Symmetry Restored GCM Based on Time-Reversal Breaking States

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Workshop on
The future of multireference DFT
Warsaw, Poland, 25-26 June 2015

People involved

- Identifying problems with general functionals in MR EDF:
  M. B., T. Duguet, D. Lacroix, B. Avez, B. Bally, P.-H. Heenen
- construction of a Skyrme-type 3-body pseudo-potential:
  J. Sadoudi (thesis work in Saclay + postdoc in Bordeaux),
  T. Duguet, J. Meyer, M. Bender

particle-number projector

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

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

$$|JMq\rangle = \sum_{K=-J}^{+J} f_J(K) \ \hat{P}^J_{MK} \ \hat{P}^Z \ \hat{P}^N \, |\text{MF}(q)\rangle = \sum_{K=-J}^{+J} f_J(K) \, |JM(qK)\rangle$$

$f_J(K)$ 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, while the sum over K collapses, $f_J(K) \sim \delta_{K0}$

Configuration mixing by the symmetry-restored Generator Coordinate Method

Superposition of projected self-consistent mean-field states $|\mathrm{MF}(\mathbf{q})\rangle$ differing in a set of collective and single-particle coordinates $\mathbf{q}$

$$|NZJM\nu\rangle = \sum_{\mathbf{q}} \sum_{K=-J}^{+J} f_{J,\kappa}^{NZ}(\mathbf{q}, K)\, \hat{P}^J_{MK}\, \hat{P}^Z\, \hat{P}^N\, |\mathrm{MF}(\mathbf{q})\rangle = \sum_{\mathbf{q}} \sum_{K=-J}^{+J} f_{J\nu}^{NZ}(\mathbf{q}, K)\, |NZ\, JM(\mathbf{q}K)\rangle$$

with weights $f_{J\nu}^{NZ}(\mathbf{q}, K)$.

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

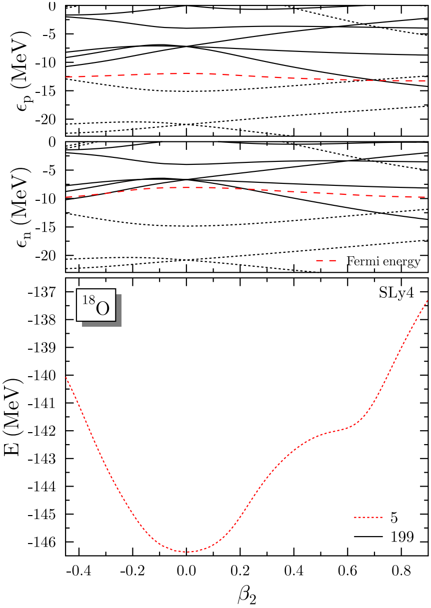
$$\sum_{\mathbf{q}'} \sum_{K'=-J}^{+J} \left[\mathcal{H}_J^{NZ}(\mathbf{q}K, \mathbf{q}'K') - E_{J,\nu}^{NZ}\, \mathcal{I}_J^{NZ}(\mathbf{q}K, \mathbf{q}'K')\right] f_{J,\nu}^{NZ}(\mathbf{q}'K') = 0$$

with

$$\mathcal{H}_J(\mathbf{q}K, \mathbf{q}'K') = \langle NZ\, JM\, \mathbf{q}K|\hat{H}|NZ\, JM\, \mathbf{q}'K'\rangle \quad \text{energy kernel}$$
$$\mathcal{I}_J(\mathbf{q}K, \mathbf{q}'K') = \langle NZ\, JM\, \mathbf{q}K|NZ\, JM\, \mathbf{q}'K'\rangle \quad \text{norm kernel}$$

Angular-momentum projected GCM gives the

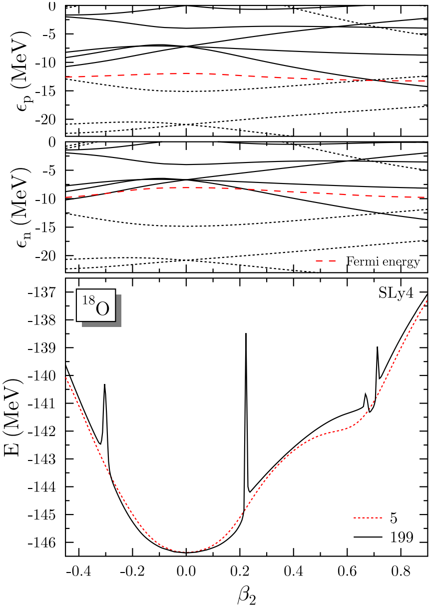
- correlated ground state for each value of J
- spectrum of excited states for each J



- pure particle-number projection

M. B., T. Duguet, and D. Lacroix Phys. Rev. C 79 (2009) 044319

What kind of functionals to use? Problems with existing ones



- pure particle-number projection

M. B., T. Duguet, and D. Lacroix Phys. Rev. C 79 (2009) 044319

(LDB-) Regularisation: A non-solution to the problem

- Lacroix, Duguet, & Bender, PRC 79 (2009) 044318, proposed a physics-based regularization scheme of the EDF that allows for the use of (almost) standard functionals for which numerically efficient high-quality parameterizations can be easily constructed.
- In a nutshell, one tries to remove self-interaction and self-pairing contributions to the EDF that are multiplied with unphysical weights.
- Problem: complicated formalism, requires construction of the canonical basis of a very general canonical (Bogoliubov) transformation.
- Problem: Works properly only in particle-number projection.
- Problem: Combined particle-number and angular-momentum projection projection does not converge and sum rules are not fulfilled
- Problem: two ways of defining the regularisation of GCM that are not equivalent $\Rightarrow$ need to average
- In angular-momentum projection of time-reversal-invariance-breaking states small components take unphysical energies (with regularization this might become worse than without).

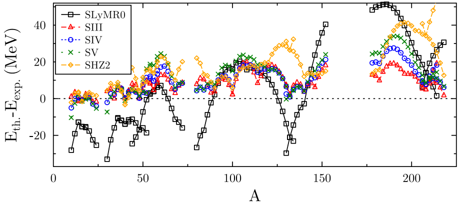
Bender, Avez, Bally, Duguet, Heenen, Lacroix, *in preparation for too long*

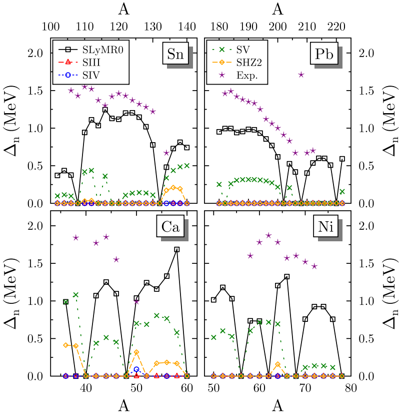
First try: SLyMR0

$$
\begin{aligned}
\hat{v} = {} & t_0 \left(1 + x_0 \hat{P}_\sigma\right) \hat{\delta}_{r_1 r_2} \\
& + \frac{t_1}{2} \left(1 + x_1 \hat{P}_\sigma\right) \left(\hat{\mathbf{k}}_{12}^{\prime 2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12}^{2}\right) \\
& + t_2 \left(1 + x_2 \hat{P}_\sigma\right) \hat{\mathbf{k}}_{12}^{\prime} \cdot \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12} \\
& + \mathrm{i}\, W_0 \left(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2\right) \cdot \hat{\mathbf{k}}_{12}^{\prime} \times \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12} \\
& + u_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1}\right) \\
& + v_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \hat{\delta}_{r_3 r_4} + \hat{\delta}_{r_1 r_2} \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_2 r_4} + \cdots\right)
\end{aligned}
$$

J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta T154 (2013) 014013

Proof-of-principle: Does using Hamiltonians remove all problems?





