Symmetry restoration with the nuclear EDF: The quest for a good methodology

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September 13th, 2011

ESNT Sep 2011, Saclay

Ouline of the talk

Quest for a methodology

- Symmetry breaking in nuclear physics
- Nuclear EDFs and extensions for the GCM
- Requirements, problems and what to avoid
- Some ideas to tackle the issue

Other technical problems

- Sign of the norm (pfaffian variations)
- Overlap for multiquasiparticle configurations

Other approaches

- Mapping to exactly solvable models for pairing

Symmetry breaking

Spontaneus symmetry breaking is a extremely fruitful concept to understand nuclear structure phenomenology

- Nuclear superfluidity (Particle number, BCS like w.f.)
- Rotational bands (Rotational symmetry)
- Octupole bands (Parity)
- Translational invariance

1. Intrinsic wave functions treated at the mean field level
2. Coupling between symmetry related degrees of freedom (Euler angles in rotational symmetry) and intrinsic (deformed) states can be neglected to some extent ...
3. Exact symmetry restoration required for a more precise description (correlation energy, selection rules)

Effective interactions

Bare nucleon-nucleon

Bare nucleon-nucleon interaction well known at long distances. At short distances the repulsive core is less known. Three body forces are more or less understood.

Short range in-medium correlations

Short range in-medium correlations (Pauli blocking) ”cancel out” the repulsive core and yield a smooth effective in medium interaction

Effective interactions

Handling of short range correlations requires Brueckner-like methods which are extremely hard to implement in finite nuclei. The smooth effective in-medium interaction is replaced by phenomenological effective interactions like Skyrme, Gogny or RFM

Skyrme/Gogny

Non-relativistic Skyrme like/Gogny

Central part, spin-orbit, Coulomb and a phenomenological density dependent term.

- Skyrme: Zero range central part $\delta(\vec{r} - \vec{r}\,')$ + gradient terms
- Gogny: Finite range central part $\exp(-(\vec{r} - \vec{r}\,')^2/\mu^2)$

Density dependent term (strongly repulsive)

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

α is usually non-integer

EDF: Replace $E[\Phi\rangle] = \langle\Phi|H|\Phi\rangle + V_{DD}[\langle\Phi|\rho|\Phi\rangle]$ by a functional $E[\rho]$ (modern Skyrme, BCP, etc)

This is not DFT !

Restoring symmetries

PNP as an example

$$|\Psi^N\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$$

Projected Energy ?

In a pure hamiltonian framework the overlap $\langle\varphi_0|H|\varphi_1\rangle$ is required to compute the projected energy.

How to deal with density dependent interactions ?

$$E[|\Phi_0\rangle,|\Phi_1\rangle] = \langle\Phi_0|H|\Phi_1\rangle + V_{DD}[???]$$

or general EDF ?.

Transition density prescription

Hamiltonian overlap

GWT says that

$$\frac{\langle \Phi_0 | \hat{H} | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle}$$

has the same functional form as the energy but in terms of the transition density and pairing tensors

$$\rho_{01\,kl} = \frac{\langle \Phi_0 | c_l^+ c_k | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \quad \kappa_{01\,kl} = \frac{\langle \Phi_0 | c_l c_k | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \ldots$$

Prescription

For the calculation of energy overlaps use

$$\langle \Phi_0 | H | \Phi_1 \rangle + V_{DD}[\rho_{01}]$$

for DD interactions or $E[\rho_{01}, \kappa_{01}, \kappa_{10}]$ for EDF

Consistency checks

The transition density prescription has the right limit when $|\Phi_1\rangle \rightarrow |\Phi_0\rangle$ but

- ρ_{01}, etc are, in general, complex quantities (non-hermitian V_{DD}!!). Need to make sure the final energy is real
- breaks (spatial) symmetries (rotational, parity). Make sure energy is a scalar under symmetry transformation
- Consistent with the underlying mean field (definition of chemical potentials)

The same should be used for configuration mixing (GCM in nuclear physics)

- Consistent with RPA in the small amplitude limit of configuration mixing

Also to be considered

Generalizations

- Statistical admixtures (finite temperature)
- Odd-A systems and multiquasiparticle excitations

Problems

- When $\langle \Phi_0 | \Phi_1 \rangle = 0$ the transition density ρ_{01} diverges. However, physical quantities are well defined, because strict enforcement of the Pauli principle yields to the cancelation of divergencies. Similar to self-energy problem. Solved (partially) by some people in the audience.
  Specially bad for multiquasiparticle excitations
- Definition of ρ_{01}^{α} for non integer α and complex ρ_{01} (Riemman sheets) $e^{i\varphi/\alpha}$, $e^{i\varphi/\alpha+2\pi/\alpha}$, ...

