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

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

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

Express single-particle operators in terms of one set of quasiparticle operators

$$a^+_i = \sum_\nu\left(\tilde{U}^{0*}_{i\nu}\,\tilde{\alpha}^+_\nu + \tilde{V}^0_{i\nu}\,\tilde{\alpha}_\nu\right) \qquad \text{with } \tilde{U}^0 = U^0 D \text{ and } \tilde{V}^0 = V^0 D$$

to define quasiparticle wave functions $\begin{pmatrix}|\phi_\nu\rangle\\ |\varphi_{\bar{\nu}}\rangle\end{pmatrix} = \sum_i \begin{pmatrix}\tilde{U}^{0\,T}_{\nu i}\\ \tilde{V}^{0\,+}_{\nu i}\end{pmatrix}|i\rangle$

associated with $\{\tilde{\alpha}_\nu,\tilde{\alpha}^+_\nu\}$ in the single-particle basis.

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 is

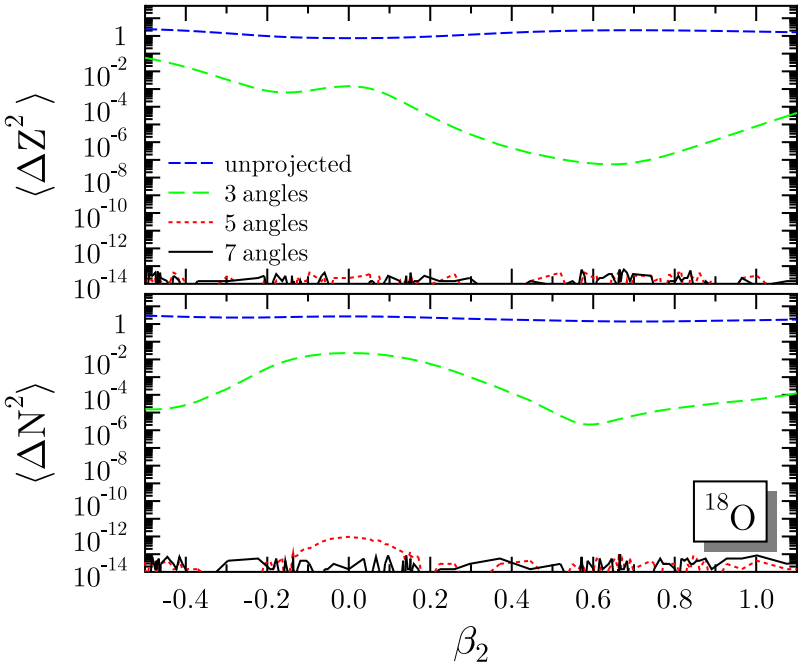
$$\begin{aligned} \mathcal{E}^N_{CG} &= \sum_{\mu>0}\left[\frac{1}{2}\left(\bar{v}^{\rho\rho}_{\mu\mu\mu\mu}+\bar{v}^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}}+\bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}}+\bar{v}^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu}\right)-\bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}}\right]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

