Pfaffians in nuclear structure theory

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Stockholm, September, 2014

Computational Challenges in Nuclear and Many-Body Physics

Outline

- Computational challenges in beyond-mean-field theories (nuclear physics)
  Configuration mixing
  (Collective variables, multiquasiparticles)
  Symmetry restoration
  (Angular momentum, isospin, particle number)
- Traditional approaches: Overlaps (Onishi formula) and operator overlaps (GWT) between HFB mean field w.f.
  Sign problem
  Combinatorial explosion
  Combining different bases
- Solution:
  pfaffians in Nuclear Structure based on fermionic coherent state techniques

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

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

U, V are HFB amplitudes

HFB wave function $|\phi\rangle$

$|\phi\rangle$ is the vacuum of β_μ ($\beta_\mu|\phi\rangle = 0$) 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 Quadrupole, Octupole, particle number fluctuations, etc
  2. Multi-quasiparticle excitations $\beta^+_\mu \beta^+_\nu |\phi\rangle$, $\beta^+_\mu \beta^+_\nu \beta^+_\rho \beta^+_\sigma |\phi\rangle$
- Restore broken symmetries (spontaneously or deliberatedly broken)

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

- $\langle\phi|\phi'\rangle$ ($\langle\phi(Q)|\phi(Q')\rangle$ or $\langle\phi(Q)|\hat{R}|\phi(Q')\rangle$, $\hat{R}$ symmetry op)
- $\langle\phi|\hat{O}|\phi'\rangle$ ($\hat{O}$ is a N-body generic operator)
- $\langle\phi|\beta_1\ldots\beta_r\bar{\beta}_1^+\ldots\bar{\beta}_s^+|\phi'\rangle$
- $\langle\phi|\beta_1\ldots\beta_r\hat{O}\bar{\beta}_1^+\ldots\bar{\beta}_s^+|\phi'\rangle$

$|\phi\rangle$ 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, ...)

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

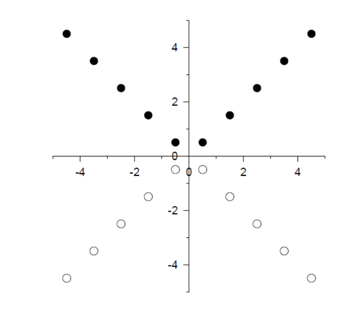
Contractions

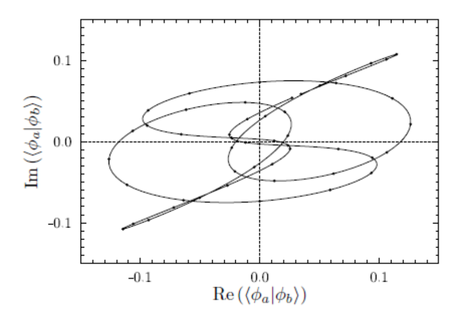
$$\frac{\langle\phi|\beta_\mu\beta_\nu|\phi'\rangle}{\langle\phi|\phi'\rangle} \qquad \frac{\langle\phi|\bar{\beta}_\sigma^+\bar{\beta}_\tau^+|\phi'\rangle}{\langle\phi|\phi'\rangle} \qquad \frac{\langle\phi|\beta_\mu\bar{\beta}_\tau^+|\phi'\rangle}{\langle\phi|\phi'\rangle}$$

Combinatorial explosion:
$(r+s-1)$!! terms in the sum (11)!!=10395

Sign of HFB overlaps

The sign of $\langle\phi|\phi'\rangle$ is undefined (square root) when computed with the Onishi formula. This is a problem as overlaps are used in sums





Of the order of 10^{8-10} overlaps required in typical calculations for a single nucleus. Large variety of nuclei (spherical, deformed, ...) call for a robust determination of the sign.