Real energies

- The transition density is in general a complex quantity but

$$E = \int dq dq' f^*(q) f(q') \langle q|\hat{H}|q'\rangle$$

$$E^* = \int dq dq' f(q) f^*(q') \langle q|\hat{H}|q'\rangle^*$$

and

$$\langle q|\hat{H}|q'\rangle^* = \langle q'|\hat{H}^\dagger|q\rangle \qquad \hat{H}^\dagger[\rho_{q,q'}] = \hat{H}[\rho_{q',q}]$$

Therefore

$$E = E^*$$

R. R-G, J.L.E, L.M.R.; Nuclear Physics A709 (2002) 201

Symmetry requirements (AMP)

For rotational invariant (scalar) hamiltonians we have

- $\langle \Psi_{IM} | \hat{H} | \Psi_{I'M'} \rangle = \delta_{II'} \delta_{MM'} \langle \Psi_{IM} | \hat{H} | \Psi_{IM} \rangle$
- $\langle \Psi_{IM} | \hat{H} | \Psi_{IM} \rangle = \langle \Psi_{I} | \hat{H} | \Psi_{I} \rangle$

$$|\Psi_{IM}\rangle = \frac{2I+1}{8\pi^2} \sum_K g_K \int d\Omega \mathcal{D}^{I*}_{MK}(\Omega) \hat{R}(\Omega) |\Phi\rangle = \sum_K g_K \hat{P}^I_{MK} |\Phi\rangle$$

This is a consequence of $[\hat{R}(\Omega), \hat{H}] = 0$ as it implies

$$\langle \Phi | \hat{R}^\dagger(\Omega') H \hat{R}(\Omega) | \Phi \rangle = \langle \Phi | H \hat{R}(\Omega' - \Omega) | \Phi \rangle$$

and therefore

$$\langle \Phi | {P^I_{MK}}^\dagger H P^{I'}_{M'K'} | \Phi \rangle = \langle \Phi | H {P^I_{MK}}^\dagger P^{I'}_{M'K'} | \Phi \rangle = \delta_{II'} \delta_{MM'} \langle \Phi | H P^{I'}_{KK'} | \Phi \rangle$$

For DD interactions we should have

$$\langle\Phi|\hat{R}^{\dagger}(\Omega')H_{DD}[\Omega',\Omega]\hat{R}(\Omega)|\Phi\rangle = \langle\Phi|H_{DD}[0,\Omega'-\Omega]\hat{R}(\Omega'-\Omega)|\Phi\rangle$$

that holds because

$$\hat{R}^{\dagger}(\Omega')\rho(\vec{R},\Omega',\Omega)\hat{R}(\Omega) = \rho(\vec{R},0,\Omega'-\Omega)\hat{R}(\Omega'-\Omega)$$

with

$$\rho(\vec{R},\Omega',\Omega) = \frac{\langle\Phi|\hat{R}^{\dagger}(\Omega')\hat{\rho}(\vec{R}))\hat{R}(\Omega)|\Phi\rangle}{\langle\Phi|\hat{R}^{\dagger}(\Omega')\hat{R}(\Omega)|\Phi\rangle}$$

R. R-G, J.L.E, L.M.R.; Nuclear Physics A709 (2002) 201

Mean field chemical potential

1. At the mean field level and when a symmetry is broken the routhian $\langle \hat{H} - \lambda \hat{N} \rangle$ is minimized with the constraint $\langle \hat{N} \rangle = N$.
2. The chemical potential λ is determined by the condition of having the gradient of the Routhian H' perpendicular to the gradient of the constraint

$$\lambda = \frac{\langle \hat{H} \Delta \hat{N} \rangle}{\langle \Delta \hat{N}^2 \rangle}$$

3. Deduced from minimizing the particle number projected energy evaluated in an approximate way (the Kamlah expansion)

Mean field chemical potential

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

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 $E^N_{M=1} = \langle\Phi|(H - h_1(\hat{N} - N))|\Phi\rangle$ with

$$h_1 = \frac{\hat{I}h(\varphi)_{|\varphi=0}}{\langle\Delta\hat{N}^2\rangle} = \frac{\langle\hat{H}\Delta\hat{N}\rangle}{\langle\Delta\hat{N}^2\rangle}$$

The minimum of $E^N_{M=1}$ with the constraint $\langle\Phi|\hat{N}|\Phi\rangle = N$ is equivalent to minimizing $\langle\Phi|(H - h_1\hat{N})|\Phi\rangle$

Mean field chemical potential

1. For density dependent forces the chemical potential is computed in the same way but we have an extra rearrangement term

$$\langle(\hat{H}+\partial\hat{\Gamma})\Delta\hat{N}\rangle-\lambda\langle\Delta\hat{N}^2\rangle=0 \quad \partial\hat{\Gamma}=\sum_{ij}\langle\frac{\delta H}{\delta\rho}\varphi_i^*\varphi_j\rangle c_i^\dagger c_j$$

2. To get $h_1=\lambda$ for EDFs we must have

$$h_1=\frac{\hat{I}h(\varphi)_{|\varphi=0}}{\langle\Delta\hat{N}^2\rangle}=\frac{\langle(\hat{H}+\partial\hat{\Gamma})\Delta\hat{N}\rangle}{\langle\Delta\hat{N}^2\rangle}$$

RPA

The RPA equation can be derived as a special limit of the Time Dependent Mean Field (HF or HFB) equations.