The origin of the poles VI

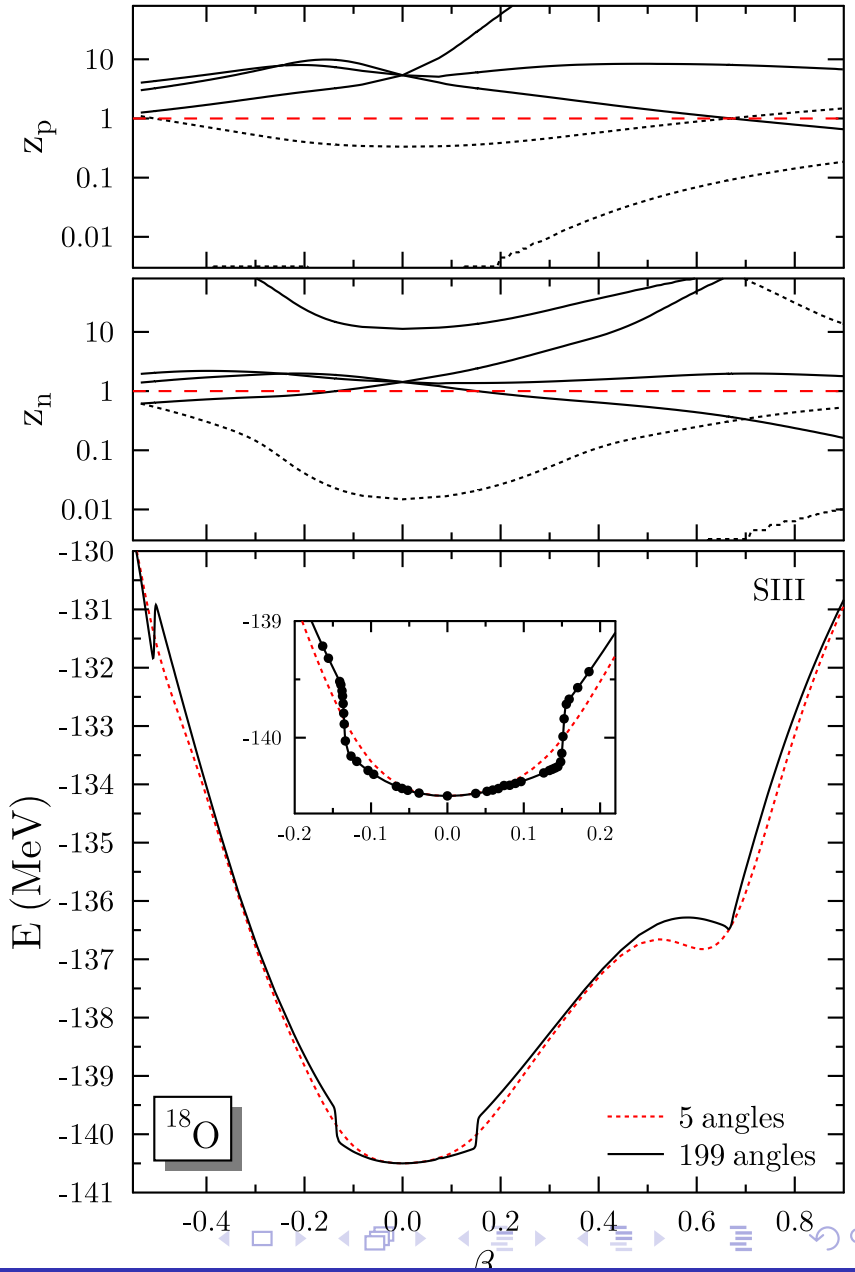
- The poles turn out to be a consequence of using the GWT to motivate the multi-reference energy functional
- They appear in terms that are spurious self-interactions or spurious self-pairing, the former known for long from condensed-matter DFT.
- self-interaction is related to broken antisymmetry of 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?

