On pairing correlations as they appear in configuration mixing of symmetry-restored self-consistent mean-field states

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Espace de Structure Nucléaire Théorique

XIII Nuclear Physics Workshop Maria and Pierre Curie
Pairing & beyond – 50 years of the BCS model
Kazimiersz Dolny, Poland, September 28 2006

The starting point: Self-consistent mean-field models with pairing – HFB

Assumptions and features

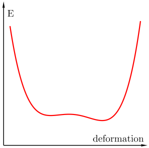
- independent quasi-particle states (HFB states)
- self-consistency
- stationary states $\Rightarrow$ equations-of-motion
- full model space of occupied states
- universal effective interaction or energy density functional (no agreement about a unique interaction yet, though: Skyrme, Gogny, Fayans, relativistic Lagrangians, . . . ; many parameterizations thereof)
- Intuitive interpretation in terms of $\left\{ \begin{array}{l} \text{shapes of a nuclear liquid} \\ \text{shells of single-particle states} \end{array} \right.$

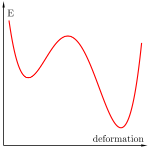
Self-Consistent Mean Field Models: Limitations and problems

- limited access to spectroscopy
  – rotational bands in well-deformed nuclei through cranking
  – harmonic vibrations from linear response theory (QRPA);
  (no coupling between excitation modes).
- nuclei are described in a body-fixed intrinsic frame
- symmetry breaking. Mean-field states are not eigenstates of

particle number	for HFB states (pairing)
momentum	for finite nuclei
angular momentum	for deformed nuclei
parity	for octupole-deformed nuclei

  done on purpose: adds *n*p-*n*h and p-p shell-model correlations but still missing correlations related to symmetry restoration, and difficult connection to the lab frame for spectroscopic observables





- arbitrary when energy changes slowly with collective coordinate (transitional nuclei)
- interpretation of coexisting minima: mean-field states with different deformation are not orthogonal and are coupled by the interaction.

Correlations within and beyond the mean field – semantics

- static correlations: deviation of a single deformed and paired mean-field state from a spherical Slater determinant.
  (described by a deformed HFB state)
- dynamical correlations: fluctuations around a given mean-field state (described by a coherent superposition of many mean-field states)
- All short-range correlations are assumed to be contained in the effective interaction.

Going Beyond the Mean Field I: Projection (After Variation)

$$\underbrace{|JMN_0Z_0q\rangle}_{\text{projected state}} = \frac{1}{\mathcal{N}} \sum_{K=-J}^{+J} \underbrace{F_K^{J*}}_{K \text{ mixing weight}} \hat{P}^J_{MK} \hat{P}_{N_0} \hat{P}_{Z_0} \underbrace{|q\rangle}_{\text{mean-field state}}$$

- particle-number projector (separately for protons and neutrons)

$$\hat{P}_{N_0} = \frac{1}{2\pi} \int_0^{2\pi} d\phi_N \; e^{i\phi_N(\hat{N}-N_0)}$$