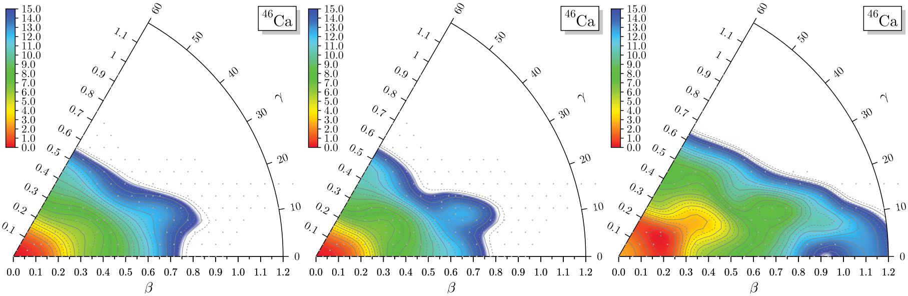
- it is impossible to fullfil the usual nuclear matter constraints , to have stable interactions and attractive pairing
- no "best fit" possible
- very bad performance compared to standard general functionals

J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta T154 (2013) 014013

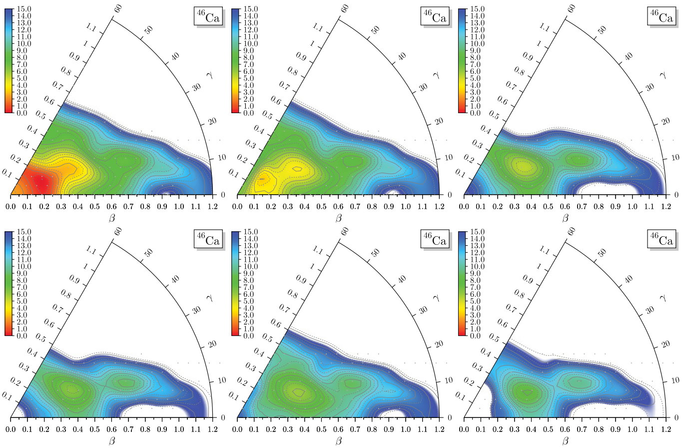
⇒ see talk by B. Bally lateron for angular-momentum and particle-number projected GCM of blocked triaxial one-quasiparticle states

B. Bally, doctoral thesis, Université de Bordeaux (2014)

B. Bally, B. Avez, M. B., and P.-H. Heenen, PRL 113 (2014) 162501

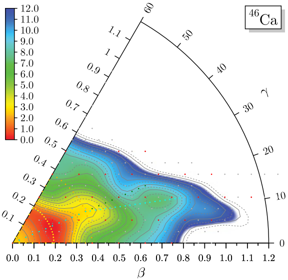


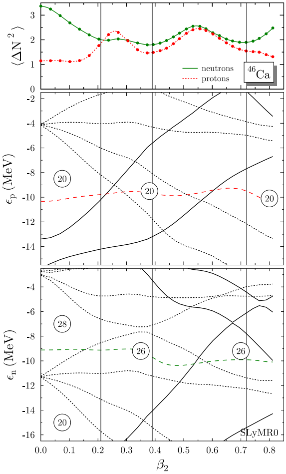
Left: Non-projected total energy of the HFB vacua (without LN correction) relative to the spherical configuration. Middle: $N = 26$, $Z = 20$ projected total energy of the HFB vacua relative to the spherical configuration. Right: Energy of the projected $N = 26$, $Z = 20$, $J = 0$ HFB vacua.



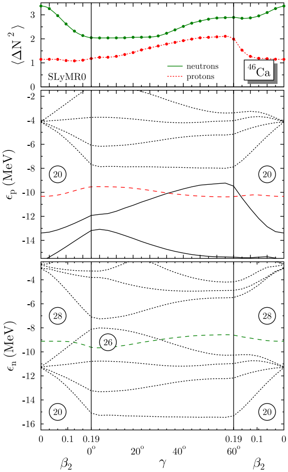
Top row: Right: Energy of the $J = 0$ HFB vacua. Middle: Energy of the lowest K-mixed $J = 2$ projected state . Right: Energy of the second K-mixed $J = 2$ state . Bottom row: Right: Energy of the $J = 3$ state. Middle: Energy of the lowest K-mixed $J = 4$ projected state. Right: Energy of the second K-mixed $J = 4$ state. The total energy is relative to the minimum of the $J = 0$ energy surface. All states are projected on $N = 26$, $Z = 20$,

Fun with SLyMR0 – ^{46}Ca



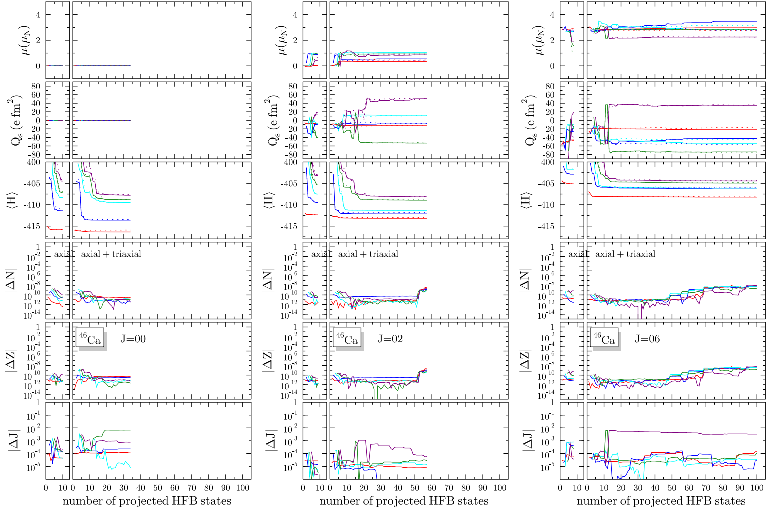


Nilsson diagram along the path indicated by cyan dots. Vertical bars indicate the deformation of the minima.



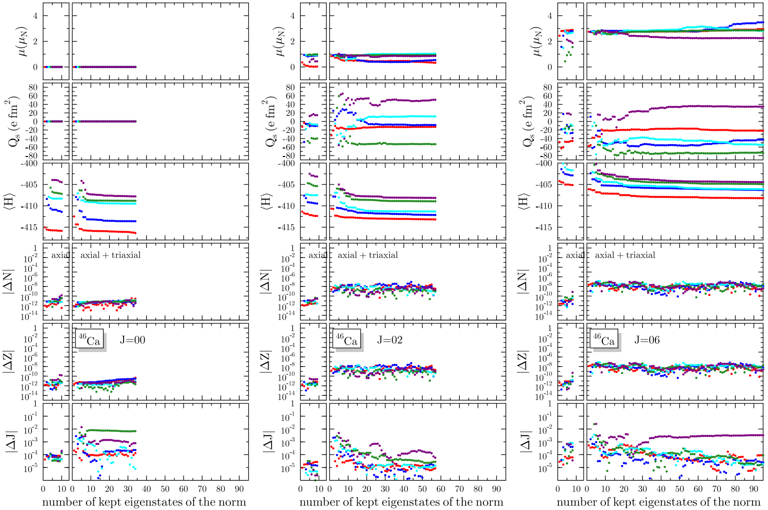
Nilsson diagram for a closed path through indicated by yellow dots.