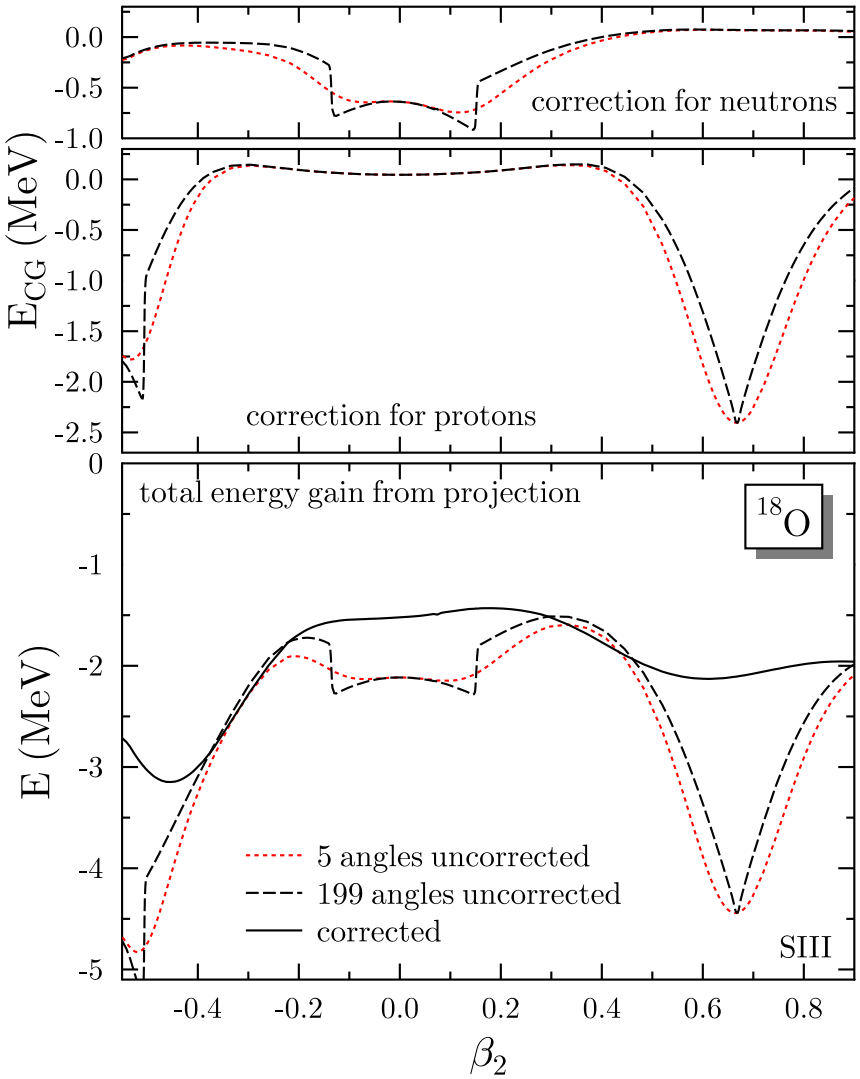
Corrected PNP: ^{18}O I

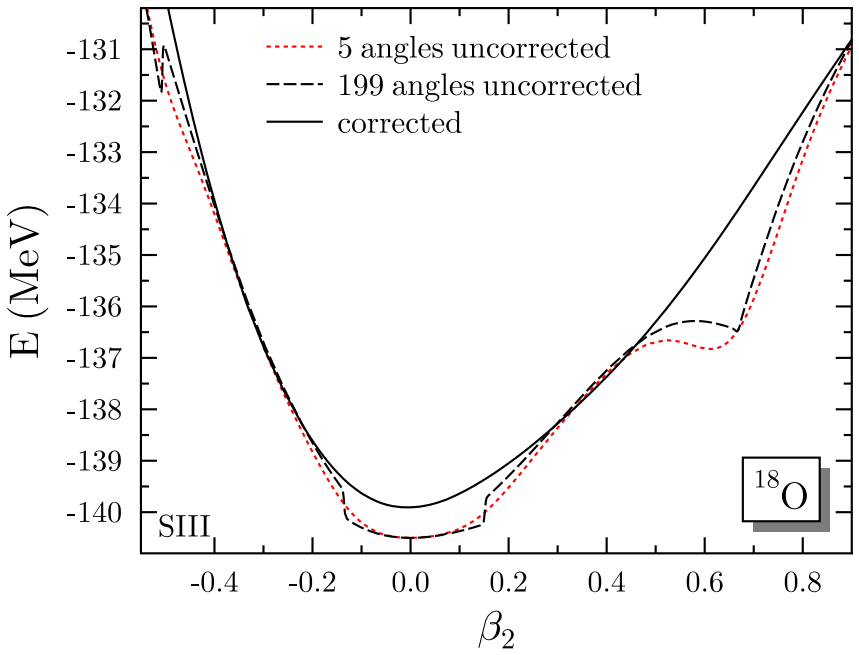


- calculations with SIII (bilinear in density of given isospin, no divergence)
- projected wave function and all operator matrix elements are converged with $L = 5$ discretization points of the gauge space integral
- the projected energy functional does *not* converge with $L = 199$ points