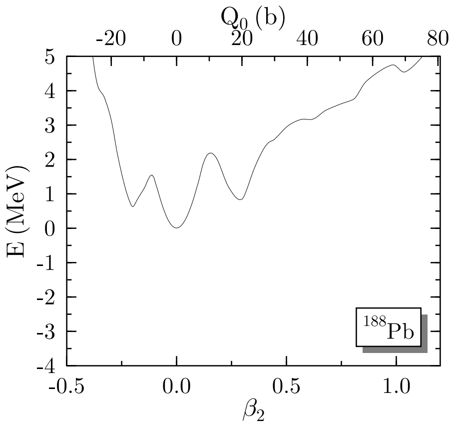
- angular-momentum projector

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

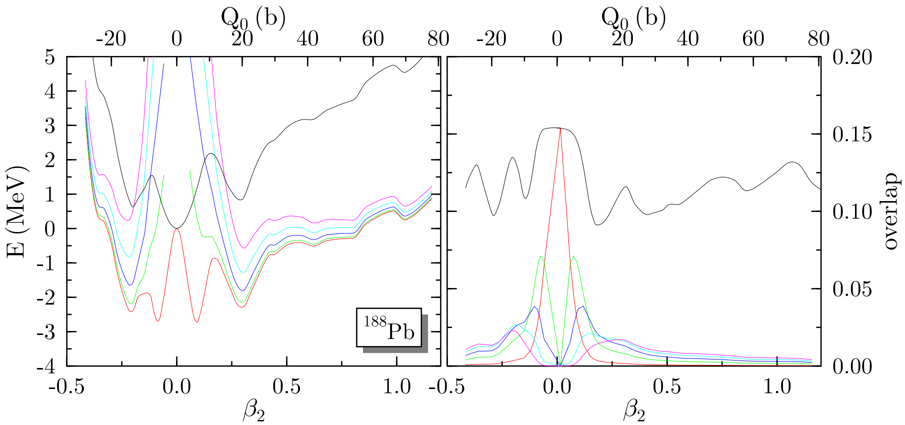
Significantly simplified for matrix elements of axial states
— one rotation angle only, no K mixing

$$\hat{P}^J_{M0} = \frac{2J+1}{2} \int_0^{\pi} d\beta \; \sin(\beta) \; d^J_{M0}(\beta) \; \hat{R}(0,\beta,0)$$

Going Beyond the Mean Field I: Projection (After Variation)



Going Beyond the Mean Field I: Projection (After Variation)



Going Beyond the Mean Field II: Configuration Mixing via the Generator Coordinate Method

mixed projected many-body state:

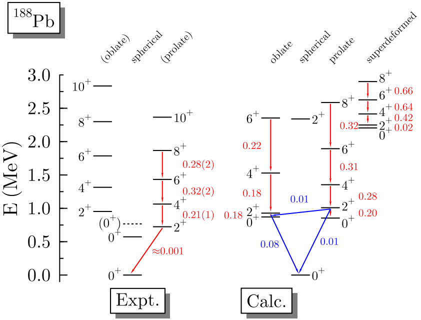
$$|JMi\rangle = \sum_q f_{Ji}(q)\, |JMq\rangle \qquad \begin{cases} |JMq\rangle & \text{projected mean-field state} \\ f_{Ji}(q) & \text{weight function} \end{cases}$$

stationarity: $\frac{\delta}{\delta f_{Ji}^*(q)} \frac{\langle JMi|\hat{H}|JMi\rangle}{\langle JMi|JMi\rangle} = 0 \quad \Rightarrow$ Hill-Wheeler-Griffin equation

$$\sum_{q'} \left[\mathcal{H}_J(q,q') - E_i\, \mathcal{I}_J(q,q')\right] f_{J,i}(q') = 0 \qquad \begin{cases} \mathcal{H}_J(q,q') = \langle JMq|\hat{H}|JMq'\rangle \\ \mathcal{I}_J(q,q') = \langle JMq|JMq'\rangle \end{cases}$$

- correlated ground state (for each J)
- spectrum of excited states (from orthogonalisation to the ground state)
- the weight functions $f_k^J(q)$ are not orthonormal $\Rightarrow$ orthonormal collective wave functions are obtained as $g_k(q) = \sum_{q'} \mathcal{I}^{1/2}(q,q')\, f_k(q')$
- Projection is a special case of the GCM, where the group structure determines the collective path and the weight function.
- Angular momentum-projection is part of the "quadrupole correlations", as it mixes states with different orientations of the quadrupole tensor.

