Particle number restoration: its implementation and impact in nuclear structure calculations

XIII Nuclear Physics Workshop
Maria and Pierre Curie
Pairing and Beyond- 50 Years of the BCS Model

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The Pairing interaction plays a very important role in the description of the low-lying spectrum of atomic nuclei

in the ground state

- Binding energies
- Mass parabolas
- J^{π} of the ground state

and the excited states

- Level density around Fermi surface
- Moments of inertia
- Collective masses

The standard nuclear pairing interaction favors the coupling of like nucleons to $J = 0$ to maximize the spatial overlap

similar to a Cooper pair in the theory of superconductivity

mean field description in terms of BCS wave functions

$$|\varphi\rangle = \prod (u_k + v_k a_k^+ a_{\bar{k}}^+)|-\rangle$$

or the more general HFB wave function

$$|\varphi\rangle = \prod \beta_k |-\rangle$$

$$\beta_k = \sum U_{lk} c_l + V_{lk} c_l^+$$

both the BCS and HFB wave functions do not have a definite number of particles and therefore both violate one of the "symmetries" of the hamiltonian (preservation of particle number)

the mean field approximation leads to spontaneous symmetry breaking in the wave function

Nice mechanism to incorporate correlations into the mean field wave function

but it is unphysical as the real wave function of the atomic nucleus has to preserve the symmetries of the hamiltonian in the traditional sense

Not important in Condense Matter as the consequences of symmetry restoration in observables go as the inverse of the number of particles (degrees of freedom)

but relevant in Nuclear Physics

If it is required to have

- Wave functions with the right symmetries
- not to loose the simplicity of the mean field and the correlations included by the spontaneous symmetry breaking mechanism

Particle Number Projected (PNP) wave functions

$$|\Psi^N\rangle = \hat{P}^N|\Phi\rangle$$

- $|\Phi\rangle$ is a HFB wave function
- $\hat{P}^N = \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{i(\hat{N}-N)\varphi}$

Why the hassle if we have so many exactly solvable models at hand ?
In Nuclear Physics pp and ph channels are strongly interconnected

Projected energy

$$E^N = \frac{\langle\Phi|HP^N|\Phi\rangle}{\langle\Phi|P^N|\Phi\rangle} = \frac{\int d\varphi h(\varphi) e^{-iN\varphi}}{\int d\varphi n(\varphi) e^{-iN\varphi}} \qquad \begin{matrix} n(\varphi) \\ h(\varphi) \end{matrix} = \langle\Phi| \begin{matrix} 1 \\ H \end{matrix} e^{i\hat{N}\varphi}|\Phi\rangle$$

Hamiltonian overlap $h(\varphi)$ and norm $n(\varphi)$ are evaluated with the help of the extended Wick theorem

Kamlah expansion

$$h(\varphi) = \sum_{m=0}^{M} h_m \hat{I}^m n(\varphi) \text{ with } \hat{I} = -i\partial_\varphi - \langle N\rangle.$$

For M=1 we have $E^N_{M=1} = \langle\Phi|H - h_1(\hat{N} - N)|\Phi\rangle$
The minimum of $E^N_{M=1}$ with the constraint $\langle\Phi|\hat{N}|\Phi\rangle = N$ is equivalent to minimizing $\langle\Phi|(H - h_1\hat{N})|\Phi\rangle$
For M=2 we have $E^N_{M=2} = \langle\Phi|H - h_1(\hat{N} - N) - h_2(\hat{N} - N)^2|\Phi\rangle$
An expansion in terms of powers of $(\hat{N} - N)^2$

There are two main variational strategies to determine the intrinsic HFB wave funtction $|\Phi\rangle$