Fun with SLyMR0 – ^{46}Ca



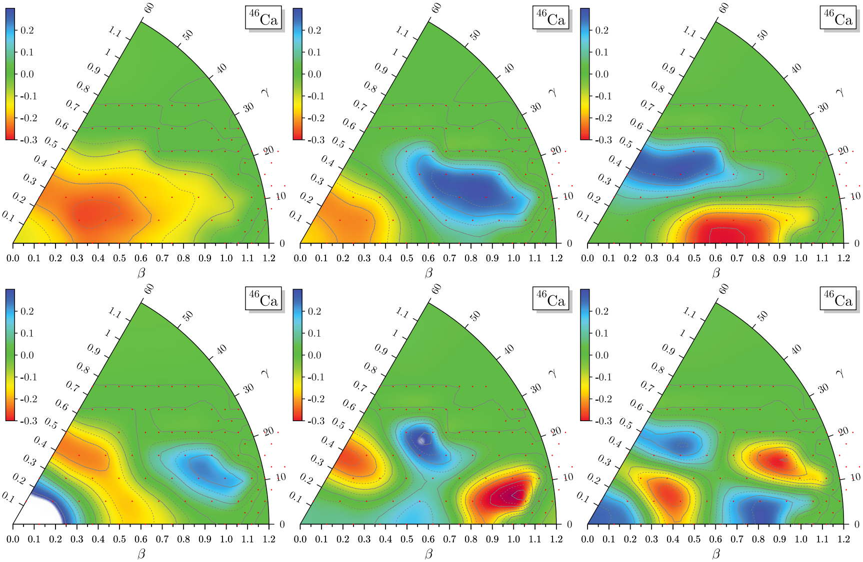
Convergence of various properties of the five lowest GCM states for $J = 0$, 2 and 6 as a function of the number of states out of the basis of projected states.

Fun with SLyMR0 – ^{46}Ca



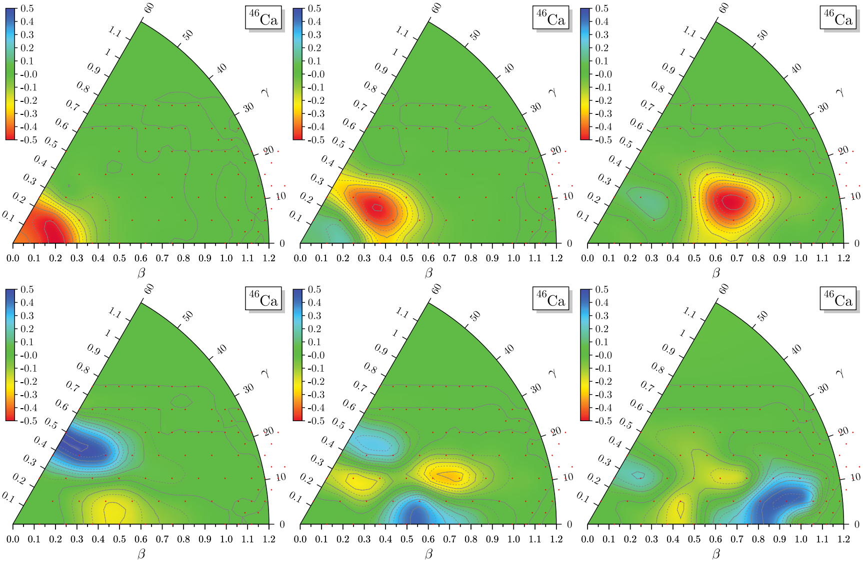
Convergence of various properties of the five lowest GCM states for $J = 0$, 2 and 6, in a basis that combines *all* projected states as a function of the number of kept eigenstates of the norm.

Fun with SLyMR0 – ^{46}Ca



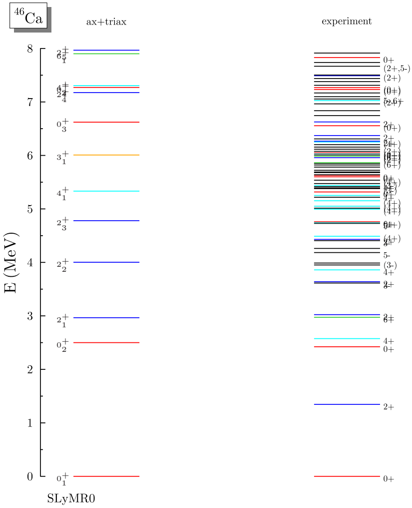
Lowest eigenstates of the norm for $J = 0$.

Fun with SLyMR0 – ^{46}Ca



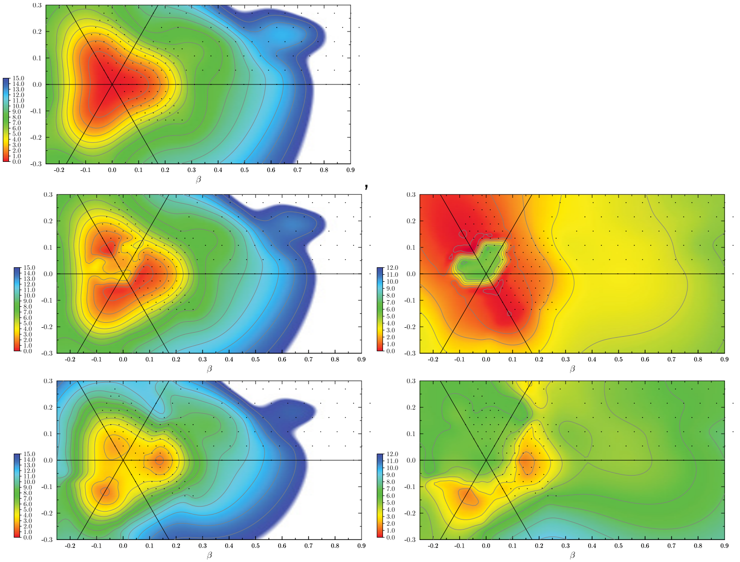
Lowest eigenstates of the Hamiltonian for $J = 0$.

Fun with SLyMR0 – ^{46}Ca



- There is a sequence of "seniority-2" states with $J^{\pi} = 2^{+}$, 4^{+}, 6^{+} that in the shell-model is easily obtained by coupling two neutron holes in the $1f_{7/2}-$shell to these angular momenta.
- These are non-collective; hence, cannot be describes by "traditional" GCM.

Fun with SLyMR0 and diabatic states – ^{46}Ca

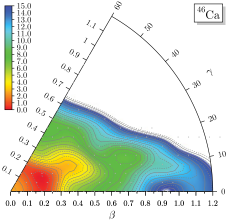


mean-field energy relative to non-cranked spherical state (left) and mean value of J_z (right) for states cranked to $\hbar\omega = 0$ (top), 0.5 (middle) and 0.7 MeV (bottom).