Going Beyond the Mean Field II: Configuration Mixing via the Generator Coordinate Method

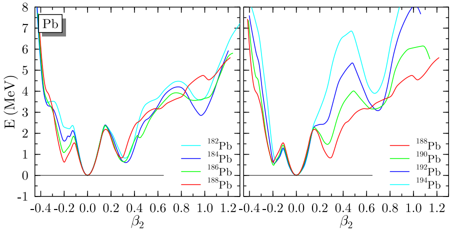


$$B(E2; J'_{k'} \to J_k) = \frac{e^2}{2J'+1} \sum_{M=-J}^{+J} \sum_{M'=-J'}^{+J'} \sum_{\mu=-2}^{+2} |\langle JMk|\hat{Q}_{2\mu}|J'M'k'\rangle|^2$$

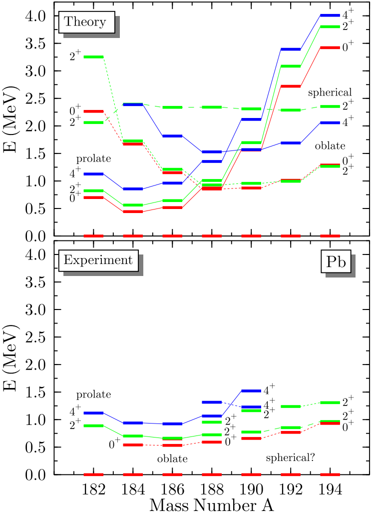
$$\beta_2^{(t)}(J_k) = \frac{4\pi}{3R^2A} \sqrt{\frac{B(E2; J_k \to J'_k - 2)}{(J\,0\,2\,0\,|(J-2)\,0)^2 e^2}} \quad \text{with} \quad R = 1.2\,A^{1/3}$$

M. B., P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303. Experiment: A. Dewald, private communication

Shape coexistence in the neutron-deficient Pb region

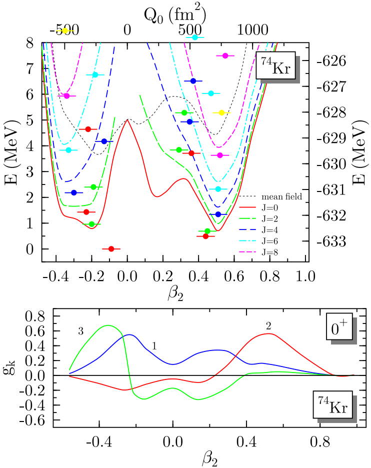


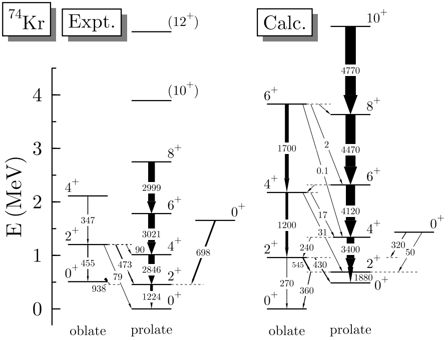
- SLy6+density-dependent pairing
- There are no adjustable parameters!
- excitation energy of the projected GCM bandheads is different from that of the mean-field minima.
- projected GCM gives prolate (oblate) bands also in nuclei without prolate (oblate) mean-field minimum
- calculated spectra are too spread out



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

Shape coexistence in the neutron-deficient Kr region



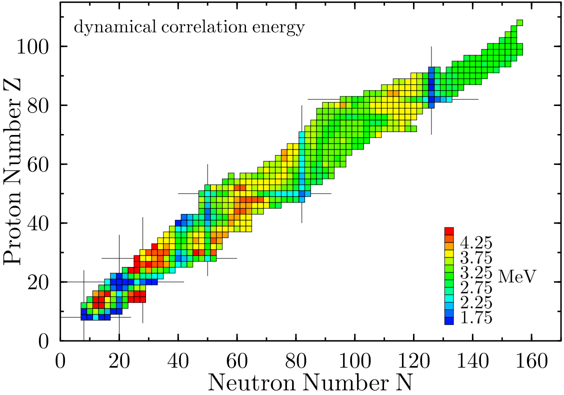


- SLy6+density-dependent pairing
- There are no adjustable parameters. . .