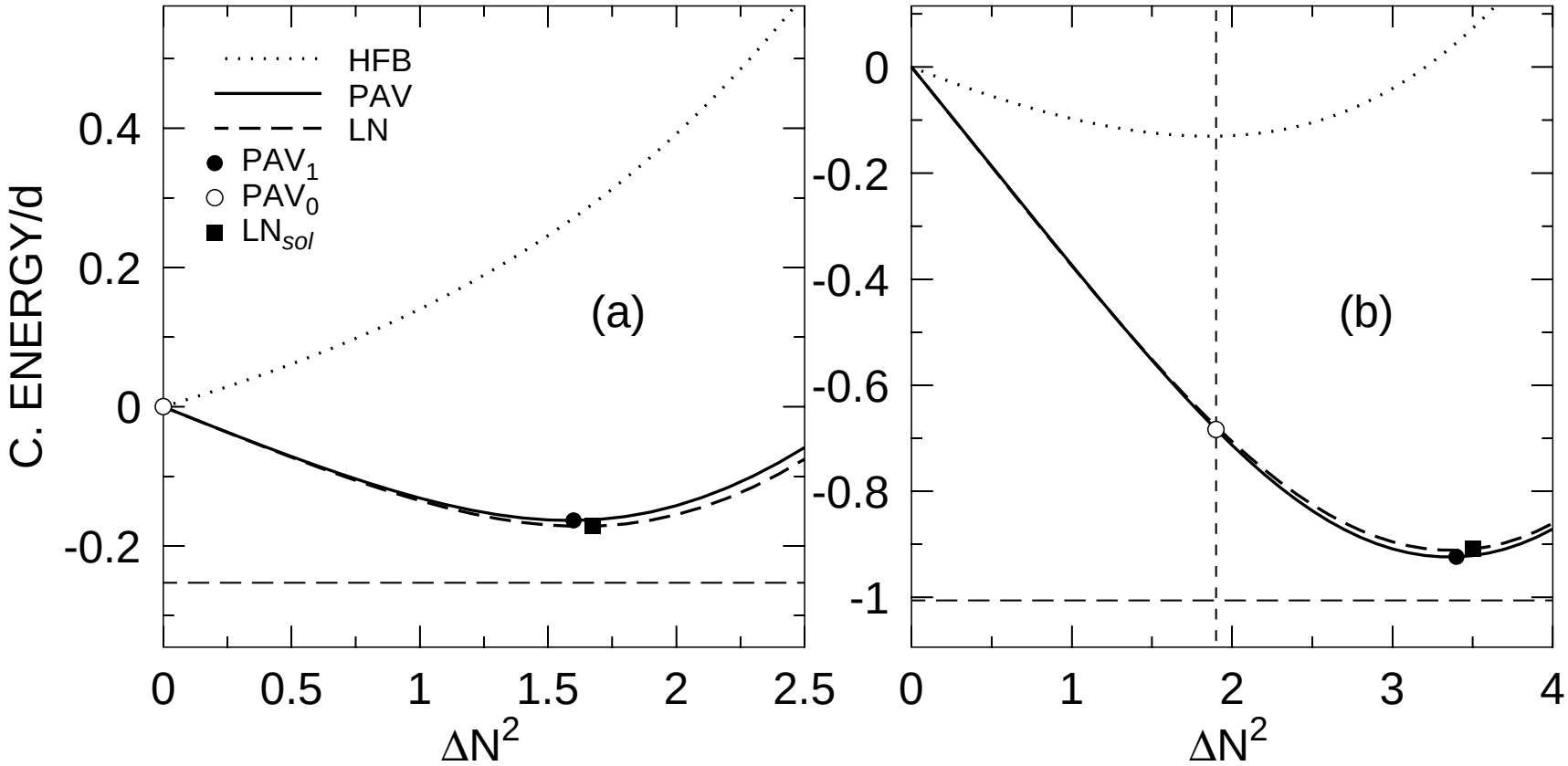
- Variation after projection (VAP) $|\Phi\rangle$ is determined as to minimize the projected energy E^N
- Projection after variation (PAV). $|\Phi\rangle$ is determined as to minimize the intrinsic HFB energy. E^N is computed afterwards

The most relevant degree of freedom related to PNP is the particle number fluctuation $\langle\Phi|\Delta N^2|\Phi\rangle$