Corrected PNP: ^{18}O II





Shift invariance

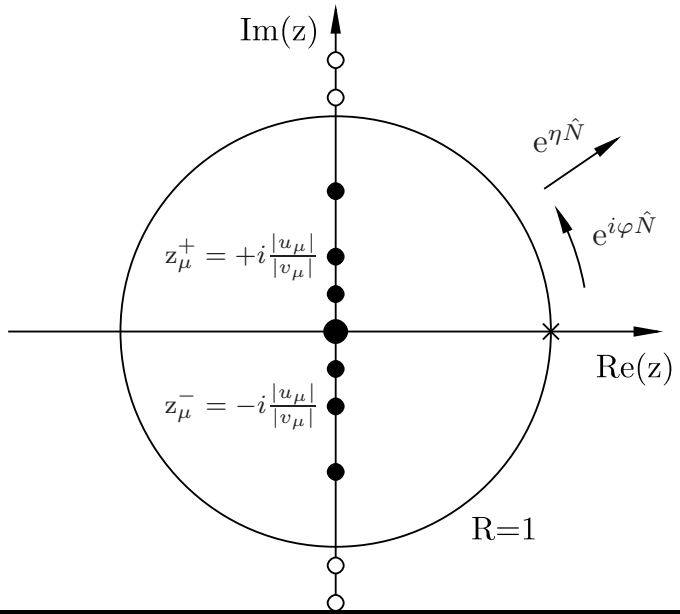
- Shift transformation

$$|\Phi_{\varphi-i\eta}\rangle = e^{\eta\hat{N}}\,|\Phi_{\varphi}\rangle$$

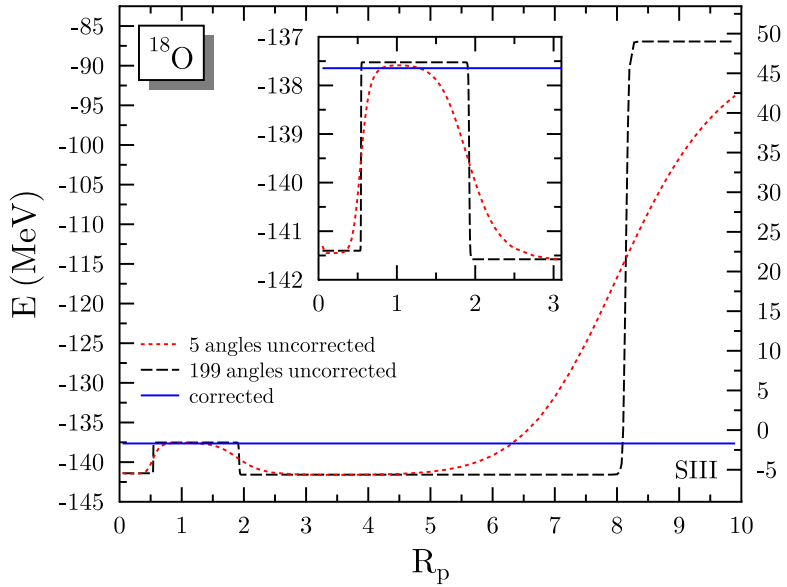
- shifts radius of complex contour interal

$$\int_0^{2\pi}\frac{d\varphi}{2\pi\,c_N^2}e^{-i\varphi N}|\Phi_{\varphi-i\eta}\rangle = \oint_R\frac{dz}{2i\pi}\frac{1}{z^{N+1}}|\Phi_{\varphi}\rangle$$

- Operators that commute with $\hat{N}$ are shift invariant



- the uncorrected projected energy functional is not
- steps far from the standard contour $R_p = 1$ ($\Leftrightarrow$ Fermi level) can be huge
- the corrected projected energy functional is shift invariant



energy as a function of the radius R_p of the integration contour of protons at $Q = 500$ fm^2, $\beta_2 = 0.371$ and using $R_n = 1$.

(Radius weighted) Sum rules I

From

$$\sum_{N\geq 0} |\Psi^N\rangle\langle\Psi^N| = \sum_{N\geq 0} \hat{P}^N = 1$$

follows a sumrule for operator matrix elements

$$\langle\Phi_1|\hat{O}|\Phi_R\rangle = \langle\Phi_1|\hat{O}e^{\eta\hat{N}}|\Phi_1\rangle = \sum_{N\geq 0}\langle\Phi_1|\hat{O}e^{\eta\hat{N}}|\Psi^N\rangle\,\langle\Psi^N|\Phi_1\rangle = \sum_{N\geq 0} c_N^2(R)\,O^N$$

A general EDF does not correspond to an operator, and there is no equivalent to "inserting a complete 1" when having an EDF.
$\Rightarrow$ start from the tail-end and sum over Fourier components, which leads to

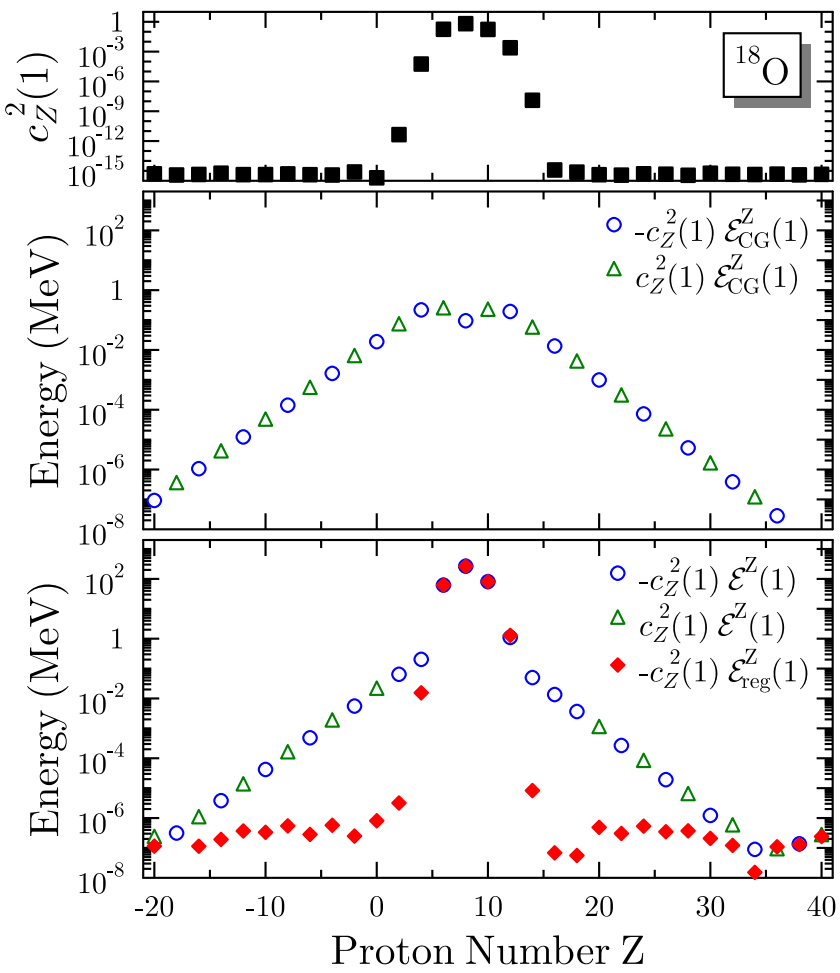
$$\sum_{N=0}^{+\infty} |c_N|^2\,\mathcal{E}^N = \mathcal{E}[\rho,\kappa,\kappa^*]$$