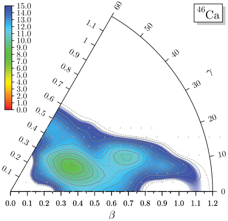
Fun with SLyMR0 and diabatic states – ^{46}Ca

seniority 0

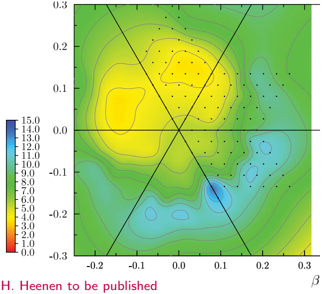
N, Z, $J = 0$ projected



N, Z, $J = 6$ projected



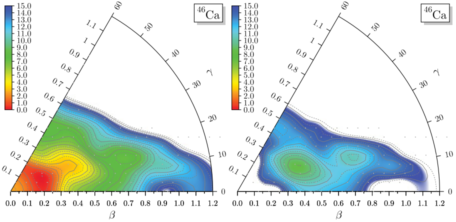
seniority 2, lowest N, Z, $J = 6$ projected



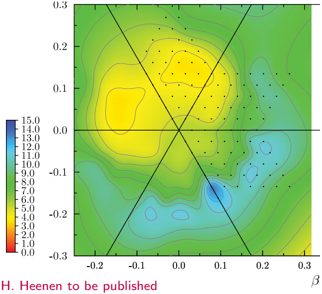
M. B.& P.-H. Heenen to be published

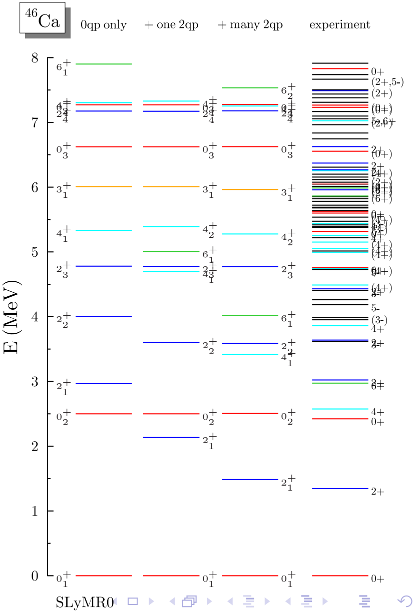
seniority 0

N, Z, $J = 0$ projected N, Z, $J = 6$ projected



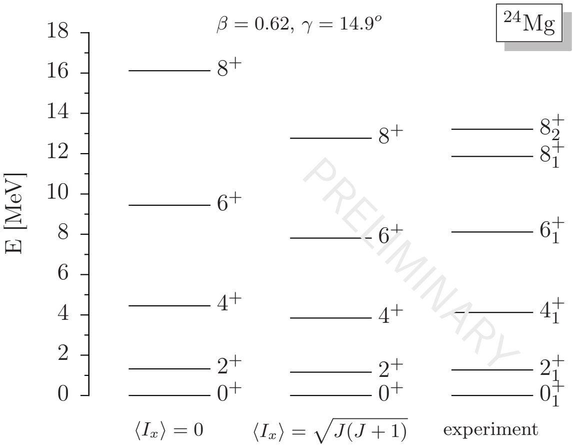
seniority 2, lowest N, Z, $J = 6$ projected





M. B.& P.-H. Heenen to be published

Projection of cranked states for collective rotation



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

- compression of excitation spectrum
- projecting the states cranked to I does not lead to the lowest energy for $J = I$ states.

3-body terms of 2nd order in gradients

The most general *central* Skyrme-type 3-body force up to 2nd order in gradients has been constructed by J. Sadoudi with a dedicated formal algebra code

1. write down all possible 3-body pseudo-potentials compatible with symmetry requirements (invariance under time reversal, space inversion, rotations, translations, isospin rotations, ...
2. derive complete functional in particle-hole and $T = 1$ pairing channels as HFB expectation value of the pseudo-potential with the help of a dedicated *in-house* formal algebra code.
3. separate the linearly independent terms in the pseudo-potential from the redundant ones by SVD of the matrix that relates the coupling constants of the *functional* with those of the *pseudo potential*.
4. derive mean fields and pairing fields
5. derive properties of infinite nuclear matter for symmetric, polarized symmetric, neutron and polarized neutron matter, including effective masses and Landau parameters.

J. Sadoudi, T. Duguet, J. Meyer, M. B., PRC 88 (2013) 064326

3-body terms of 2nd order in gradients

- structure

$$
\begin{aligned}
\hat{v}_{123} = & \, u_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \right) \\
& + \frac{u_1}{2} \left[1 + y_1 P^{\sigma}_{12} \right] \left(\hat{\mathbf{k}}_{12} \cdot \hat{\mathbf{k}}_{12} + \hat{\mathbf{k}}'_{12} \cdot \hat{\mathbf{k}}'_{12} \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
& + \frac{u_1}{2} \left[1 + y_1 P^{\sigma}_{31} \right] \left(\hat{\mathbf{k}}_{31} \cdot \hat{\mathbf{k}}_{31} + \hat{\mathbf{k}}'_{31} \cdot \hat{\mathbf{k}}'_{31} \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\
& + \frac{u_1}{2} \left[1 + y_1 P^{\sigma}_{23} \right] \left(\hat{\mathbf{k}}_{23} \cdot \hat{\mathbf{k}}_{23} + \hat{\mathbf{k}}'_{23} \cdot \hat{\mathbf{k}}'_{23} \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \\
& + u_2 \left[1 + y_{21} P^{\sigma}_{12} + y_{22} (P^{\sigma}_{13} + P^{\sigma}_{23}) \right] \left(\hat{\mathbf{k}}_{12} \cdot \hat{\mathbf{k}}'_{12} \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
& + u_2 \left[1 + y_{21} P^{\sigma}_{31} + y_{22} (P^{\sigma}_{32} + P^{\sigma}_{12}) \right] \left(\hat{\mathbf{k}}_{31} \cdot \hat{\mathbf{k}}'_{31} \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\
& + u_2 \left[1 + y_{21} P^{\sigma}_{23} + y_{22} (P^{\sigma}_{21} + P^{\sigma}_{31}) \right] \left(\hat{\mathbf{k}}_{23} \cdot \hat{\mathbf{k}}'_{23} \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1}
\end{aligned}
$$

J. Sadoudi, T. Duguet, J. Meyer, M. B., PRC 88 (2013) 064326

- implementation in spherical HFB code
- implementation in 3d SR and MR EDF codes
- implemtation into semi-infinite nuclear matter code
- implementation into code calculating linear response in infinite homogeneous matter
- first preliminary fits have been achieved (⇒ Karim Bennaceur's talk)

Table: Three-body terms labeled by their parameters that have been considered in earlier (non-systematic) work as indicated by $+$.

Ref.	u_0	u_1	$u_1 y_1$	u_2	$u_2 y_{21}$	$u_2 y_{22}$
Blaizot et al. (1975)	+	+	−	−	−	−
Liu et al. (1975)	+	+	−	−	−	−
Onishi et al. (1978)	+	−	−	+	+	−
Waroquier et al. (1983)	+	+	−	−	−	−
Arima et al. (1986)	+	+	−	+	+	−
Zheng et al. (1990)	+	+	−	−	−	−
Liu et al. (1991)	+	+	+	+	+	−

(cf. Table III of J. Sadoudi, T. Duguet, J. Meyer, M. B., PRC 88 (2013) 064326 for complete references)