- Restricted VAP (RVAP) A restricted variational space where $\langle\Phi|\Delta N^2|\Phi\rangle$ is used as variational parameter

If the approximate Kamlah expansion is used for E^N and M=2 then RVAP becomes the Lipkin Nogami method

An example in a very simple model



T.R.Rodriguez, J.L. Egido and LMR Phys. Rev. C72 064303 (2005)

- Until recently PNP had been implemented only in model calculations with restricted configuration spaces (a couple of major shells) and simplified interactions (PPQ hamiltonian)
- In the 90's the Lipkin Nogami method was very popular and was used with Skyrme and Gogny forces
- Recently the full PNP+VAP has been implemented with the Gogny force and PNP+LN has been implemented with Skyrme interactions
- Full VAP is still computationally expensive
- Technical difficulties are also present as well as some more fundamental problems of how to define the density dependent term typical of Skyrme or Gogny forces for PNP energy functionals.

Technical difficulties: the pole problem

- The pole problem appears in the evaluation of two-body operator overlaps when the norm overlap $\langle\Phi|e^{i\varphi\hat{N}}|\Phi\rangle$ becomes zero.
- $\langle\Phi|e^{i\varphi\hat{N}}|\Phi\rangle = 0$ when one of the BCS occupancies v_k equals $1/2$ and $\varphi = \pi/2$
- In this case the overlap

$$\langle\Phi|c_k^+ c_l^+ c_m c_n e^{i\varphi\hat{N}}|\Phi\rangle = (\sum \text{Contractions})\langle\Phi|e^{i\varphi\hat{N}}|\Phi\rangle$$

is finite but each of the contractions in $\sum \text{Contractions}$ diverges. There is a cancellation between the direct, exchange and pairing contractions.

M. Anguiano, J.L. Egido and LMR, Nucl Phys A696, 467 (2001)

A real problem as it is common to discard some contributions of some parts of the interaction for the Skyrme or Gogny forces. The most usual is the case of the Coulomb interaction.
Bad for VAP but you may be lucky with PNP+LN

The solution is to consider all contributions, direct, exchange and pairing for each piece of the interaction

and then you live happily forever after ..... except for a bad guy called Coulomb

but considering Coulomb exchange and pairing multiplies by a factor 6-7 the computing time for the finite range Gogny force.
For Zero range forces like Skyrme you will be force to introduce into your computational scheme the hassle of finite range forces ... or to find a way to regularize the divergences (ask Michael Bender)

The density dependence problem

Skyrme and Gogny interactions are very popular at the mean field level as they allow the calculations of many nuclear properties all over the Nuclide Chart with the same set of parameters
Most of theirs sucess comes from their density dependence

$$V_{DD}(\rho) = t_3\delta(\vec{r}_1 - \vec{r}_2)\rho^{\alpha}(\frac{1}{2}(\vec{r}_1 + \vec{r}_2))$$

- Phenomenological and very hard (if not impossible) to deduced them from first principles
- They produce a strongly repulsive interaction energy
- State dependent interaction:
  To compute $\langle\Phi|\hat{H}_{DD}|\Phi\rangle$ use $\hat{H}_{DD} = f[\rho]$ with $\rho = \langle\Phi|\hat{\rho}|\Phi\rangle$

In the GCM and projection one has to deal with linear combinations of mean field wave functions (HF or HFB) $|\Phi(q)\rangle$

$$|\Psi\rangle = \int dq f(q)|\Phi(q)\rangle$$

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\int dqdq' f^*(q)f(q')\mathcal{H}(q,q')}{\int dqdq' f^*(q)f(q')\mathcal{N}(q,q')}$$

Hamiltonian and norm overlaps

$$\mathcal{H}(q,q') = \langle\Phi(q)|\hat{H}|\Phi(q')\rangle \quad \mathcal{N}(q,q') = \langle\Phi(q)|\Phi(q')\rangle$$

Evaluated with the extended Wick's theorem for overlaps

For the GCM+GOA second derivatives of $\mathcal{H}(q,q')$ are needed

how to define the DD interaction for hamiltonian overlaps ?