For Density Dependent forces (Blaizot&Gogny) the interaction matrix elements entering the RPA equation are given by the second derivative

$$\frac{\delta^2 E}{\delta \rho_{ij} \delta \rho_{kl}}$$

Rearrangement terms ! that is, derivatives of the DD interaction have to be considered in the RPA matrix elements

The RPA can also be derived from the GCM (*)

- $|\mathbf{Z}\rangle = \exp(\sum_{\mu\nu} Z_{\mu\nu}\alpha^+_\mu\alpha^+_\nu)|\psi_0\rangle$ and $|\Psi\rangle = \int d\mathbf{Z} f(\mathbf{Z})|\mathbf{Z}\rangle$
- Expand $\langle\mathbf{Z}'|\hat{H}|\mathbf{Z}\rangle/\langle\mathbf{Z}'|\mathbf{Z}\rangle$ up to second order
- Assume Gaussian overlaps $\langle\mathbf{Z}'|\mathbf{Z}\rangle \propto \exp(-\mathbf{Z}'^*\mathbf{Z})$
- Introduce the above in the Hill-Wheeler equation
- After some manipulations the RPA equation is obtained

and the only way to get the same rearrangement terms as in the standard derivation of the RPA is to have a density dependent term depending upon $\mathbf{Z}'^*$ and $\mathbf{Z}$.

(*) Jancovici&Schiff, Brink &Weiguny

Symmetry preserving density ?

Some people claim it is better to use symmetry preserving densities in the DD term

1. Very appealing in doing projection as it preserves the symmetries in the interaction.
2. Let us consider, for simplicity, parity projection. Intrinsic wave functions have an octupole moment Q_3 different from zero. The projector to good parity p is given by

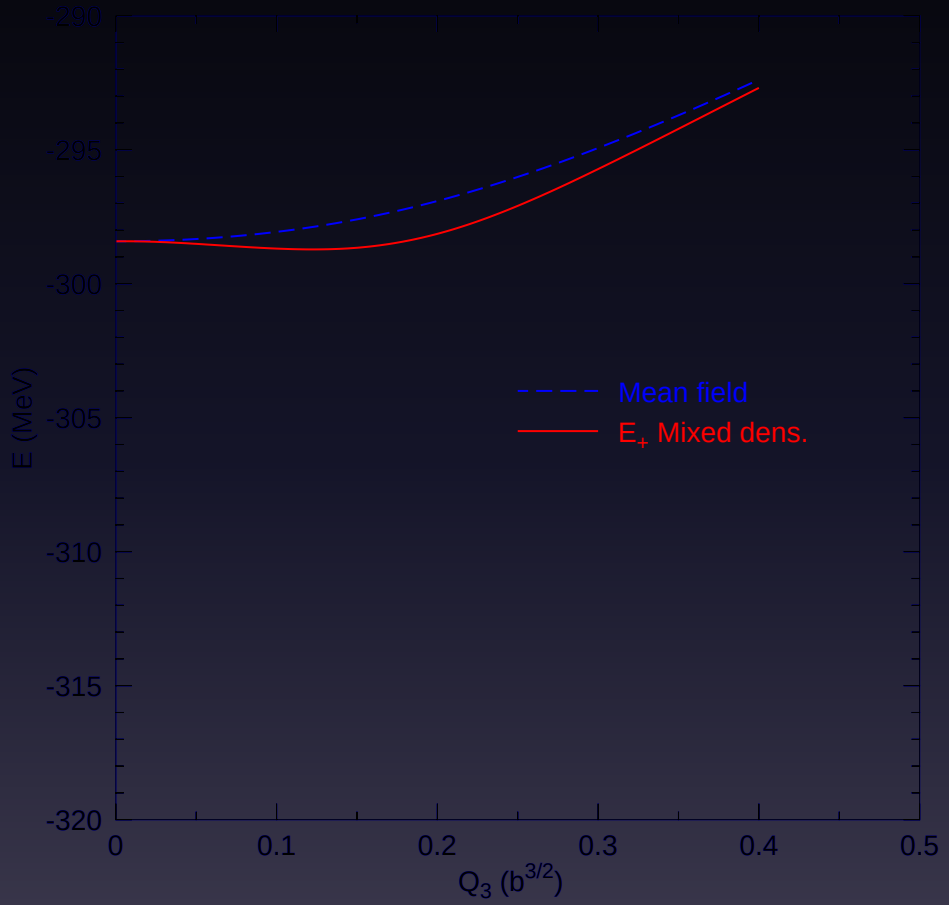
$$\hat{P}_p = 1 + p\Pi$$

3. The correlated density to be used is the one projected to positive parity

$$\rho_{Proj} = \frac{\langle\Psi|(1+\Pi)\hat{\rho}(1+\Pi)|\Psi\rangle}{\langle\Psi|(1+\Pi)(1+\Pi)|\Psi\rangle}$$