The normal part of the functional

$$
\begin{aligned}
\mathcal{E}^{\rho\rho\rho} = \sum_{t=0,1} \Big\{ & B_t^{\rho}\, \rho_t\, \rho_t\, \rho_0 + B_t^{s}\, \mathbf{s}_t \cdot \mathbf{s}_t\, \rho_0 + B_t^{\tau}\, \rho_t\, \tau_t\, \rho_0 + B_t^{\tau s}\, \tau_t\, \mathbf{s}_t \cdot \mathbf{s}_0 \\
& + B_t^{T}\, \mathbf{s}_t \cdot \mathbf{T}_t\, \rho_0 + B_{t\bar{t}}^{T}\, \mathbf{s}_t \cdot \mathbf{T}_{\bar{t}}\, \rho_1 + B_t^{\nabla\rho}\, (\boldsymbol{\nabla}\rho_t) \cdot (\boldsymbol{\nabla}\rho_t)\, \rho_0 + B_t^{j}\, \mathbf{j}_t \cdot \mathbf{j}_t\, \rho_0 \\
& + \sum_{\mu\nu} \Big[B_t^{\nabla s}\, (\nabla_\mu s_{t,\nu})(\nabla_\mu s_{t,\nu})\, \rho_0 + B_t^{J}\, J_{t,\mu\nu} J_{t,\mu\nu}\, \rho_0 \\
& + B_{t\bar{t}}^{\nabla\rho s}\, (\nabla_\mu \rho_t)(\nabla_\mu s_{\bar{t},\nu})\, s_{1,\nu} + B_t^{\nabla\rho s}\, (\nabla_\mu \rho_t)(\nabla_\mu s_{t,\nu})\, s_{0,\nu} \\
& + B_t^{Js}\, j_{t,\mu}\, J_{t,\mu\nu}\, s_{0,\nu} + B_{t\bar{t}}^{Js}\, j_{t,\mu}\, J_{\bar{t},\mu\nu}\, s_{1,\nu} \Big] \\
& + \sum_{\mu\nu\lambda\kappa} \epsilon_{\nu\lambda\kappa} \Big[B_t^{\nabla sJ}\, (\nabla_\mu s_{t,\nu})\, J_{t,\mu\lambda}\, s_{0,\kappa} + B_{t\bar{t}}^{\nabla sJ}\, (\nabla_\mu s_{t,\nu})\, J_{\bar{t},\mu\lambda}\, s_{1,\kappa} \Big] \Big\} \\
& + B_{10}^{s}\, \mathbf{s}_1 \cdot \mathbf{s}_0\, \rho_1 + B_{10}^{\tau}\, \rho_1\, \tau_0\, \rho_1 + B_{10}^{\tau s}\, \tau_0\, \mathbf{s}_1 \cdot \mathbf{s}_1 + B_{10}^{\nabla\rho}\, (\boldsymbol{\nabla}\rho_1) \cdot (\boldsymbol{\nabla}\rho_0)\, \rho_1 \\
& + \sum_{\mu\nu} B_{10}^{\nabla s}\, (\nabla_\mu s_{1,\nu})(\nabla_\mu s_{0,\nu})\, \rho_1 + B_{10}^{j}\, \mathbf{j}_1 \cdot \mathbf{j}_0\, \rho_1 + \sum_{\mu\nu} B_{10}^{J}\, J_{1,\mu\nu}\, J_{0,\mu\nu}\, \rho_1
\end{aligned}
$$

- 8 terms are the usual central two-body terms $\times \rho_0$, the other 15 have different vector and/or isospin coupling.

A word on isospin pair densities I

- The particle-hole part of the energy density functional is usually represented in isospin representation
- The pairing part of the energy density functional is usually represented in proton-neutron representation

In the case with p-p and n-n pairing, $|\text{HFB}_n\rangle \otimes \text{HFB}_p\rangle$

$$\kappa(\mathbf{r}\sigma q, \mathbf{r}'\sigma' q') \equiv \langle\Phi| a_{\mathbf{r}'\sigma' q'} a_{\mathbf{r}\sigma q} |\Phi\rangle \quad \text{with} \quad \kappa(\mathbf{r}\sigma q, \mathbf{r}'\sigma' q') = -\kappa(\mathbf{r}'\sigma' q', \mathbf{r}\sigma q)$$

There is no local proton or neutron anomalous density $\kappa_q(\mathbf{r})$ analogous to $\rho_q(\mathbf{r}) = \sum_\sigma \rho(\mathbf{r}\sigma q, \mathbf{r}\sigma q)$

$$\kappa_q(\mathbf{r}) = \sum_\sigma \kappa(\mathbf{r}\sigma q, \mathbf{r}\sigma q) = -\sum_\sigma \kappa(\mathbf{r}\sigma q, \mathbf{r}\sigma q) = 0$$

Define pairing density instead

$$\tilde{\rho}_q(\mathbf{r}) \equiv \sum_\sigma (-\sigma)\kappa(\mathbf{r}\sigma q, \mathbf{r} - \sigma q) = -\sum_\sigma (-\sigma)\kappa(\mathbf{r} - \sigma q, \mathbf{r}\sigma q) \neq 0$$

But there is no isoscalar or isovector pairing density $\tilde{\rho}_t$ analogous to

$$\rho_0(\mathbf{r}) \equiv \sum_{\sigma q} \rho(\mathbf{r}\sigma q, \mathbf{r}\sigma q)$$

$$\rho_{1,\mathfrak{a}}(\mathbf{r}) \equiv \sum_{\sigma q' q} \rho(\mathbf{r}\sigma q, \mathbf{r}\sigma q')\, \tau_{\mathfrak{a}, q' q} \quad \rightarrow \quad \rho_{1,1} = \rho_{1,2} = 0, \quad \rho_{1,3} = \rho_p(\mathbf{r}) - \rho_n(\mathbf{r})$$

Pairing densities

$$\breve{\rho}_0(\mathbf{r}) \equiv \sum_{\sigma q} (-\sigma)(-q)\,\kappa(\mathbf{r}\sigma q, \mathbf{r} - \sigma - q) = \sum_{\sigma q} \sigma\, q\, \kappa(\mathbf{r} - \sigma - q, \mathbf{r}\sigma q) = 0$$

$$\breve{\rho}_{1,\mathfrak{a}}(\mathbf{r}) \equiv \sum_{\sigma q' q} (-\sigma)(-q')\,\kappa(\mathbf{r}\sigma q, \mathbf{r} - \sigma - q')\,\tau_{\mathfrak{a},q' q}$$

- the first ($\mathfrak{a} = 1$) and second ($\mathfrak{a} = 2$) isovector components of all normal densities are zero,
- all isoscalar pairing densities are zero,
- the third component ($\mathfrak{a} = 3$) of all isovector pairing densities is zero.

E. Perlinska, S. G. Rohoziński, J. Dobaczewski, W. Nazarewicz, PRC **69**, 014316 (2004)

S. G. Rohoziński, J. Dobaczewski, W. Nazarewicz, PRC 81, 014313 (2010)

$$\mathcal{P}_n \equiv \frac{1}{2}\left(\mathcal{P}_0 + \mathcal{P}_{1,3}\right) \qquad \mathcal{P}_p \equiv \frac{1}{2}\left(\mathcal{P}_0 - \mathcal{P}_{1,3}\right)$$

$$\tilde{\mathcal{P}}_n \equiv \frac{1}{2}\left(\breve{\mathcal{P}}_{1,1} + \mathrm{i}\breve{\mathcal{P}}_{1,2}\right) \qquad \tilde{\mathcal{P}}_p \equiv \frac{1}{2}\left(\breve{\mathcal{P}}_{1,1} - \mathrm{i}\breve{\mathcal{P}}_{1,2}\right)$$