Experiment: E. Clément *et al.* (unpublished), A. Görgen *et al.* Eur. Phys. J. A26 (2005) 153

M. B., P. Bonche, P.-H. Heenen, Phys. Rev. C 74 (2006) 024312.

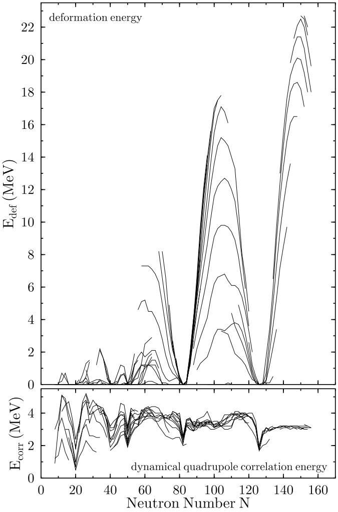
Quadrupole Correlation Energy from Projection and Configuration Mixing

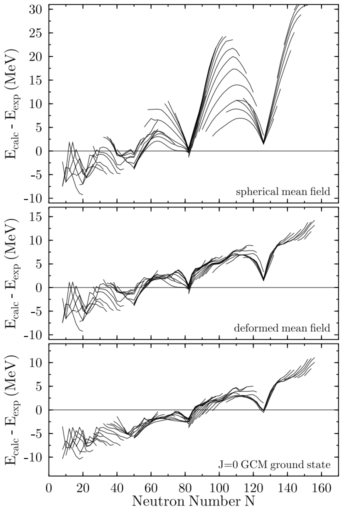


- numerical evaluation of the projected GCM kernels using an GOA-inspired approach optimized for ground states losing information on excited states

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 69 (2004) 034340
M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

Static and Dynamic Quadrupole Correlation Energies





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

Technical aspects I. Pairing correlation in the mean-field states

- The HFB method breaks down to HF whenever the level density around the Fermi energy is small. This is often the case around minima of a mean-field energy curve (for at least one nucleon species) This is a deficiency of the HFB method and contradicts experiment, which still shows signatures of pairing.
- Problem I: The missing pairing correlation energy of the HF states leads to a supression of these states in the collective wave function, when fed into the Hill-Wheeler-Griffin equation (see the following transparencies)
- Problem II: HF states with different deformation might be orthogonal (imagine two HF states with good parity where a different number of negative parity single-particle states is occupied) which completely decouples these states in the GCM.
- Consequence: pairing correlations should be enforced for all mean-field states entering a GCM calculation

Technical aspects I. Pairing correlation in the mean-field states

- We generate the mean-field states with the Lipkin-Nogami (LN) method

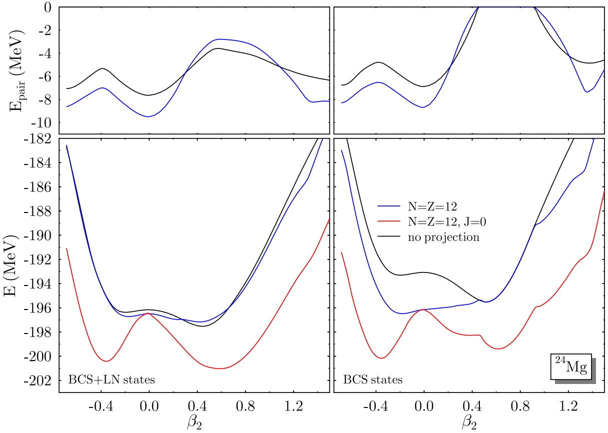
$$\delta\Big[\hat{H} - \sum_{q=n,p}\Big(\lambda_{1,q}\hat{N}_q + \lambda_{2,q}\hat{N}_q^2\Big)\Big] = 0$$

  with the usual auxiliary condition that $\langle \hat{N}_q \rangle = N_{q,0}$ and a second one that fixes $\lambda_{2,q}$.
- The LN method is an approximation to projection on particle number before variation, introducing an energy correction that estimates the energy gain from projection.