$$\langle\Phi(q)|\hat{H}|\Phi(q')\rangle$$

A prescription is required for the calculation of the density dependent part of $\langle\Phi(q)|\hat{H}|\Phi(q')\rangle$ in order to compute energies
As it may lead to a complex and/or symmetry breaking density dependent term we have to make sure it yields energies that are

1. real numbers
2. invariant under symmetry transformations (scalar)

we also want to have a framework consistent with the underlying mean field approximation

1. Reduce to the mean field DD term when $|\Phi(q)\rangle = |\Phi(q')\rangle$
2. Produce consistent results for "mean field like" quantities like
   - Chemical potentials
   - RPA equation

Mixed density $\rho_{q,q'} = \langle\Phi(q)|\hat{\rho}|\Phi(q')\rangle / \langle\Phi(q)|\Phi(q')\rangle$
For PNP $\rho_{\varphi} = \langle\Phi|\hat{\rho}e^{i\varphi\hat{N}}|\Phi\rangle / \langle\Phi|e^{i\varphi\hat{N}}|\Phi\rangle$

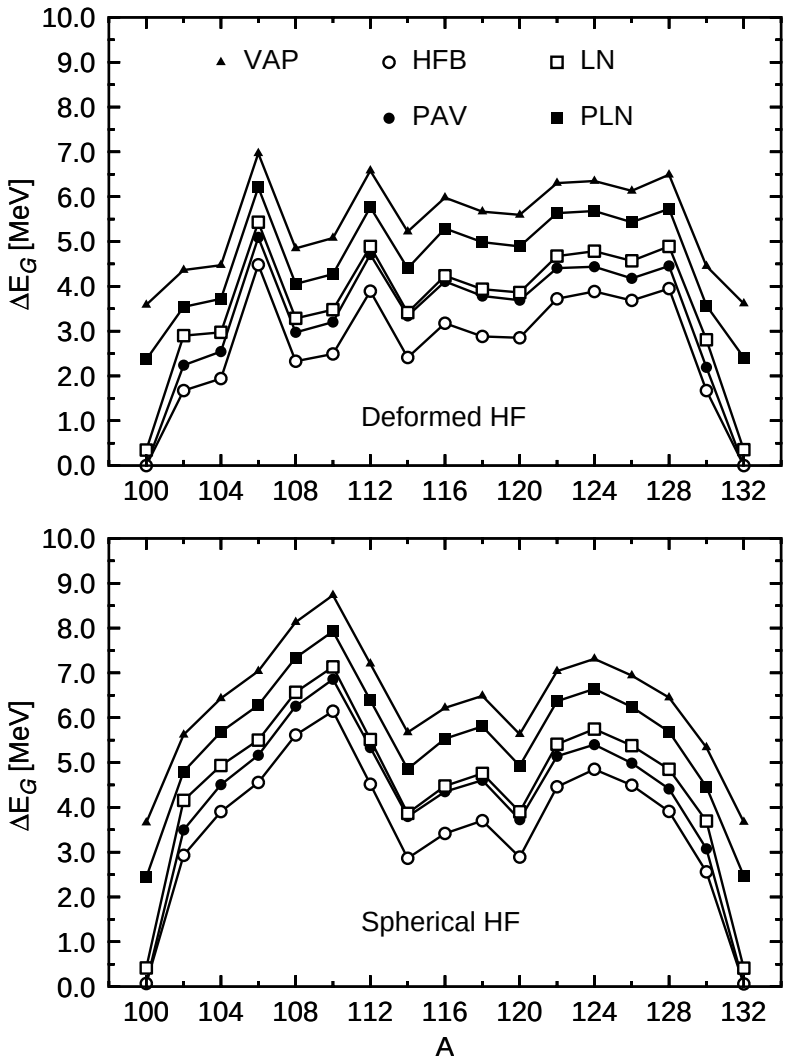
Caveats

- As the mixed density is complex in general and is raised to the power α (1/3 typically) which Riemman sheet should be chosen for the evaluation of $\rho^{\alpha}(\vec{r})$?
- What to do if $\langle \Phi | e^{i\varphi \hat{N}} | \Phi \rangle = 0$?
  - In this case the mixed density diverges !
    But the singularity is integrable if $\alpha < 1$

These questions need to be addressed before we can move forward in the use of PNP with effective forces like Gogny, Skyrme

if you close your eyes and use another prescription (the projected density prescription) not consistent but real and not diverging then you can obtain some results ... (I am not so pesimistic ...)