There also is a sum rule for spurious energy

$$\sum_{N=0}^{+\infty} |c_N|^2\,\mathcal{E}^N_{CG} = 0$$

Who has ordered negative particle numbers ???

(Radius weighted) Sum rules II



SR interaction energy (without kinetic energy)

$$\mathcal{E}[\rho,\kappa,\kappa^*] = -410.3403 \text{ MeV}$$

sum over physical components $Z > 0$

$$\sum_{Z>0} c_Z^2(1)\,\mathcal{E}^Z(1) = -410.3550 \text{ MeV}$$

sum over all $Z \gtrless 0$

$$\sum_{Z=-\infty}^{+\infty} c_Z^2(1)\,\mathcal{E}^Z(1) = -410.3403 \text{ MeV}$$

$Z = 0$ component

$$c_Z^2(1)\,\mathcal{E}^{Z=0}(1) = c_Z^2(1)\,\mathcal{E}^{Z=0}_{CG}(1) = 0.0189 \text{ MeV}$$

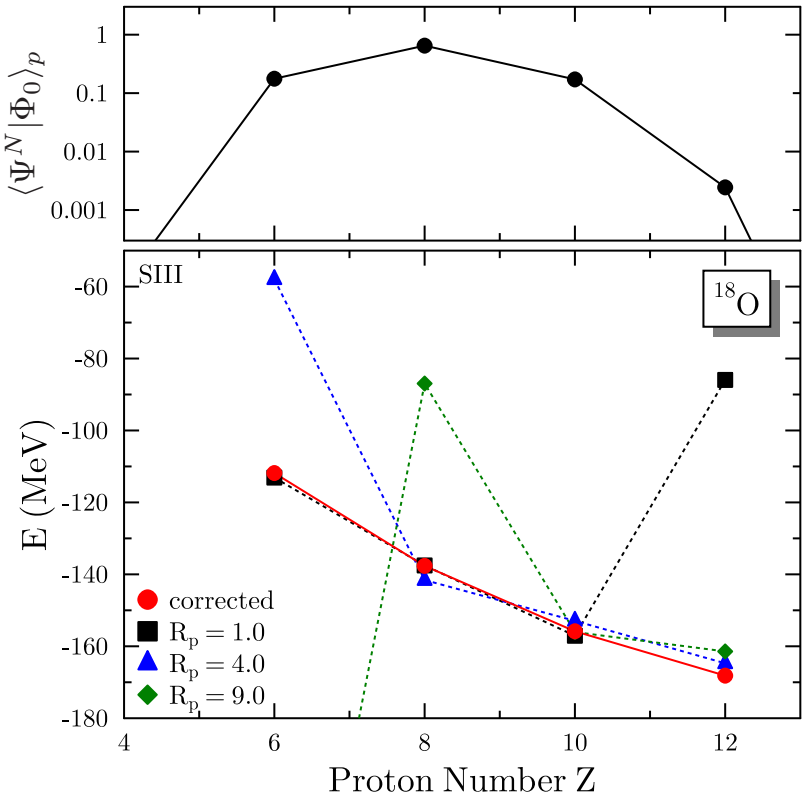
sum correction over all $Z \gtrless 0$

$$\sum_{Z=-\infty}^{+\infty} c_Z^2(1)\,\mathcal{E}^Z_{CG}(1) = 0.0000 \text{ MeV}$$

sum regularized EDF over $Z > 0$

$$\sum_{Z>0} c_Z^2(1)\mathcal{E}^Z_{REG}(1) = -410.3403 \text{ MeV}$$

(Radius weighted) Sum rules III



Weight of the normalized state projected on various values of Z in the SR vacuum (top panel) and decomposition of the energy into Z components for three different radii of the integration contour for protons (bottom panel) for ^{18}O at $\beta_2 = 0.371$. All states are projected on $N = 10$ with $R_n = 1$.

