Pfaffians in nuclear structure theory

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Unraveling the complexity of nuclear systems. ECT* Trento

Outline

- Motivation for beyond-mean-field theories
  Mean field (HFB) not enought in many situations
  Collective and single particle degrees of freedom
  Symmetry restoration

- Overlaps (Onishi formula) and operator overlaps (GWT) between HFB mean field w.f.
  Sign problem
  Combinatorial explosion
  Different bases

- Solution to some of the problems:
  pfaffians in Nuclear Structure

Mean field in nuclear structure

- The atomic nucleus is made of fermions (protons and neutrons)
- Short range correlation favor the formation of nuclear Cooper pair
- Mean field theory is Hartree- Fock- Bogoliubov (HFB), a generalization of HF + BCS

Quasiparticles

$$\beta_\mu^+ = \sum_k U_{k\mu} c_k^+ + V_{k\mu} c_k$$

U, V are HFB amplitudes

HFB wave function

$|\phi\rangle$ is the vacuum of β_μ and therefore $|\phi\rangle = \prod_\mu \beta_\mu|\rangle$

Beyond mean-field

Going beyond the Hartree- Fock- Bogoliubov (HFB) mean field theory is the only microscopic way to unify ”collective” and ”single particle” models of nuclear structure

Procedure

- Generate sets of wave functions according to ”relevant” collective or single particle variables and do configuration mixing
  1. Constraints on relevant degrees of freedom: Quadrupole, Octupole, etc or Pairing
  2. Multi-quasiparticle excitations
- Restore broken symmetries (spontaneous or deliberated)

Gives access to excited states and improves gs description

Modern EDFs (Skyrme, Gogny, Relativistic) have reached reasonable accuracy on bulk properties over the Mass Table

Goal: Implement beyond mean field with modern EDFs

Configuration mixing

Generator coordinate method (GCM) wave function

$$|\Psi\rangle = \int dQ\, f(Q)|\phi(Q)\rangle + \sum_{ij} \int dQ\, f_{ij}(Q)\, \beta_i^+ \beta_j^+ |\phi(Q)\rangle \ldots$$

Amplitudes f, f_{ij}, etc from variational principle

Overlaps required

- $\langle\phi|\phi'\rangle$
- $\langle\phi|\hat{O}|\phi'\rangle$
- $\langle\phi|\beta_1 \ldots \beta_r \bar{\beta}_1^+ \ldots \bar{\beta}_s^+|\phi'\rangle$
- $\langle\phi|\beta_1 \ldots \beta_r \hat{O} \bar{\beta}_1^+ \ldots \bar{\beta}_s^+|\phi'\rangle$

$|\phi\rangle$ and $|\phi'\rangle$ are HFB wave functions

Symmetry breaking

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

PNP as an example

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

- $\langle\Phi|e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$
- $\langle\Phi|\hat{O}e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$
- $\langle\Phi|\beta_1\ldots\beta_r\bar{\beta}_1^+\ldots\bar{\beta}_s^+\,e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$
- $\langle\Phi|\beta_1\ldots\beta_r\hat{O}\bar{\beta}_1^+\ldots\bar{\beta}_s^+\,e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$

$e^{-i\varphi(\hat{N}-N)}|\Phi\rangle$ is a HFB wave function (Thouless theorem)

Tools: Onishi formula and GWT

Onishi formula

$$\langle \phi | \phi' \rangle = \pm \sqrt{\det(U^+ U' + V^+ V')}$$

sign undefined !