$$E_{\text{LN}} = E - \sum_{q=n,p} \lambda_2 \langle (\hat{N}_q - N_{q,0})_q^2 \rangle$$

- It has the attractive side-effect that pairing correlations never break down.
- The quality of the LN energy correction term has been doubted, particularly in the weak-pairing regime. But we do not make use of the LN energy correction, only of the LN wave function, that we project on good particle number afterwards.

Technical aspects I. Why not to project non-LN states



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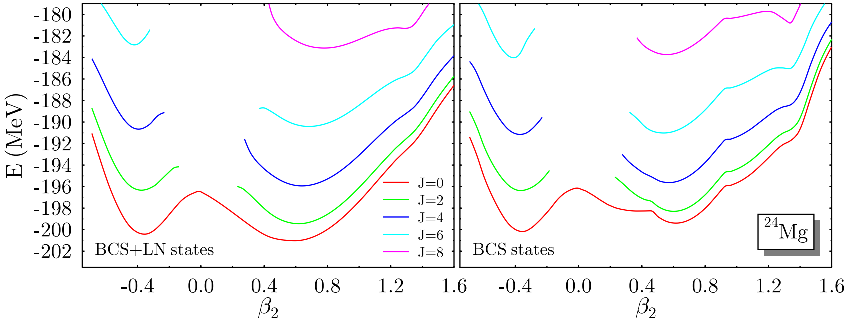

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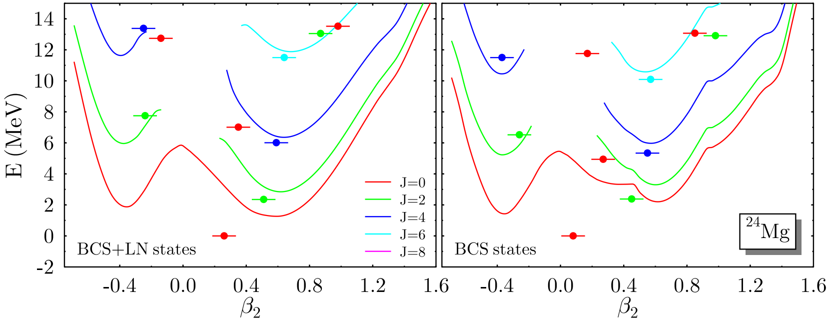


Technical aspects II. Off-diagonal matrix elements

- Off-diagonal matrix elements of two HFB states with average particle numbers N_0 and Z_0 do *not* have this average particle number anymore.
- Solution I: add Lagrange multipliers to the Hill-Wheeler Griffin equation to enforce the desired average particle number

$$\sum_{q'} \left[\mathcal{H}_J(q,q') - E_i\,\mathcal{I}_J(q,q') - \lambda_n \mathcal{N}_J(q,q') - \lambda_z \mathcal{Z}_J(q,q')\right] f_{J,i}(q') = 0$$

  Madrid, projected GCM with the Gogny Force,
  Zagreb-München, projected GCM with relativistic Lagrangians
- Solution II: project on particle number, and use the usual Hill-Wheeler Griffin equation

Particle-number projection might appear as the more elegant solution, but there is a price to pay

- Onishi's formula for the overlap of two arbitrary HFB states does not determine the sign of the (usually complex) overlap. The absolute phase has to be followed during the calculation, which for particle number migh be difficult as the overlap oscillates very fast.
- There might be divergences in the projected energy