RHS figure from B. Avez and M. Bender, Phys. Rev. C 85, 034325

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 symmetry helps (Kramers degeneracy, matrices have a block structure with two identical blocks)
- Neergard's method: M^+N has double degenerate eigenvalues c_i. Then $\langle\phi|\phi'\rangle = \prod_i(1 + c_i)$ where the product runs over half the eigenvalues
- Continuity argument: $\langle\phi(q))|\phi(q' + \Delta q)\rangle$ from $\langle\phi(q))|\phi(q')\rangle$ and $\langle\phi(q)|\phi(q)\rangle = 1$

Difficulties

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

Recently a new formula to evaluate the overlap has been obtained [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 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

$$1 = \int d\mu(\mathbf{z})|\mathbf{z}\rangle\langle\mathbf{z}| \quad \text{with} \quad \mu(\mathbf{z}) = \exp(-\mathbf{z}^*\mathbf{z})$$

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

HFB wave functions are parametrized with Thouless theorem

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

in terms of the skew-symmetric $M^{(i)} = (V_i U_i^{-1})^*$. The evaluation of the overlap involves 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

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

This 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 to 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 (2011))

The advantages of the present approach are

- Calculation of eigenvalues avoided
- Can be extended to the evaluation of traces of density matrix operators (finite temperature)†.
- Performant 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 **C79**, 021302(R) (2009)
(*) L.M. Robledo, Phys Rev **C84**, 014307 (2011)

Multi-quasiparticle overlaps

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

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

The overlap between un-normalized wave functions

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

With the contractions

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

$$\langle\tilde{\phi}|\tilde{\phi}'\rangle = (-1)^n \mathrm{pf} \begin{bmatrix} V^T U & V^T V'^* \\ -V'^\dagger V & U'^\dagger V'^* \end{bmatrix}$$

If $\mathcal{R}$ is a symmetry operator

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

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

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

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

$p_{\mu_j m} = \bar{V}_{m\mu_j}$, $p'_{\nu_j m} = \bar{V}'_{m\nu_j}$

$q_{\mu_j m} = \bar{U}_{m\mu_j}$, $q'_{\nu_j m} = \bar{U}'_{m\nu_j}$

p, q dimension $r \times 2n$, p', q' dimension $a \times 2n$

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 (finite) bases

Very often the quasiparticle operators of $|\phi\rangle$ and $|\phi'\rangle$ are defined in terms of different single particle (finite) bases $c^+_{(0)i}$ and $c^+_{(1)j}$ that do not span the same Hilbert subspace, i.e. $c^+_{(0)i}$ can not be writen in terms of the $c^+_{(1)j}$.

- Translated localized bases (eg HO)

  $\exp[-(x-x_0)^2] = \exp[-x^2]\exp[2x]\exp[-x_0^2]$ and $\exp[2x]$ is not a polynomial.

- Rotated bases (eg deformed HO)
- Different oscillator lengths

Previous formulas assume implicitly equal bases

Solution(*): Given the two basis $c^+_{(0)i}$ and $c^+_{(1)j}$ define the non orthogonal extended basis $A^+_\mu = \{c^+_{(0)i}, c^+_{(1)j}\}$ of dimension $N_{(0)} + N_{(1)}$.

Orthogonalize this basis to get B^+_μ.

Express quasiparticle operators in terms of this basis with appropriate Bogoliubov amplitudes.

A little algebra yields

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

where T is the (rectangular) overlap matrix $\{c^+_{(0)i}, c^+_{(1)j}\}$

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

Connection with GWT

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

equals (up to a phase) to

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

Aitken's formula: If

$$A = \begin{pmatrix} T & Q \\ -Q^T & S \end{pmatrix} \qquad \mathrm{pf}(A) = \mathrm{pf}(T)\mathrm{pf}(S + Q^T T^{-1} Q)$$

Note that $\mathrm{pf}(T) \approx \langle \phi | \phi' \rangle$ and therefore the whole set of contractions is in $\mathrm{pf}(S + Q^T T^{-1} Q)$. Work in progress !

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

- Connection between the pfaffian formula and GWT and analysis of the structure of T^{-1}
- 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.