Operator and multiquasiparticle overlaps use the Generalized Wick Theorem (Balian and Brezin, Hara, Gaudin, ...)

$$\frac{\langle \phi | \beta_1 \ldots \beta_r \bar{\beta}_1^+ \bar{\beta}_s^+ | \phi' \rangle}{\langle \phi | \phi' \rangle} = \sum \mathrm{Contractions}$$

Contractions

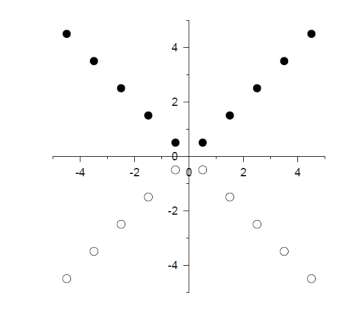
$$\frac{\langle \phi | \beta_\mu \beta_\nu | \phi' \rangle}{\langle \phi | \phi' \rangle} \qquad \frac{\langle \phi | \bar{\beta}_\sigma^+ \bar{\beta}_\tau^+ | \phi' \rangle}{\langle \phi | \phi' \rangle} \qquad \frac{\langle \phi | \beta_\mu \bar{\beta}_\tau^+ | \phi' \rangle}{\langle \phi | \phi' \rangle}$$

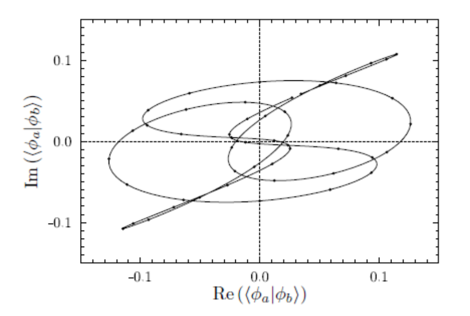
Combinatorial explosion: $(r+s-1)!!$ terms in the sum

Sign of HFB overlaps

The sign of $\langle\phi|\phi'\rangle$ is undefined (square root)

Overlaps computed on a mesh of discrete points and used in sums (relative sign is important).





Not a minor problem: 10^{8-10} overlaps required in typical calculations for a single nucleus. Large variety of nuclei (spherical, deformed, paired, ...). Therefore, a robust determination of the sign of the overlaps is required.

RHS figure from B. Avez and M. Bender, PRC 85, 034325 (2012)

Dealing with the sign

$$\langle\phi|\phi'\rangle = \pm\sqrt{\det(U^+U' + V^+V')} = \pm\sqrt{\det(U^+U')\det(1 + M^+N)}$$

- Time reversal helps (Kramers degeneracy, the matrix in the first determinant has a block structure with two identical blocks)
- 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 $\mathrm{T}r[\hat{D}]$ (finite temperature).
- Continuity requires a lot of "intelligence" when the overlap is close to zero and/or there are may collective variables.

A new formula to evaluate the overlap has been proposed [1]

The formula relies on the powerful concept of Fermion Coherent States $|\mathbf{z}\rangle$ parametrized in terms of the anti-conmuting elements z_k and z_k^* of a Grassmann algebra and defined by the conditions (eigenvalue problem)

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

and

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

The coherent states satisfy a closure relation

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

[1] *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 is carried out by introducing the closure relation

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

and using the properties of $|\mathbf{z}\rangle$

$$e^{\frac{1}{2}\sum_{kk'} M^{(0)\,*}_{kk'} a_{k'} a_k}|\mathbf{z}\rangle = e^{\frac{1}{2}\sum_{kk'} M^{(0)\,*}_{kk'} z_{k'} z_k}|\mathbf{z}\rangle$$

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

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

Pfaffian

$\mathrm{pf}A$ 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 $R = \begin{pmatrix} 0 & r_{12} & r_{13} & r_{14} \\ -r_{12} & 0 & r_{23} & r_{24} \\ -r_{13} & -r_{23} & 0 & r_{34} \\ -r_{14} & -r_{24} & -r_{34} & 0 \end{pmatrix}$
  $\mathrm{pf}(R) = r_{12}r_{34} - r_{13}r_{24} + r_{14}r_{23}$
- $\mathrm{pf}(T^t RT) = \det(T)\mathrm{pf}(R)$
- Minor-like expansion formula
- $\mathrm{pf}(R) = \sqrt{\det(R)}$