The anomalous part of the functional

$$
\begin{aligned}
\mathcal{E}^{\kappa\kappa\rho} = \sum_{\mathfrak{a}=1,2} \Big\{ & B_0^{\breve\rho}\,\breve\rho^*_{1,\mathfrak{a}}\breve\rho_{1,\mathfrak{a}}\,\rho_0 + B_0^{\breve\tau^*}\,\breve\tau^*_{1,\mathfrak{a}}\breve\rho_{1,\mathfrak{a}}\,\rho_0 + B_0^{\breve\tau}\,\breve\rho^*_{1,\mathfrak{a}}\breve\tau_{1,\mathfrak{a}}\,\rho_0 + B_0^{\breve\rho\tau}\,\breve\rho^*_{1,\mathfrak{a}}\breve\rho_{1,\mathfrak{a}}\,\tau_0 \\
& + B_0^{\nabla\breve\rho}(\boldsymbol{\nabla}\breve\rho^*_{1,\mathfrak{a}})\cdot(\boldsymbol{\nabla}\breve\rho_{1,\mathfrak{a}})\rho_0 + B_0^{\nabla\breve\rho^*\breve\rho}(\boldsymbol{\nabla}\breve\rho^*_{1,\mathfrak{a}})\breve\rho_{1,\mathfrak{a}}\cdot(\boldsymbol{\nabla}\rho_0) + B_0^{\breve\rho^*\nabla\breve\rho}\breve\rho^*_{1,\mathfrak{a}}(\boldsymbol{\nabla}\breve\rho_{1,\mathfrak{a}})\cdot(\boldsymbol{\nabla}\rho_0) \\
& + \mathrm{i}B_0^{\nabla\breve\rho^* j}(\boldsymbol{\nabla}\breve\rho^*_{1,\mathfrak{a}})\breve\rho_{1,\mathfrak{a}}\cdot\mathbf{j}_0 + \mathrm{i}B_0^{\nabla\breve\rho j}\breve\rho^*_{1,\mathfrak{a}}(\boldsymbol{\nabla}\breve\rho_{1,\mathfrak{a}})\cdot\mathbf{j}_0 \\
& + \sum_{\mu\nu}\big[B_0^{\breve J}\breve J^*_{1,\mathfrak{a},\mu\nu}\breve J_{1,\mathfrak{a},\mu\nu}\,\rho_0 + B_0^{\breve J^*\breve\rho}\breve J^*_{1,\mathfrak{a},\mu\nu}\breve\rho_{1,\mathfrak{a}}J_{0,\mu\nu} + B_0^{\breve\rho^*\breve J}\breve\rho^*_{1,\mathfrak{a}}\breve J_{1,\mathfrak{a},\mu\nu}J_{0,\mu\nu} \\
& + \mathrm{i}B_0^{\nabla\breve\rho^*\breve J}(\nabla_\mu\breve\rho^*_{1,\mathfrak{a}})\breve J_{1,\mathfrak{a},\mu\nu}s_{0,\nu} + \mathrm{i}B_0^{\breve J^*\nabla\breve\rho}\breve J^*_{1,\mathfrak{a},\mu\nu}(\nabla_\mu\breve\rho_{1,\mathfrak{a}})\,s_{0,\nu} \\
& + \mathrm{i}B_0^{\breve J^*\nabla s}\breve J^*_{1,\mathfrak{a},\mu\nu}\breve\rho_{1,\mathfrak{a}}(\nabla_\mu s_{0,\nu}) + \mathrm{i}B_0^{\breve J\nabla s}\breve\rho^*_{1,\mathfrak{a}}\,\breve J_{1,\mathfrak{a},\mu\nu}(\nabla_\mu s_{0,\nu})\big] \\
& + \sum_{\mu\nu\lambda\kappa}\epsilon_{\nu\lambda\kappa}\big[\,\mathrm{i}B_0^{\breve J^2 s}\,\breve J^*_{1,\mathfrak{a},\mu\nu}\,\breve J_{1,\mathfrak{a},\mu\lambda}\,s_{0,\kappa}\big]\Big\} \\
& + \sum_{\mathfrak{a},\mathfrak{b}=1,2}\sum_{\mathfrak{c}=3}\epsilon_{\mathfrak{a}\mathfrak{b}\mathfrak{c}}\Big\{\mathrm{i}B_1^{\breve\rho}\breve\rho^*_{1,\mathfrak{a}}\,\breve\rho_{1,\mathfrak{b}}\,\rho_{1,\mathfrak{c}} + \mathrm{i}B_1^{\breve\tau^*}\,\breve\tau^*_{1,\mathfrak{a}}\,\breve\rho_{1,\mathfrak{b}}\,\rho_{1,\mathfrak{c}} + \mathrm{i}B_1^{\breve\tau}\breve\rho^*_{1,\mathfrak{a}}\breve\tau_{1,\mathfrak{b}}\rho_{1,\mathfrak{c}} \\
& + \mathrm{i}B_1^{\breve\rho\tau}\,\breve\rho^*_{1,\mathfrak{a}}\,\breve\rho_{1,\mathfrak{b}}\,\tau_{1,\mathfrak{c}} + \mathrm{i}B_1^{\nabla\breve\rho}(\boldsymbol{\nabla}\breve\rho^*_{1,\mathfrak{a}})\cdot(\boldsymbol{\nabla}\breve\rho_{1,\mathfrak{b}})\rho_{1,\mathfrak{c}} + \mathrm{i}B_1^{\nabla\breve\rho^*\breve\rho}(\boldsymbol{\nabla}\breve\rho^*_{1,\mathfrak{a}})\breve\rho_{1,\mathfrak{b}}\cdot(\boldsymbol{\nabla}\rho_{1,\mathfrak{c}}) \\
& + \mathrm{i}B_1^{\breve\rho^*\nabla\breve\rho}\breve\rho^*_{1,\mathfrak{a}}(\boldsymbol{\nabla}\breve\rho_{1,\mathfrak{b}})\cdot(\boldsymbol{\nabla}\rho_{1,\mathfrak{c}}) + B_1^{\nabla\breve\rho^* j}(\boldsymbol{\nabla}\breve\rho^*_{1,\mathfrak{a}})\breve\rho_{1,\mathfrak{b}}\cdot\mathbf{j}_{1,\mathfrak{c}} + B_1^{\nabla\breve\rho j}\breve\rho^*_{1,\mathfrak{a}}(\boldsymbol{\nabla}\breve\rho_{1,\mathfrak{b}})\cdot\mathbf{j}_{1,\mathfrak{c}} \\
& + \sum_{\mu\nu}\Big[\mathrm{i}B_1^{\breve J}\breve J^*_{1,\mathfrak{a},\mu\nu}\breve J_{1,\mathfrak{b},\mu\nu}\rho_{1,\mathfrak{c}} + \mathrm{i}B_1^{\breve J^*\breve\rho}\breve J^*_{1,\mathfrak{a},\mu\nu}\breve\rho_{1,\mathfrak{b}}J_{1,\mathfrak{c},\mu\nu} + \mathrm{i}B_1^{\breve\rho^*\breve J}\breve\rho^*_{1,\mathfrak{a}}\breve J_{1,\mathfrak{b},\mu\nu}J_{1,\mathfrak{c},\mu\nu} \\
& + B_1^{\nabla\breve\rho^*\breve J}(\nabla_\mu\breve\rho^*_{1,\mathfrak{a}})\breve J_{1,\mathfrak{b},\mu\nu}s_{1,\mathfrak{c},\nu} + B_1^{\breve J^*\nabla\breve\rho}\breve J^*_{1,\mathfrak{a},\mu\nu}(\nabla_\mu\breve\rho_{1,\mathfrak{b}})s_{1,\mathfrak{c},\nu} + B_1^{\breve J^*\nabla s}\breve J^*_{1,\mathfrak{a},\mu\nu}\breve\rho_{1,\mathfrak{b}}(\nabla_\mu s_{1,\mathfrak{c},\nu}) \\
& + B_1^{\breve J\nabla s}\breve\rho^*_{1,\mathfrak{a}}\breve J_{1,\mathfrak{b},\mu\nu}(\nabla_\mu s_{1,\mathfrak{c},\nu})\Big] + \sum_{\mu\nu\lambda\kappa}\epsilon_{\nu\lambda\kappa}\Big[B_1^{\breve J^2 s}\breve J^*_{1,\mathfrak{a},\mu\nu}\breve J_{1,\mathfrak{b},\mu\lambda}s_{1,\mathfrak{c},\kappa}\Big]\Big\}
\end{aligned}
$$