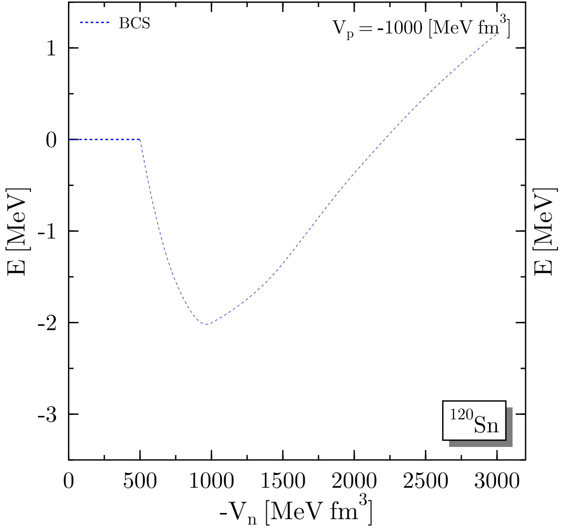
Dynamical pairing correlations I. Motivation

- All results shown so far were obtained with particle-number projection after variation.
- As for angular-momentum projection of quadrupole-deformed states, the minimum of the projected energy might not coincide with the minimum of the unprojected curve
- one has to calculate an energy curve, project and find the minimum
- Difficulty: finding a constraint that does not introduce spurious effects into the wave functions (similar to multipole constraints on the density, that create spurious pockets in the single-particle potential if not cut properly at large radii)
- This might contribute to the resolution of one of our standard problems: calculations which include a mixing of states with different pairing gap in a schematic microscopic Bohr-Hamiltonian lead to a larger density of excited levels. (there are other sources of similar significance as well)

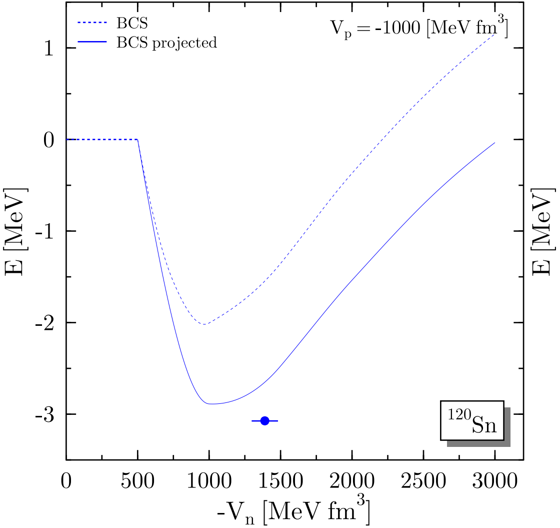
Dynamical pairing correlations II. An illustrative example

- neutron pairing effects only: the proton pairing strength is fixed at the usual value.
- "poor man's constraint" on neutron pairing correlations using a "generating pairing strength" when constructing the BCS or LN state.
- After that, the energy is recalculated without iteration using the usual pairing strength
- This procedure has some similarities with a constraint on the pairing gap in schematic models of dynamical pairing.
- Then, the states with different "generating pairing strength" are mixed in the GCM.

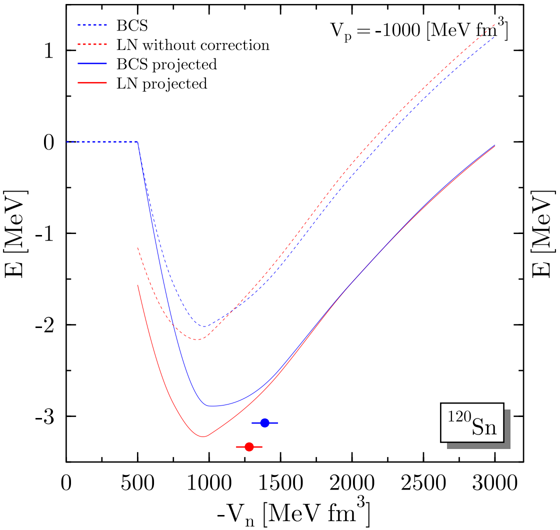
Dynamical pairing correlations II. An illustrative example