Numerical evaluation

- Straightforward using Householder (orthogonal) transformations to bring the matrix in tridiagonal form

$$\mathrm{pf}\begin{pmatrix} 0 & r_{12} & 0 & 0 \\ -r_{12} & 0 & r_{23} & 0 \\ 0 & -r_{23} & 0 & r_{34} \\ 0 & 0 & -r_{34} & 0 \end{pmatrix} = r_{12}r_{34}$$

- Aitken's block diagonalization formula can be used

$$\begin{pmatrix} \mathbb{I} & 0 \\ Q^T R^{-1} & \mathbb{I} \end{pmatrix}\begin{pmatrix} R & Q \\ -Q^T & S \end{pmatrix}\begin{pmatrix} \mathbb{I} & -R^{-1}Q \\ 0 & \mathbb{I} \end{pmatrix} = \begin{pmatrix} R & 0 \\ 0 & S + Q^T R^{-1} Q \end{pmatrix} \quad (1)$$

- FORTRAN, Mathematica and Python routines available at CPC Software Library (CPC 182, 2213)

The advantages of the present approach are

- Calculation of eigenvalues (Neergard) avoided
- Can be extended to the evaluation of traces of density matrix operators (finite temperature).
- Performing algorithms for the numerical evaluation of the Pfaffian exist.
- Fully occupied levels (v=1) can be easily handled to avoid in a very clean way the indeterminacy that appear in this case[(*)]
- Empty levels (v=0) can also be handled reducing computational burden even more[(*)]

[(*)] L.M.Robledo, Phys Rev C84, 014307 (2011)

Another derivation

Note that

$$\langle|\beta_1\beta_2\bar{\beta}_3\bar{\beta}_4|\rangle = r_{12}r_{34} - r_{13}r_{24} + r_{14}r_{23}$$

where r_{ij} are the contractions

$$\mathrm{pf}\begin{pmatrix} 0 & r_{12} & r_{13} & r_{14} \\ -r_{12} & 0 & r_{23} & r_{24} \\ -r_{13} & -r_{23} & 0 & r_{34} \\ -r_{14} & -r_{24} & -r_{34} & 0 \end{pmatrix} = r_{12}r_{34} - r_{13}r_{24} + r_{14}r_{23}$$

from here

$$\langle|\beta_1 \ldots \beta_P \bar{\beta}_1 \ldots \bar{\beta}_Q|\rangle = \mathrm{pf}(S_{ij})$$

where S_{ij} is the skew symmetric $(P+Q) \times (P+Q)$ matrix such that S_{ij} $i < j$ are the possible contractions

$$\langle|\beta_k\beta_l|\rangle \quad \langle|\beta_k\bar{\beta}_r|\rangle \quad \langle|\bar{\beta}_r\bar{\beta}_s|\rangle$$

$$\langle\tilde{\phi}|\tilde{\phi}'\rangle = \langle|\beta_{2n}\ldots\beta_1\beta'^+_1\ldots\beta'^+_{2n}|\rangle = (-1)^n \mathrm{pf} S$$

Contractions

$$\langle|\beta_\mu\beta_\nu|\rangle = V^T U \quad \langle|\beta_\mu\beta'^+_\nu|\rangle = V^T V'^* \quad \langle|\beta'^+_\mu\beta'^+_\nu|\rangle = U'^+ V'^*$$

$$\langle\tilde{\phi}|\tilde{\phi}'\rangle = (-1)^n \mathrm{pf}\left[\begin{array}{cc} V^T U & V^T V'^* \\ -V'^\dagger V & U'^\dagger V'^* \end{array}\right]$$

If R is a symmetry operator

$$\langle\tilde{\phi}|\mathcal{R}|\tilde{\phi}'\rangle = (-1)^n \mathrm{pf}\left[\begin{array}{cc} V^T U & V^T R^T V'^* \\ -V'^\dagger R V & U'^\dagger V'^* \end{array}\right]$$

R is the matrix of matrix elements of $\mathcal{R}$

G.F. Bertsch and L.M. Robledo, PRL 108, 042505 (2012)