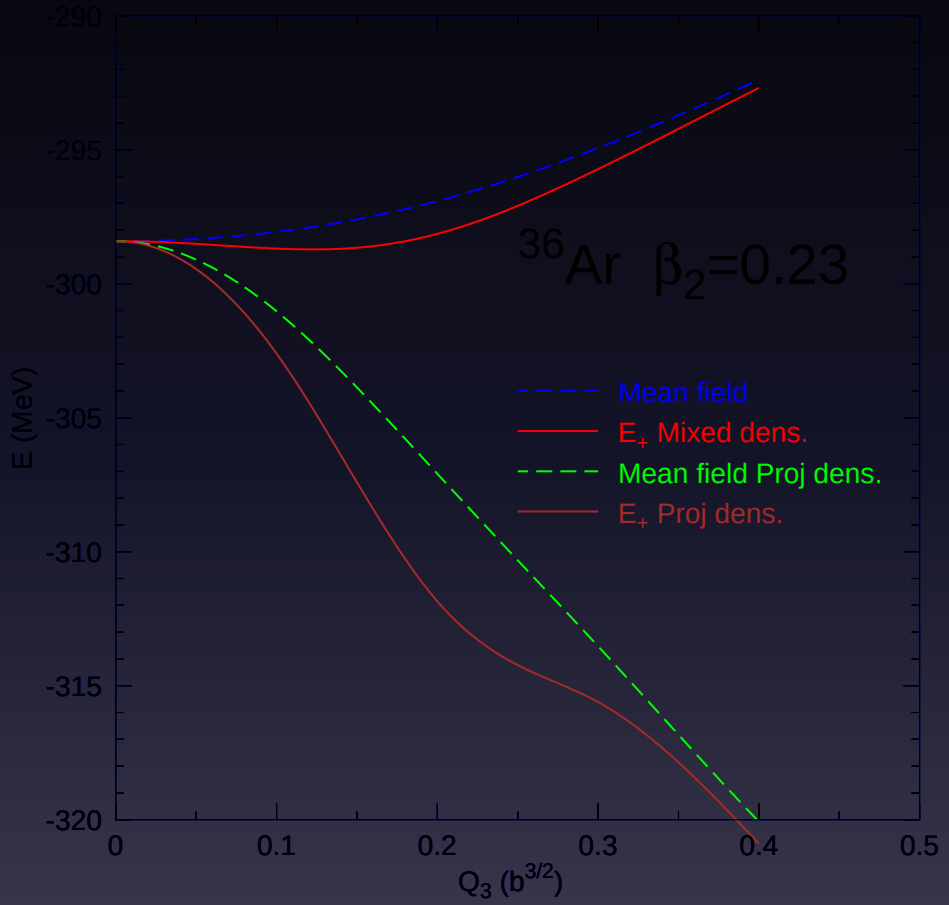
Such that $\rho_{Proj}(-\vec{r}) = \rho_{Proj}(\vec{r})$

An example



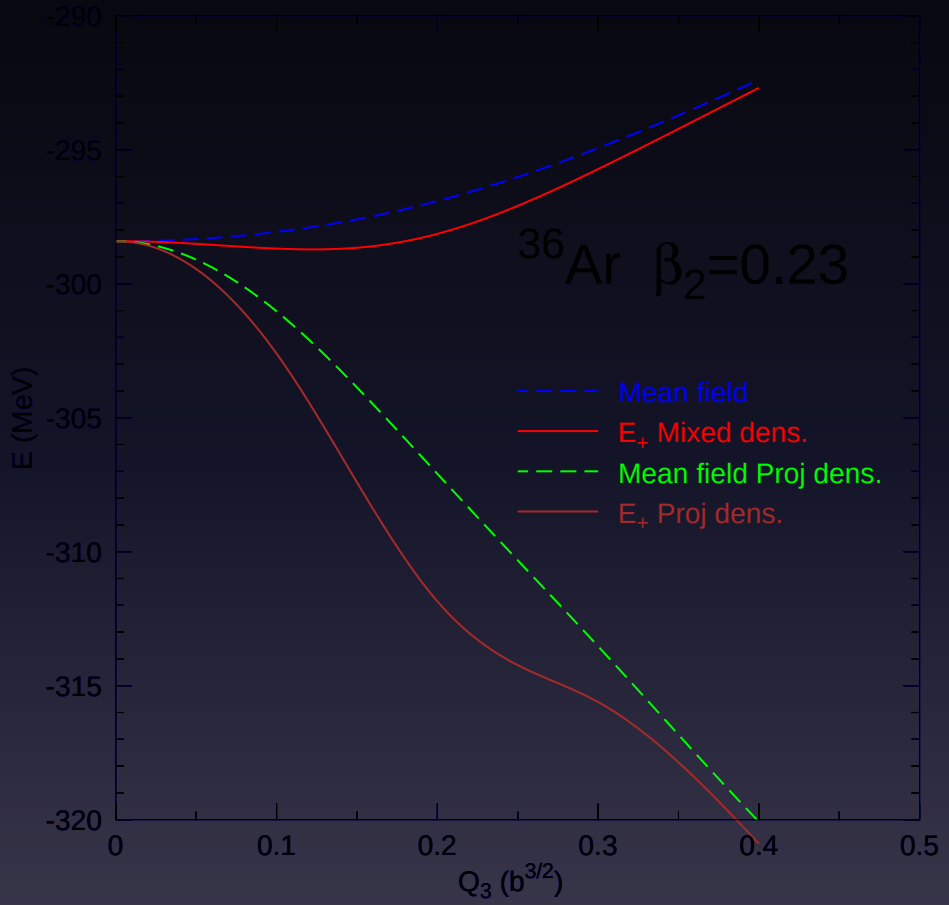
L.M.Robledo, Jour of Phys G37, 064020 (2010)