- at each spurious step, the decomposition of the energy over all N components changes
- Small spurious energies in components with large weight c_N^2 do not prevent large spurious energies in components with small weight $c_{N'}^2$

(Non-radius weighted) Sum rules

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

Contribution from isolated poles. I neutron levels in ^{18}O

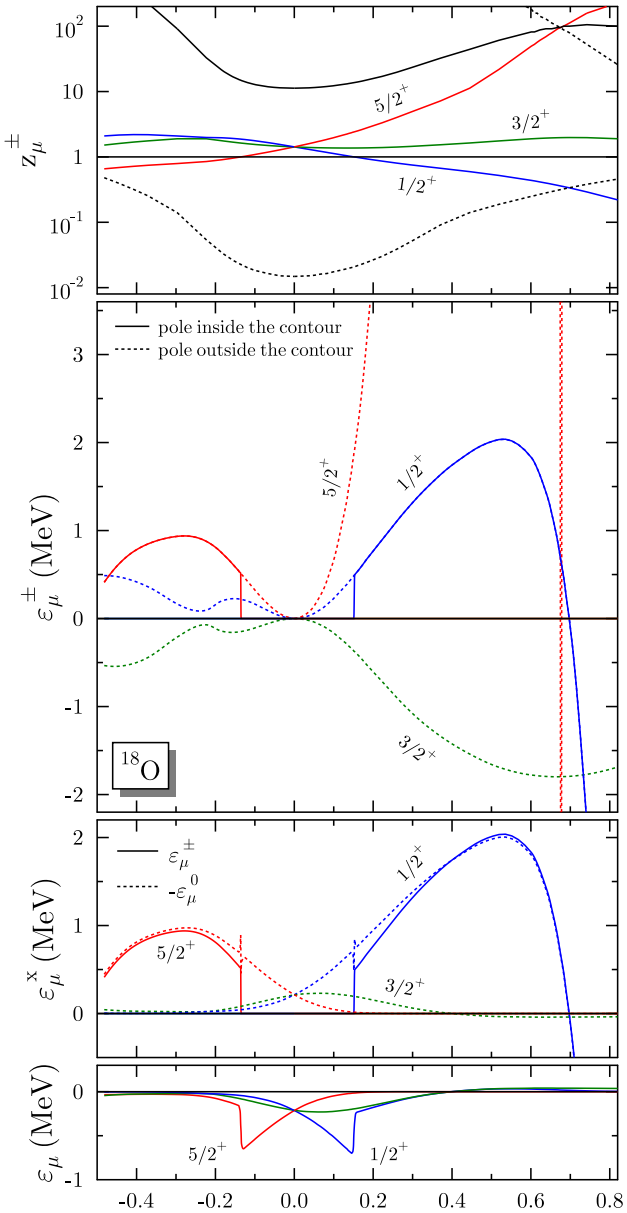
contribution from individual levels

$$\mathcal{E}^N_{CG} = \sum_{\mu>0} \varepsilon_\mu = \sum_{\mu>0} \varepsilon^0_\mu + \sum_{\substack{\mu>0 \\ |z^\pm_\mu|<R}} \varepsilon^\pm_\mu$$

$\varepsilon^\pm_\mu$ is proportional to $u^4 v^4$ times the residue of a pole at $z^\pm_\mu$

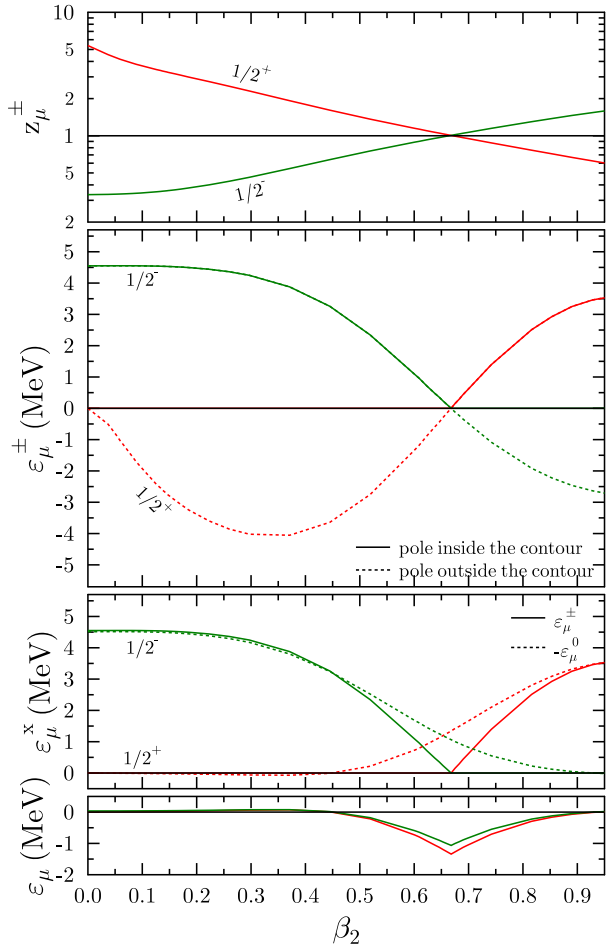
$$\begin{aligned} & \mathcal{R}e_{CG}(z^\pm_\mu) \\ &= \sum_{z_i = z^\pm_\mu} \mathcal{R}es(z_i) \left[\frac{\left(z^2-1\right)^2 \prod_{\substack{\nu>0 \\ \nu\neq\mu}} \left(u^2_\nu + v^2_\nu z^2\right)}{v^2_\mu z^{N+1} \left(z - i\frac{|u_\mu|}{|v_\mu|}\right)\left(z + i\frac{|u_\mu|}{|v_\mu|}\right)} \right] \\ &= -\frac{1}{v^6_\mu} \left(\frac{v_\mu}{u_\mu}\right)^{N+2} \frac{1+(-1)^N}{2\, i^N} \prod_{\substack{\nu>0 \\ \nu\neq\mu}} \frac{u^2_\nu v^2_\mu - v^2_\nu u^2_\mu}{v^2_\mu} \end{aligned}$$