Most general multi-quasiparticle overlap

$$\langle\phi|\bar{\beta}_{\mu_r}\cdots\bar{\beta}_{\mu_1}\mathcal{R}\bar{\beta}'^{\dagger}_{\nu_1}\cdots\bar{\beta}'^{\dagger}_{\nu_s}|\phi'\rangle = (-1)^n(-1)^{r(r-1)/2}\frac{\det C^* \det C'}{\prod_\alpha^n v^*_\alpha v'_\alpha}$$

$$\times \mathrm{pf}\begin{bmatrix} V^T U & V^T \mathbf{p}^\dagger & V^T R^T \mathbf{q}'^T & V^T R^T V'^* \\ -\mathbf{p}^* V & \mathbf{q}^* \mathbf{p}^\dagger & \mathbf{q}^* R^T \mathbf{q}'^T & \mathbf{q}^* R^T V'^* \\ -\mathbf{q}' R V & -\mathbf{q}' R \mathbf{q}^\dagger & \mathbf{p}' \mathbf{q}'^T & \mathbf{p}' V'^* \\ -V'^\dagger R V & -V'^\dagger R \mathbf{q}^\dagger & -V'^\dagger \mathbf{p}'^T & U'^\dagger V'^* \end{bmatrix}.$$

$p_{\mu_j m} = \bar{V}_{m\mu_j}$ (dimension $r \times 2n$)
$q_{\mu_j m} = \bar{U}_{m\mu_j}$ (dimension $s \times 2n$)

Valid for ”blocked HFB states” (odd-A nuclei)
Avoids combinatorial explosion !
$\langle\phi|\beta_1\beta_2\beta_3\hat{H}\beta'^\dagger_4\beta'^\dagger_5\beta'^\dagger_6|\phi'\rangle$ is the energy of 1p-1h excitations in odd-A nuclei. It involves $9!! = 945$ terms

Different bases

Very often the quasiparticle operators of $|\phi\rangle$ and $|\phi'\rangle$ are defined in terms of different single particle bases that do not span the same Hilbert subspace

- Translated
- Rotated
- Different oscillator lengths (for instance in fission)

Previous formulas assume equal bases

Solution: Simply take $\mathcal{R}$ as the operator transforming one basis into another (non unitary in general). R in the above formulas becomes the matrix of the overlap between the two basis.

Beware of the non orthgonaliy of R !

Applications to other fields

Symmetry restoration is becoming popular

- Condensed matter physics (Yannouleas and Landman)
- Quantum chemistry (Scuseria)
  1. Particle number
  2. Spin
  3. Translational invariance

Quantities given in terms of ρ and κ

$$\langle \phi | \mathcal{R} | \phi' \rangle = (-1)^n \prod_{\alpha}^{n} v_\alpha v'_\alpha \det D^* \det D' \mathrm{pf} \begin{bmatrix} -\rho^{-1}\kappa & R^T \\ -R & \rho'^{*\,-1}\kappa'^{*} \end{bmatrix}$$

Conclusions and perspectives

Technical problems arising in the evaluation of HFB overlaps are solved easily using expressions based on pfaffians

- Sign of the overlap
- Combinatorial explosion
- Different expressions for even-even and odd-A
- Different bases

Perspectives

- Implementation of results in a computational code for symmetry restoration
- Pfaffian formulas and Gaudin's theorem (GWT at finite temperature).

Johann Friedrich Pfaff (sometimes spelled Friederich; born Stuttgart, 22 December 1765, died Halle, 21 April 1825) was a German mathematician. He was described as one of Germany’s most eminent mathematicians during the 19th century. He studied integral calculus, and is noted for his work on partial differential equations of the first order (Pfaffian systems as they are now called) which became part of the theory of differential forms; and as Carl Friedrich Gauss’s formal research supervisor.

Two announcements:

- ECT* workshop on the theoretical description of odd-mass nuclei to be held from the 25th to the 29th of September 2017
- Nuclear structure conference in Madrid in December 2017