An example



L.M.Robledo, Jour of Phys G37, 064020 (2010)

An example



1. $E_{DD} \propto \int d^3\vec{r}\rho^{\tau}(\vec{r})\rho^{\tau'}(\vec{r})\rho^{\alpha}(\vec{r})$
2. $\rho_{Proj}(\vec{r}) \approx \rho(\vec{r}) + \rho(-\vec{r})$
3. Integrand decreases
4. $t_3 \approx 1400$ MeV

Meaningless prescription!

L.M.Robledo, Jour of Phys G37, 064020 (2010)

A proposal

Inspired by the RPA use the expansion to second order of $V_{DD}(\rho)$ instead of $V_{DD}(\rho_{01})$.
In the evaluation of $\langle\Phi|V_{DD}(\rho(\varphi))e^{i\varphi N}|\Phi\rangle$ replace $V_{DD}(\rho(\varphi))$ by

$$V_{DD}(\rho) + \frac{\delta V_{DD}}{\delta\rho}\frac{\delta\rho}{\delta\varphi}\varphi + \frac{1}{2}\frac{\delta^2 V_{DD}}{\delta\rho^2}\frac{\delta^2\rho}{\delta\varphi^2}\varphi^2$$

Advantages

1. No diverging density in V_{DD}
2. No ”non-integer root of complex number” problem

Self-energy still remains through the HFB density ρ
Work in progress !

Other proposals

- Obtain the equivalent of the Slater approximation but for overlaps of the Coulomb interaction (Density Matrix Expansion ?) to better understand the problem
- Use “local expressions” like the Kamlah expansion (supplemented with topGOA ideas) to get rid of difficulties (think of LN and PNP).
- Use Skyrme or Gogny to derive the parameters of simpler models like the Pairing+Quadrupole or exactly solvable pairing models which are free from patogolies

Multiquasiparticle overlaps

A natural way to incorporate correlations is to consider linear combinations of multi- quasiparticle excitations

$$|\Psi\rangle = C_0|\varphi\rangle + \sum_{i,j} C_{i,j}\beta_i^+\beta_j^+|\varphi\rangle + \sum_{i,j,k,l} C_{i,j,k,l}\beta_i^+\beta_j^+\beta_k^+\beta_l^+|\varphi\rangle + \ldots$$

This can also be extended to ”odd” systems (one, three, five quasiparticle excitations, ...)
An alternative to ”cranking” wave functions (PSM) using axial intrinsic configurations.
Requires the evaluation of Multicuasiparticle overlaps like

$$\langle\varphi|\beta_i\beta_j\beta_k\beta_l c_m^+ c_n^+ c_p c_q \beta_r^+\beta_s^+\beta_t^+\beta_u^+|\varphi\rangle$$

that can be evaluated with the standard Wick’s theorem ...

... by considering 11 !! (10 395) contractions
(the combinatorial explosion)

things get worse if we consider instead

$$\langle\varphi|\beta_i\beta_j\beta_k\beta_l c_m^+ c_n^+ c_p c_q \tilde{\beta}_r^+ \tilde{\beta}_s^+ \tilde{\beta}_t^+ \tilde{\beta}_u^+ |\tilde{\varphi}\rangle$$

with different HFB vacuums and quasiparticle operators because that requires the use of the Generalized Wick's theorem (GWT) with its more involved contractions

In [1] a new way to evaluate those overlaps, free from the combinatorial explosion, has been obtained. It makes use of a limiting procedure on the contractions provided by the Statistical Wick's theorem.

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[1] *Generalized Wick's theorem for multiquasiparticle overlaps as a limit of Gaudin's theorem*, S. Perez-Martin and L.M. Robledo, Phys. Rev. C76, 064314 (2007)

Statistical Wick's (Gaudin's) theorem

Same as the standard Wick's theorem but for statistical averages

$$\frac{\mathrm{Tr}[\hat{D}\hat{O}]}{\mathrm{Tr}[\hat{D}]} = \sum \mathrm{Contractions}$$

here $\hat{O}$ is a product of creation and annihilation operators.

$$\hat{O} = \beta^{+}_{k_1}\beta_{k_2}\beta_{k_3}\ldots\beta^{+}_{k_{N-1}}\beta_{k_N}$$

Contractions: as in the standard Wick's theorem but replacing mean values by statistical traces.

$$\frac{\mathrm{Tr}[\hat{D}\beta_k\beta_l]}{\mathrm{Tr}[\hat{D}]} \quad \frac{\mathrm{Tr}[\hat{D}\beta^{+}_k\beta_l]}{\mathrm{Tr}[\hat{D}]} \quad \frac{\mathrm{Tr}[\hat{D}\beta^{+}_k\beta^{+}_l]}{\mathrm{Tr}[\hat{D}]}$$