- smallest when there are $N/2$ pairs of levels below the level in question $\Rightarrow$ levels at the Fermi energy
- $\varepsilon^\pm_\mu$ alone grows beyond all meaningful energy scales for levels far above the Fermi level



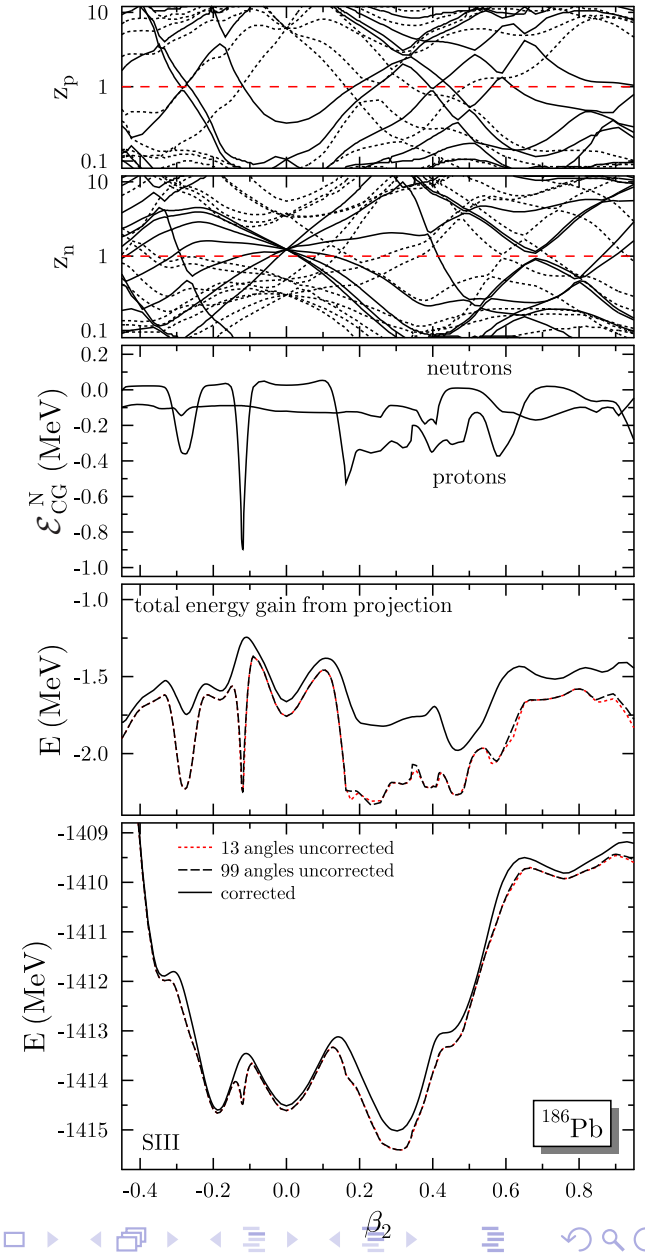
Contribution from isolated poles. II proton levels in ^{18}O

- for bilinear functionals $\varepsilon_\mu^\pm$ disappears for more than twofold degenerate levels
- ε_μ^0 still might be large
- $\Rightarrow$ spurious cusp (discontinuity) without a step where two levels cross at the Fermi level