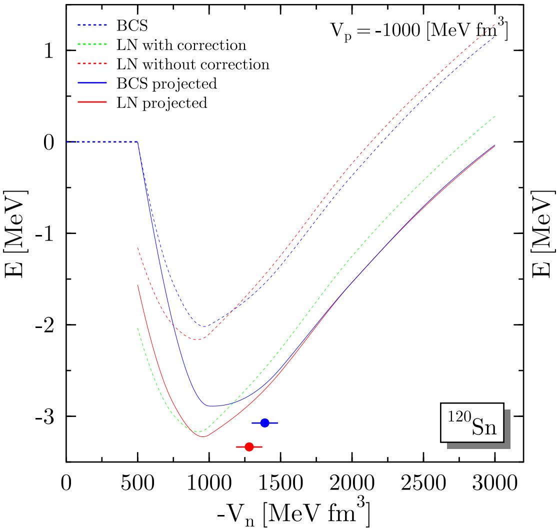
Dynamical pairing correlations II. An illustrative example



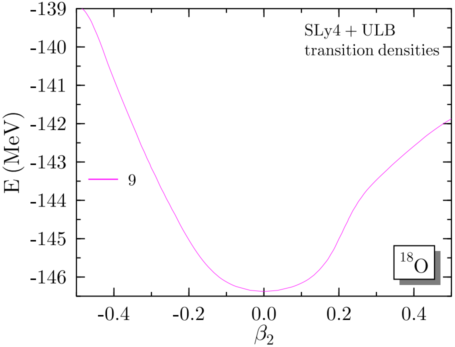
Dynamical pairing correlations II. An illustrative example



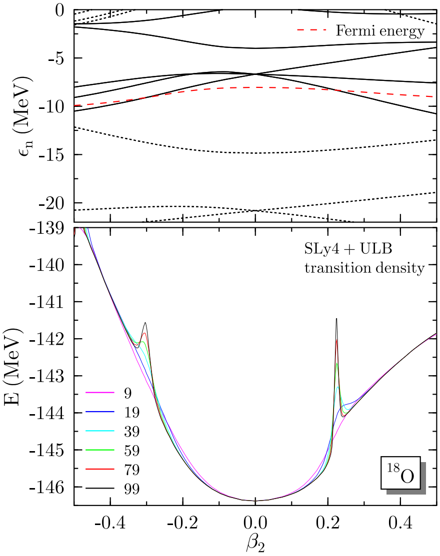
Dynamical pairing correlations II. An illustrative example



A bunch of problems: Self-pairing and divergences in the projected energy



A bunch of problems: Self-pairing and divergences in the projected energy



- Divergence when a single-particle level crosses the Fermi energy: M. Anguiano, J. L. Egido, and L. M. Robledo, Nucl. Phys. A696 (2001) 467
- Offset in the PES before and behind the crossing: M. Stoitsov, J. Dobaczewski, W. Nazarewicz, and P.-G. Reinhard (in preparation)
- this can spoil any variation after projection calculation (M. Stoitsov, J. Dobaczewski, W. Nazarewicz, private frustration)

Analysis:

- M. Anguiano, J. L. Egido, and L. M. Robledo, Nucl. Phys. A696 (2001) 467: use the same effective interaction in the particle-particle (pp) and particle-hole c(ph) hannel, do not neglect or approximate any exchange term, and you can live happily ever after
- but: when motivating effective interactions from many-body perturbation theory, the pp and ph channels are obviously different
- M. Stoitsov, J. Dobaczewski, W. Nazarewicz, P.-G. Reinhard (in preparation): divergences related to unphysical poles of the energy $\mathcal{E}(z)$ at $z_\mu^\pm = \pm i\,|u_\mu|/|v_{\bar{\mu}}|$
- M. B., T. Duguet (in preparation): There might be spurious self-pairing in nuclei, i.e. the interaction of a pair with itself, when using effective interactions. This is a generalization of the spurious self-energy known from density functional theory in condensed matter physics (J. P. Perdew and A. Zunger, Phys. Rev. B 23 (1981) 5048)
- The generalized Wick theorem by Balian and Brézin used to evaluate the matrix elements between different, but non-orthogonal, HFB states adds a second layer of spuriosity, as it introduces terms with an unphysical dependence on the gauge angle in the Hamiltonian kernel for particle number projection.