The Generalized Wick's Theorem (GWT) for overlaps has also its counterpart by considering

$$\frac{\mathrm{Tr}[\hat{D}\hat{T}\hat{O}]}{\mathrm{Tr}[\hat{D}\hat{T}]} = \sum \mathrm{Contractions}$$

where $\hat{T}$ is the operator carrying out the required canonical transformation (the exponential of a one-body operator)
The contractions are

$$\frac{\mathrm{Tr}[\hat{D}\hat{T}\beta_k\beta_l]}{\mathrm{Tr}[\hat{D}\hat{T}]} \quad \frac{\mathrm{Tr}[\hat{D}\hat{T}\beta_k^+\beta_l]}{\mathrm{Tr}[\hat{D}\hat{T}]} \quad \frac{\mathrm{Tr}[\hat{D}\hat{T}\beta_k^+\beta_l^+]}{\mathrm{Tr}[\hat{D}\hat{T}]}$$

Mean values can be expressed as the limit

$$\lim_{p_\mu \to 0} \frac{\mathrm{Tr}[\hat{D}\hat{O}]}{\mathrm{Tr}[\hat{D}]} = \lim_{p_\mu \to 0} \frac{1}{Z}(\langle \hat{O} \rangle + \sum_\mu p_\mu \langle \beta_\mu \hat{O} \beta_\mu^+ \rangle + \frac{1}{2} \sum_{\mu\nu} p_\mu p_\nu \langle \beta_\mu \beta_\nu \hat{O} \beta_\nu^+ \beta_\mu^+ \rangle + \ldots) = \langle \hat{O} \rangle$$

The idea is valid for overlaps

$$\lim_{p_\mu \to 0} \frac{\mathrm{Tr}[\hat{D}\hat{\mathcal{T}}\hat{O}]}{\mathrm{Tr}[\hat{D}\hat{\mathcal{T}}]} =$$

$$\lim_{p_\mu \to 0} \frac{1}{\bar{Z}}(\langle \hat{O}\hat{\mathcal{T}} \rangle + \sum_\mu p_\mu \langle \beta_\mu \hat{O}\hat{\mathcal{T}} \beta_\mu^+ \rangle + \frac{1}{2} \sum_{\mu\nu} p_\mu p_\nu \langle \beta_\mu \beta_\nu \hat{O}\hat{\mathcal{T}} \beta_\nu^+ \beta_\mu^+ \rangle + \ldots) =$$

$$\frac{\langle \hat{O}\hat{\mathcal{T}} \rangle}{\langle \hat{\mathcal{T}} \rangle} = \frac{\langle \varphi | \hat{O} | \bar{\varphi} \rangle}{\langle \varphi | \bar{\varphi} \rangle}$$

Also for multiquasiparticle mean values

$$\langle \beta_\mu \beta_\nu \hat{O} \beta_\nu^+ \beta_\mu^+ \rangle = \lim_{[p\to\infty]} \frac{\mathrm{T}r[\hat{D}\hat{O}]}{\mathrm{T}r[\hat{D}]}$$

where $\lim_{[p\to\infty]}$ means p_μ and p_ν tend to ∞ and the other $p's$ tend to zero.

and multiquasiparticle overlaps

$$\langle \varphi | \beta_\mu \beta_\nu \hat{O} \tilde{\beta}_\nu^+ \tilde{\beta}_\mu^+ | \tilde{\varphi} \rangle = \lim_{[p\to\infty]} \frac{\mathrm{T}r[\hat{D}\hat{O}\hat{T}]}{\mathrm{T}r[\hat{D}\hat{T}]}$$

Notice

that the above trace is expressed by the sum of the contractions of $\hat{O}$! and not of the whole operator $\beta_\mu \beta_\nu \hat{O} \tilde{\beta}_\nu^+ \tilde{\beta}_\mu^+$

Fortunately the general limit $\lim_{[p\to\infty]}$ with $p_{\mu_1}, \ldots, p_{\mu_N}$ going to ∞ and the others to zero can be "easily" performed for the contractions. The expression are "simple" and can be found in the reference paper.

Then,

to compute the general overlap

$$\langle\varphi|\beta_{\mu_1}\ldots\beta_{\mu_N}\hat{O}\tilde{\beta}^{+}_{\mu_N}\ldots\tilde{\beta}^{+}_{\mu_1}|\tilde{\varphi}\rangle$$

we need to evaluate

$$\frac{\mathrm{Tr}[\hat{D}\hat{O}\hat{T}]}{\mathrm{Tr}[\hat{D}\hat{T}]}$$

(only the contractions corresponding to $\hat{O}$ (three for a two body operator)) and then perform the limit on the contractions.

nice ... but wait ! I want to compute

$$\langle\varphi|\beta_{\mu_1}\dots\beta_{\mu_N}\hat{O}\tilde{\beta}_{\nu_N}{}^{+}\dots\tilde{\beta}_{\nu_1}{}^{+}|\tilde{\varphi}\rangle$$

no problem! notice the existence of the unitary operator

$$\hat{\mathcal{T}}_{\mu\nu} = \exp(-i\pi/2(\beta_\mu^+ - \beta_\nu^+)(\beta_\mu - \beta_\nu))$$

transforming β_μ into β_ν and viceversa ....
Things get a little bit more involved but