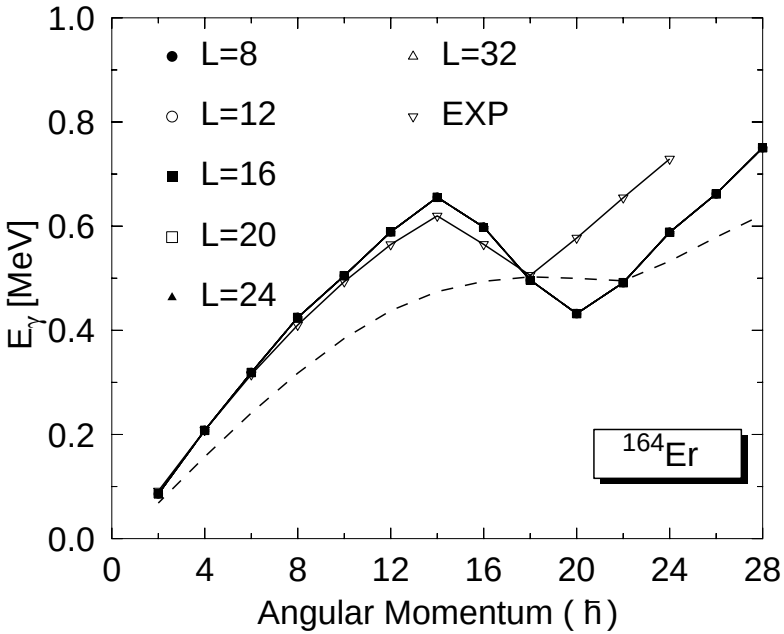
Tin isotopes

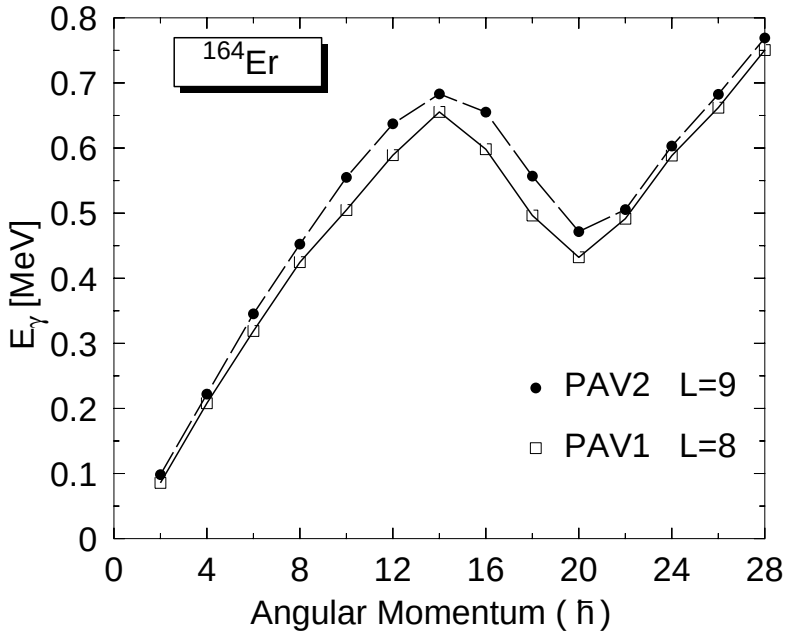


Pairing correlations in the Tin isotopes

Comparison of different theoretical approaches concerning the pairing correlation energy

Moments of inertia PAV





Moments of inertia