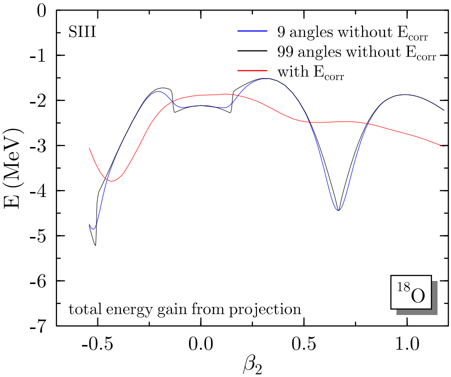
A minimal solution I

- We do not attempt to remove the spurious self-pairing entirely, but only its divergent part in PNP.
- The divergent part can be identified due to his "wrong" behaviour under rotations in gauge space (using the standard Wick theorem as guiding principle). After a few dozen pages of algebraic manipulations, one obtains for two-body interactions

$$\mathcal{E}_{\text{spu}}^{N_0} = \sum_{\mu>0} \left[\left(w^{\rho\rho}_{\mu\mu\mu\mu} + w^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}} + w^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} + w^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu} \right) - 4 w^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}} \right]$$
$$\times u_\mu^2 v_{\bar{\mu}}^4 \int_0^{2\pi} d\phi \, \frac{e^{-i\phi N_0}}{2\pi \mathcal{D}_{N_0}} \frac{e^{2i\phi}(e^{2i\phi} - 1)}{u_\mu^2 + v_{\bar{\mu}}^2 e^{2i\phi}} \prod_{\substack{\nu>0 \\ \nu\neq\mu}} (u_\nu^2 + v_{\bar{\nu}}^2 e^{2i\phi})$$

- This completely removes the contribution of the poles at $z_\mu^\pm = \pm i |u_\mu| / |v_{\bar{\mu}}|$
- This also removes part of the contribution of the poles at $z = 0$
- A similar solution for the overlap between BCS ground states and two-quasiparticle states in GCM was proposed by N. Tajima, P. Bonche, J. Dobaczewski, H. Flocard and P.-H. Heenen, Nucl. Phys. A542 (1992) 355.

A minimal solution II – PRELIMINARY results



Note that this is SIII, which uses a three-body force instead a density dependence with fractional power, as we do not know (yet?) how to correct such terms. We took the liberty to neglect the Coulomb exchange term in Slater approximation.

M. B., T. Duguet, preliminary results – please do not distribute.

Challenges for the future (related to pairing)

- (not discussed here, this would have been Karim Bennaceurs talk, had he been here): improve effective pairing interactions and their regularisation.
- Explore dynamical pairing – find suitable constraints, and find an efficient way to implement mixing of states with different proton and neutron pairing on top of angular-momentum projected GCM of quadrupole deformed states.
- Understand the divergence in particle number projection, and find a way to remove it safely. It appears probably in other projections and GCM mixing as well.
- Follow the phase, and may the force be with you!

Acknowledgements

The work presented here would have been, and the future developments will be impossible without my collaborators in this project

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Paul Bonche, SPhT, CEA Saclay, France
Thomas Duguet, NSCL/Michigan State University, USA
Hubert Flocard, CSNSM Orsay, France
Thomas Lesinski, IPN Lyon, France
Jacques Meyer, IPN Lyon, France

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