The formulas for the contractions have a closed and concise form and are free from the combinatorial explosion

See G.F. Bertsch's talk for another approach

Phase of HFB overlaps

The sign (or phase) of $\langle\varphi_0|\varphi_1\rangle$ for arbitrary HFB-like wave functions cannot be obtained from the standard formula (Onishi) $\langle\varphi_0|\varphi_1\rangle = \sqrt{\det(1 + M^+N)}$

In triaxial AMP one needs of the order of 10^{8-10} overlaps

Previously

- Neergard's method: M^+N has double degenerate eigenvalues c_i. Then $\langle\varphi_0|\varphi_1\rangle = \prod_i(1 + c_i)$ where the product runs over half the eigenvalues
- Continuity argument: $\langle\varphi(q))|\varphi(q' + \Delta q)\rangle$ from $\langle\varphi(q))|\varphi(q')\rangle$ and $\langle\varphi(q)|\varphi(q)\rangle = 1$

Difficulties

- Neergard's requires eigenvalues of general matrices; no equivalent result exists for $\mathrm{T}r[\hat{D}]$
- Continuity requires a lot of "inteligence" when the overlap is close to zero and/or there are may collective variables.

Recently a new formula to evaluate the overlap has been obtained [2]
The formula relies on the powerful concept of Fermion Coherent States $|\mathbf{z}\rangle$ parametrized in terms of the anticommuting elements z_k and z_k^* of a Grassmann algebra and given by the conditions

$$a_k|\mathbf{z}\rangle = z_k|\mathbf{z}\rangle$$

and

$$\langle\mathbf{z}|a_k^+ = z_k^*\langle\mathbf{z}|$$

The coherent states satisfy a closure relation

$$1 = \int d\mu(\mathbf{z})|\mathbf{z}\rangle\langle\mathbf{z}|$$

[2] *Sign of the overlap of Hartree-Fock-Bogoliubov wave functions*, L.M. Robledo, PHYS REV C 79, 021302(R) (2009)

Introducing the HFB wave functions in the Thouless parametrization

$$|\phi_i\rangle = \exp\left(\frac{1}{2}\sum_{kk'} M^{(i)}_{kk'} a^+_k a^+_{k'}\right)|0\rangle$$

with the skew-symmetric

$$M^{(i)} = (V_i U_i^{-1})^*$$

the evaluation of the overlap proceeds as

$$\begin{aligned}\langle\phi_0|\phi_1\rangle &= \int d\mu(\mathbf{z})\langle 0|e^{\frac{1}{2}\sum_{kk'} M^{(0)*}_{kk'} a_{k'} a_k}|\mathbf{z}\rangle \\ &\times \langle\mathbf{z}|e^{\frac{1}{2}\sum_{kk'} M^{(1)}_{kk'} a^+_k a^+_{k'}}|0\rangle\end{aligned}$$

$$\langle \phi_0 | \phi_1 \rangle = \int d\mu(\mathbf{z}) e^{\frac{1}{2}\sum_{kk'} M^{(0)\,*}_{kk'} z_{k'} z_k} e^{\frac{1}{2}\sum_{kk'} M^{(1)}_{kk'} z^*_k z^*_{k'}}$$

Introducing

$$\mathbb{M}_{\mu'\mu} = \begin{pmatrix} M^{(1)}_{k'k} & -1_{k'k} \\ 1_{k'k} & -M^{(0)\,*}_{k'k} \end{pmatrix}$$

and $z_\mu = (z^*_{k'}, z_{k'})$ then

$$\langle \phi_0 | \phi_1 \rangle = \int \prod_k (dz^*_k dz_k)\, e^{\frac{1}{2}\sum_{\mu\mu'} z_{\mu'} \mathbb{M}_{\mu'\mu} z_\mu}$$

which is a Gaussian integral well known in QFT.

$$\langle \phi_0 | \phi_1 \rangle = s_N \mathrm{pf}(\mathbb{M}) = s_N \mathrm{pf} \begin{pmatrix} M^{(1)} & -1 \\ 1 & -M^{(0)\,*} \end{pmatrix}$$

where $s_N = (-1)^{N(N+1)/2}$

$\mathrm{pf}A$ is the Pfaffian of the skew-symmetric matrix A.

- It is similar to the determinant
  for a 2×2 matrix $R = \begin{pmatrix} 0 & r_{12} \\ -r_{12} & 0 \end{pmatrix}$ we obtain $\mathrm{pf}(R) = r_{12}$
  for a 4×4 matrix $R = \begin{pmatrix} 0 & r_{12} & r_{13} & r_{14} \\ -r_{12} & 0 & r_{23} & r_{24} \\ -r_{13} & -r_{23} & 0 & r_{34} \\ -r_{14} & -r_{24} & -r_{34} & 0 \end{pmatrix}$
  $\mathrm{pf}(R) = r_{12}r_{34} - r_{13}r_{24} + r_{14}r_{23}$
- $\mathrm{pf}(T^t R T) = \det(T)\mathrm{pf}(R)$
- Minor-like expansion formula
- $\mathrm{pf}(R) = \sqrt{\det(R)}$
- The numerical evaluation of the Pfaffian is straightforward by using Householder (orthogonal) transformations to bring the matrix in tridiagonal form.
- FORTRAN, Mathematica and Python routines available (see my web page)