Generic isospin structure in case of *n*-*n* and *p*-*p* pairing

$\mathcal{P}_{1,\mathfrak{a}}, \mathcal{P}'_{1,\mathfrak{a}}$	generic normal isospin densities
$\breve{\mathcal{P}}_{1,\mathfrak{a}}, \breve{\mathcal{P}}'_{1,\mathfrak{a}}$	generic anomalous isospin densities

The generic isospin structure of the terms containing isovector densities is

$$\mathcal{P}_0\,\mathcal{P}'_0 \qquad ab$$

$$\sum_{\mathfrak{a}} \mathcal{P}_{1,\mathfrak{a}}\,\mathcal{P}'_{1,\mathfrak{a}} = \mathcal{P}_{1,3}\,\mathcal{P}'_{1,3} \qquad \mathbf{a}\cdot\mathbf{b}$$

$$\sum_{\mathfrak{a}} \breve{\mathcal{P}}^*_{1,\mathfrak{a}}\,\breve{\mathcal{P}}'_{1,\mathfrak{a}} = \breve{\mathcal{P}}^*_{1,1}\,\breve{\mathcal{P}}'_{1,1} + \breve{\mathcal{P}}^*_{1,2}\,\breve{\mathcal{P}}'_{1,2} \qquad \mathbf{A}^*\cdot\mathbf{B}$$

$$\sum_{\mathfrak{a}} \mathcal{P}_{1,\mathfrak{a}}\,\mathcal{P}'_{1,\mathfrak{a}}\,\mathcal{P}''_0 = \mathcal{P}_{1,3}\,\mathcal{P}'_{1,3}\,\mathcal{P}''_0 \qquad (\mathbf{a}\cdot\mathbf{b})\,c$$

$$\sum_{\mathfrak{a}} \breve{\mathcal{P}}^*_{1,\mathfrak{a}}\,\breve{\mathcal{P}}'_{1,\mathfrak{a}}\,\mathcal{P}''_0 = \left(\breve{\mathcal{P}}^*_{1,1}\,\breve{\mathcal{P}}'_{1,1} + \breve{\mathcal{P}}^*_{1,2}\,\breve{\mathcal{P}}'_{1,2}\right)\mathcal{P}''_0 \qquad (\mathbf{A}^*\cdot\mathbf{B})\,c$$

$$\sum_{\mathfrak{abc}} \epsilon_{\mathfrak{abc}}\breve{\mathcal{P}}^*_{1,\mathfrak{a}}\,\breve{\mathcal{P}}'_{1,\mathfrak{b}}\,\mathcal{P}''_{1,\mathfrak{c}} = \left(\breve{\mathcal{P}}^*_{1,1}\,\breve{\mathcal{P}}'_{1,2} - \breve{\mathcal{P}}^*_{1,2}\,\breve{\mathcal{P}}'_{1,1}\right)\mathcal{P}''_{1,3} \qquad (\mathbf{A}^*\times\mathbf{B})\cdot\mathbf{c}$$

Some (very) preliminary results obtained with SLyMR1

- Implementation into various codes (1d spherical HFB code, 3d time-reversal-breaking HFB code, corresponding projected energy kernel code) by J. Sadoudi
- various tools (semi-infinite nuclear matter, linear response in homogeneous infinite matter) by the Lyon group
- First fit by Robin Jodon and Karim Bennaceur

term	1d lenteur	Lagrange Esp 0.4	FD CR8 0.4	Lagrange Esp 0.8	FD CR8 0.8
rho rho	-2303.0900	-2304.5008	-2304.5007	-2307.7476	-2307.7476
tau rho	619.7104	620.6368	620.5874	622.2555	619.6135
(nabla_i rho) (nabla_i rho)	250.8967	250.8727	250.8721	251.2605	251.1661
J,ij J,ij	-1.3377	-1.3318	-1.3316	-1.3363	-1.3255
rho (nabla_i J,i)	-18.3752	-18.3406	-18.3376	-18.3539	-18.2198
rho~ rho~	-11.0146	-11.1218	-10.6793	-11.1270	-10.6856
tau~ rho~	4.3951	4.4384	4.2737	4.4452	4.2544
(nabla_i rho~) (nabla_i rho~)	0.5413	0.5395	0.5257	0.5385	0.5244
J~,ij J~,ij	0.6501	0.6424	0.6675	0.6436	0.6650
J~,ij J~,ji	0.8883	0.8777	0.9121	0.8794	0.9087
2-body normal terms	-1452.1958	-1452.6637	-1452.7104	-1453.9217	-1456.5134
2-body pairing terms	-4.5398	-4.6239	-4.3003	-4.6203	-4.3330
rho rho rho	435.6634	436.4813	436.4813	437.8326	437.8326
tau rho rho	-116.9447	-117.3016	-117.2915	-117.8265	-117.2929
(nabla_i rho) (nabla_i rho) rho	-80.5779	-80.7145	-80.6885	-80.9568	-80.0307
J,ij J,ij rho	0.6672	0.6653	0.6651	0.6713	0.6653
rho~ rho~ rho	5.0440	5.0867	4.8579	5.0925	4.8646
rho~ rho~ tau	-0.2003	-0.2024	-0.1931	-0.2030	-0.1931
tau~ rho~ rho	-2.1124	-2.1361	-2.0439	-2.1423	-2.0370
(nabla_i rho~) (nabla_i rho~) rho	-0.1761	-0.1735	-0.1714	-0.1730	-0.1670
(nabla_i rho~) rho~ (nabla_i rho)	-0.7636	-0.7626	-0.7252	-0.7619	-0.7221
J~,ij J~,ij rho	-0.1976	-0.1950	-0.2039	-0.1956	-0.2032
J~,ij rho~ J,ij	0.1824	0.1816	0.1811	0.1822	0.1805
3-body normal terms	238.8081	239.1305	239.1664	239.7207	241.1743
3-body pairing terms	1.7763	1.7987	1.7015	1.7988	1.7227
Normal energy	-1213.3877	-1213.5332	-1213.5440	-1214.2010	-1215.3391
Pairing energy	-2.7634	-2.8252	-2.5988	-2.8215	-2.6103
Total Skyrme energy	-1216.1511	-1216.3584	-1216.1428	-1217.0225	-1217.9494

SLyMR1 t1 and t2 terms

parameter	N	nphi	rho tau	(n rho)	(J,ij)^2	(j,i)^2	T,j s,j	(n s)^2	tau~ rho~	(n rho~)^2	(J~,ij)^2	sum
slymr1.full	10	9	188.3440	137.5166	-1.1522	-0.5270	0.0426	-0.0195	2.138	0.5784	0.000	326.921
slymr1.full	10	19	188.3474	137.5179	-1.1521	-0.5274	0.0425	-0.0196	2.136	0.5764	0.000	326.922
slymr1.full	10	49	188.3530	137.5200	-1.1518	-0.5280	0.0425	-0.0198	2.133	0.5730	0.000	326.922
slymr1.full	10	99	188.3546	137.5206	-1.1518	-0.5282	0.0425	-0.0198	2.132	0.5720	0.000	326.922
slymr1.full	16	9	-508.9685	-0.0908	-71.3148	49.4046	-1.4427	71.9475	419.228	258.1075	0.000	216.871
slymr1.full	16	19	-508.9650	-0.0895	-71.3147	49.4042	-1.4427	71.9474	419.226	258.1054	0.000	216.872
slymr1.full	16	49	-508.9594	-0.0874	-71.3145	49.4035	-1.4427	71.9472	419.223	258.1020	0.000	216.872
slymr1.full	16	99	-508.9578	-0.0868	-71.3145	49.4033	-1.4427	71.9472	419.222	258.1011	0.000	216.873