Corrected PNP: ^{186}Pb

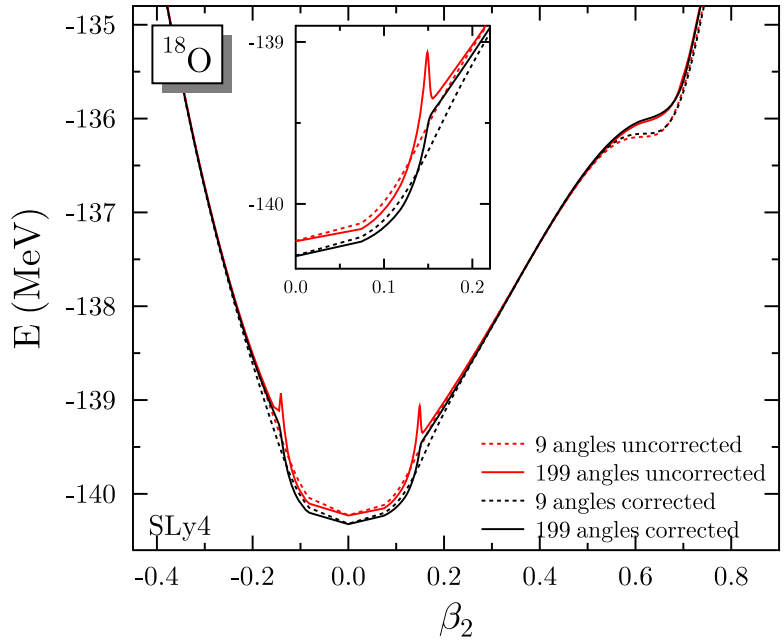
- large density of single-particle levels
  - $\Rightarrow$ large density of poles $z_\mu^\pm$
  - $\Rightarrow$ many poles crossing the Fermi surface
  - $\Rightarrow$ many steps
- the isolated proton poles give much larger steps than the densely packed neutron poles when crossing the Fermi level.
- correction might be on the same energy scale as spectroscopy of collective states

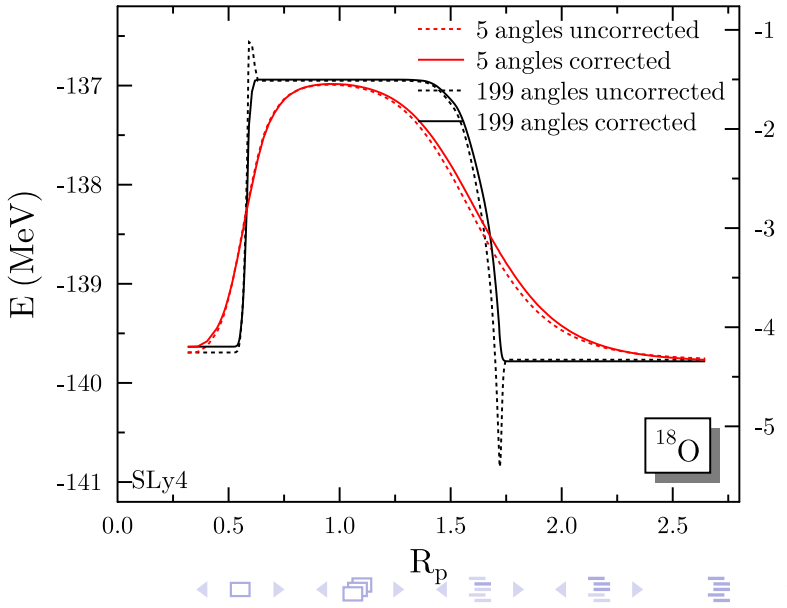


Disclaimer: the energy surface for ^{186}Pb from SIII is inconsistent with the empirical knowledge about this nucleus. The analysis of the spurious energies not compromised by that.

Non-viability of non-integer density dependencies

- there is no way to set up this correction 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" correcting for the biliear part, leaving the uncorrected density dependence
- there remains a spurious contribution from branch cuts (see Duguet *et al.* PRC 79 (2009) 044320 for complex plane analysis)





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 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.

Philosophical 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" of the energy functional and (ii) they give a contribution to sum rules for states with zero norm, for example with $N \leq 0$).

Remedies:

- 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, Warsaw)

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.

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
- divergences for terms of order > 2 in density matrices of the same isospin when a pole crosses the integration contour
- always steps or discontinutities when a pole crosses the integration contour
- spurious energy can be isolated constructing a basis that permits to use the standard Wick theorem
- only energy density functionals with density dependencies of integer power are correctable. "density dependent Hamiltonians" are *not* a priori free of anomalies

Outlook

- modification of codes: construct basis that allows the calculation of the correction
- new energy density functionals necessary (what about Coulomb exchange?)