The advantages of the present approach are

- Calculation of eigenvalues avoided
- Can be extended to the evaluation of traces of density matrix operators.
- Numerical evaluation of the Pfaffian straightforward and fast
- Fully occupied levels (v=1) can be easily handled to avoid in a very clean way the indeterminacies that appear in this case$^{(*)}$
- Empty levels (v=0) can also be handled reducing computational burden even more$^{(*)}$

See G.F. Bertsch's talk for generalizations

$^{(*)}$ L.M.Robledo, Phys Rev C84, 014307 (2011)

Mapping to simpler models

The idea

Use effective interactions valid in the whole Nuclide Chart to compute the nuclear mean field and use it to obtain parameters of simpler models like the Pairing+Quadrupole or exactly soluble pairing models.

We have implemented this idea[(*)] to map to the hyperbolic pairing model of the Richardson family of exactly integrable models. The two parameters of the model are fitted to reproduce the single particle pairing gaps Δ_i obtained with mean field calculations.

[(*)] *Exactly solvable pairing Hamiltonian for heavy nuclei*, J. Dukelsky, S. Lerma, L.M. Robledo, R. Rodriguez-Guzman, S.M.A. Rombouts

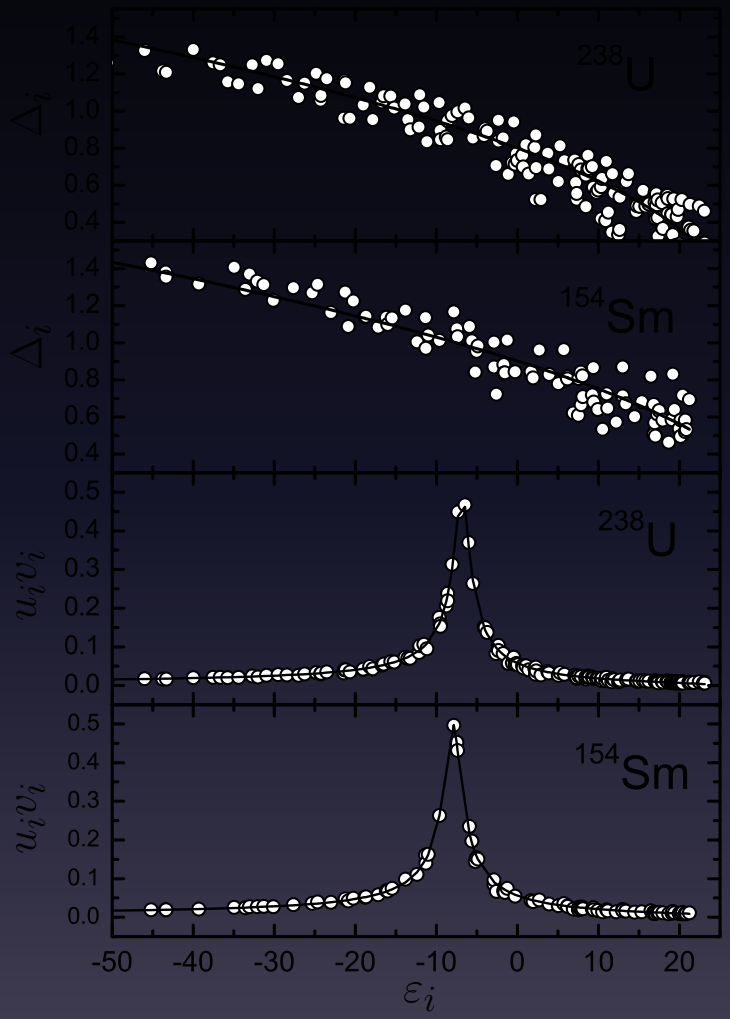
Equivalent to the $p_x + ip_y$ model

$$\begin{aligned} H &= \sum_i \varepsilon_i \left(c_i^\dagger c_i + c_{\bar{i}}^\dagger c_{\bar{i}} \right) \\ &\quad -2G \sum_{ii'} \sqrt{(\alpha - \varepsilon_i)(\alpha - \varepsilon_{i'})}\, c_i^\dagger c_{\bar{i}}^\dagger c_{\bar{i}'} c_{i'}, \end{aligned} \tag{1}$$

exact energies E_β obtained by solving

$$\sum_i \frac{s_i}{\eta_i - E_\beta} - \sum_{\beta'(\neq\beta)} \frac{1}{E_{\beta'} - E_\beta} = \frac{Q}{E_\beta}, \tag{2}$$

Parameters G and α fitted to reproduce Δ_i for each nucleus



1. Encouraging results
2. Selfconsistency
3. Nuclear table evaluation of pairing correlation energies

Conclusions

There is still a lot of work to do before having a consistent framework for symmetry restoration and configuration mixing in the nuclear EDF ...

I you want to contribute

Let the (dark side of the) force be with you ...