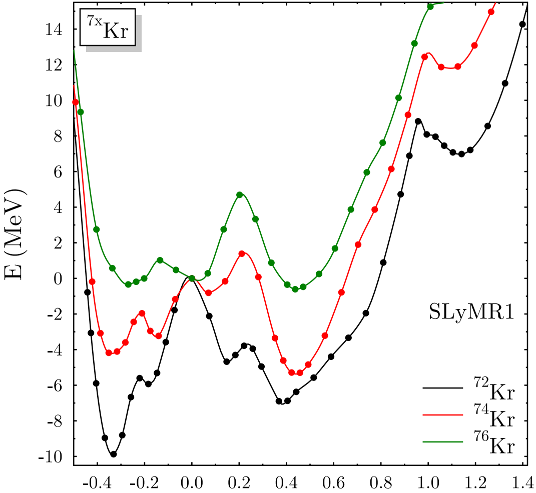
SLyMR1 3-body particle-hole terms with gradients

							(n rho)^2 rho		(n rho)(ns)s		(J,ij)^2 rho		(ns) Jij * s
parameter	ph	N	nphi	tau rho rho	tau s.s	T.s rho		(ns)^2 rho		j.j rho		j Jij s	
slymr1.u12	ph	10	9	4701.8093	-0.7998	0.0793	-575.1353	-0.5943	0.1610	-10.1486	-24.6551	0.1913	0.0340
slymr1.u12	ph	10	19	4701.6090	-0.7923	0.0794	-575.0214	-0.5902	0.1592	-10.1132	-24.7883	0.1912	0.0343
slymr1.u12	ph	10	49	4701.9386	-0.7923	0.0796	-575.1385	-0.5912	0.1590	-10.0976	-25.3188	0.1978	0.0364
slymr1.u12	ph	10	99	4703.2720	-0.8100	0.0797	-575.5858	-0.6035	0.1639	-10.1249	-26.2676	0.2061	0.0405
slymr1.u12	ph	16	9	-39021.6405	674.3819	47.9496	5569.1625	1142.6613	-143.5713	1601.0492	8376.5201	141.5929	9.2838
slymr1.u12	ph	16	19	-39022.3579	674.3954	47.9498	5569.4133	1142.6691	-143.5745	1601.0978	8376.5000	141.5932	9.2840
slymr1.u12	ph	16	49	-39021.9545	674.3950	47.9500	5569.2783	1142.6678	-143.5747	1601.1097	8375.9653	141.5999	9.2862
slymr1.u12	ph	16	99	-39020.6003	674.3772	47.9501	5568.8259	1142.6554	-143.5697	1601.0812	8375.0153	141.6083	9.2902

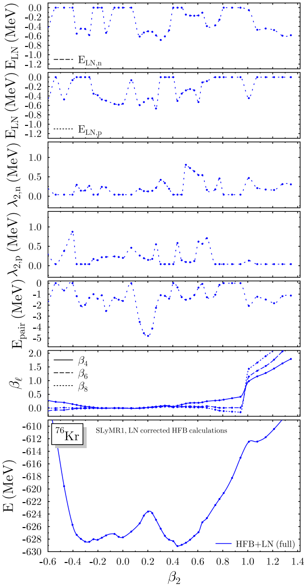
SLyMR1 3-body particle-particle terms with gradients

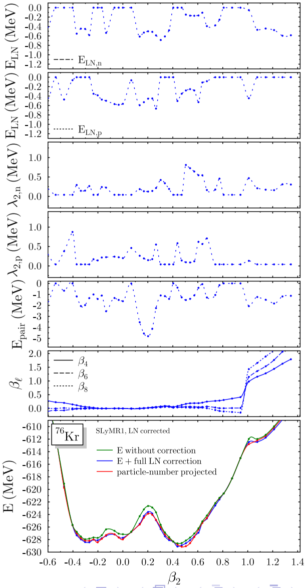
				rho~ rho~ tau		(nrho~)^2 rho		J~J~rho		j (n rho~)rho~		J~ rho~ (ns)	
parameter	pp	N	nphi		tau~ rho~		(nrho~)rho~(nrho)		J~rho~J		(n rho~)J~s		E_Skyrme
slymr1.u12	pp	10	9	52.9923	10.6258	-12.2975	11.3648	1.7275	-0.7052	-0.0285	-0.0265	-0.0181	4154.576
slymr1.u12	pp	10	19	53.3197	10.8327	-12.6713	11.2386	1.9537	-0.7785	-0.0340	-0.0327	-0.0199	4154.576
slymr1.u12	pp	10	49	53.2097	10.8258	-12.6793	10.7099	2.9412	-0.8206	-0.0335	-0.0320	-0.0189	4154.575
slymr1.u12	pp	10	99	51.9519	10.3770	-11.8584	9.7458	4.8114	-0.7757	-0.0197	-0.0161	-0.0116	4154.575
slymr1.u12	pp	16	9	7289.7021	4041.2535	1221.8195	10365.4002	3546.0851	225.7561	430.3757	402.5616	54.4158	5974.759
slymr1.u12	pp	16	19	7290.5397	4041.6231	1221.1512	10365.3966	3546.0864	225.6595	430.3673	402.5521	54.4129	5974.759
slymr1.u12	pp	16	49	7290.3974	4041.6077	1221.1414	10364.8625	3547.0744	225.6176	430.3676	402.5528	54.4139	5974.758
slymr1.u12	pp	16	99	7289.1304	4041.1565	1221.9618	10363.8971	3548.9448	225.6627	430.3815	402.5686	54.4212	5974.758

Some (very) preliminary results obtained with SLyMR1

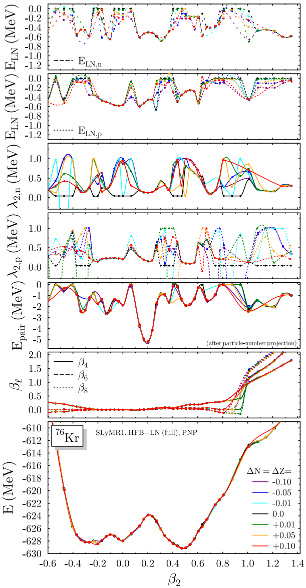


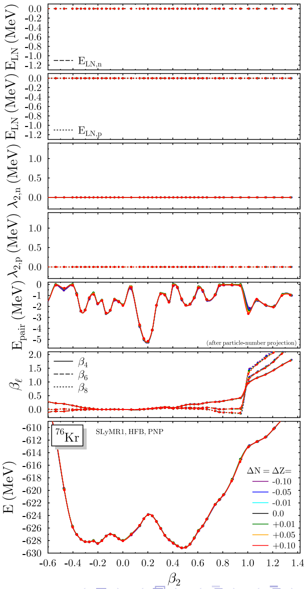
Some (very) preliminary results obtained with SLyMR1





Some (very) preliminary results obtained with SLyMR1





Take-away messages

Symmetry restoration based on time-reversal-breaking states gives access to

- coupling of collective and single-particle degrees of freedom
- angular-momentum optimization
- beyond-mean-field description of odd-A and odd-odd nuclei

From a technical point, it has been challenging as one has to solve

- "sign" problem: sign of the overlap of two HFB states
- "pole" problem: definition of the MR-EDF

Is it time for new furniture?

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Paul-Henri Heenen	Université Libre de Bruxelles

formal aspects

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Denis Lacroix	IPN Orsay

code development and benchmarking

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Jiangming Yao	Université Libre de Bruxelles

development and benchmarking of new functionals

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Dany Davesne	IPN Lyon
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Jacques Meyer	IPN Lyon
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