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A convenient implementation of the overlap between arbitrary HFB vacua for projection

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第十五届核结构会议（广西，桂林）

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1, Motivation

- Full CI (SM)

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

Observables can be extracted from $|\Psi\rangle$

Problem: Exact solutions for a many-body system are very hard to be obtained.

Mean field method (HFB)

- Hartree-Fock-Bogoliubov (HFB)transformation

$$\begin{pmatrix} \hat{\beta} \\ \hat{\beta}^{+} \end{pmatrix} = \begin{pmatrix} U^{+} & V^{+} \\ V^{T} & U^{T} \end{pmatrix} \begin{pmatrix} \hat{c} \\ \hat{c}^{+} \end{pmatrix}$$

- HFB vacuum

$$\left|\Phi\right\rangle = \hat{\beta}_1 \hat{\beta}_2 \cdots \hat{\beta}_M \left|-\right\rangle$$

- For any i

$$\hat{\beta}_i \left|\Phi\right\rangle = 0$$

Comments on HFB

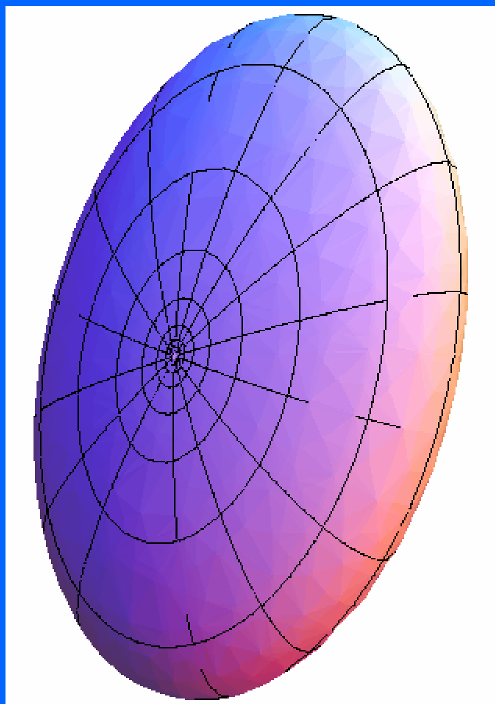
Good points:

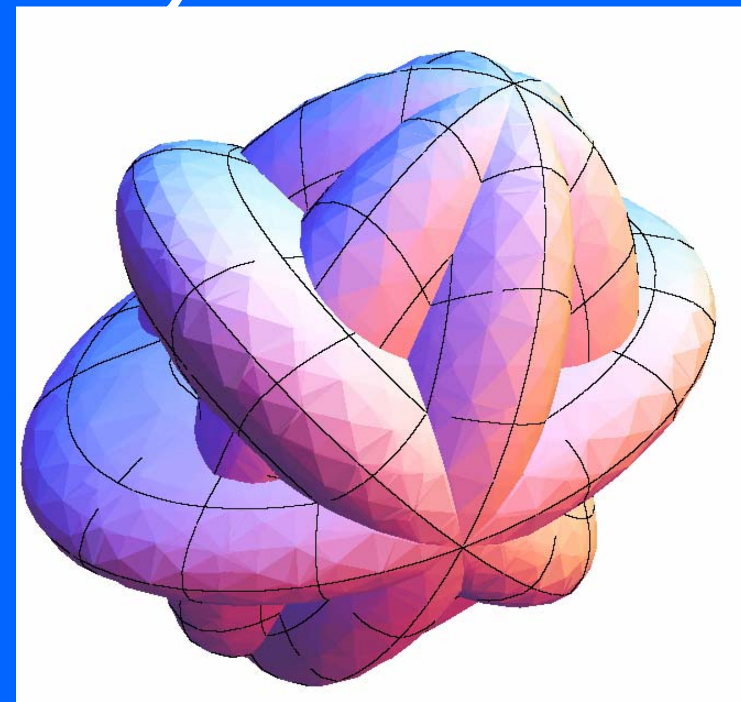
- Simplest way of studying the many-body quantum system.
- Plays central role in understanding the interacting many-body quantum system, and widely used in many fields of physics.

Bad points:

- Symmetries are broken.
- No collective correlation.

Angular momentum Projectoin





$|\Phi\rangle$

$$\hat{P}^{I}_{MK}|\Phi\rangle = \frac{2I+1}{8\pi^2}\int d\Omega D^{I}_{MK}(\Omega)\hat{R}(\Omega)|\Phi\rangle$$

A intrinsic state

projected states differed by

$K = -I, -I+1, \ldots I$

$$\left|\Phi\right\rangle = \sum_{IK} C_{IK} \left|IK\right\rangle$$

$$\begin{aligned}
P^{I_0}_{MK_0}\left|\Phi\right\rangle &= \sum_{IK} C_{IK} P^{I_0}_{MK_0}\left|IK\right\rangle \\
&= \sum_{IK} C_{IK} \frac{2I+1}{8\pi^2}\int d\Omega D^{I_0}_{MK_0}(\Omega)\hat{R}(\Omega)\left|IK\right\rangle \\
&= \sum_{IK} C_{IK} \frac{2I+1}{8\pi^2}\int d\Omega D^{I_0}_{MK_0}(\Omega)\sum_{K'} D^{I}_{K'K}(\Omega)\left|IK'\right\rangle \\
&= \sum_{IK} C_{IK} \sum_{K'} \frac{2I+1}{8\pi^2}\int d\Omega D^{I_0}_{MK_0}(\Omega) D^{I*}_{K'K}(\Omega)\left|IK'\right\rangle \\
&= \sum_{IK} C_{IK} \sum_{K'} \delta_{I_0 I}\delta_{MK'}\delta_{K_0 K}\left|IK'\right\rangle \\
&= C_{I_0 K_0}\left|I_0 M\right\rangle
\end{aligned}$$

Parity projection

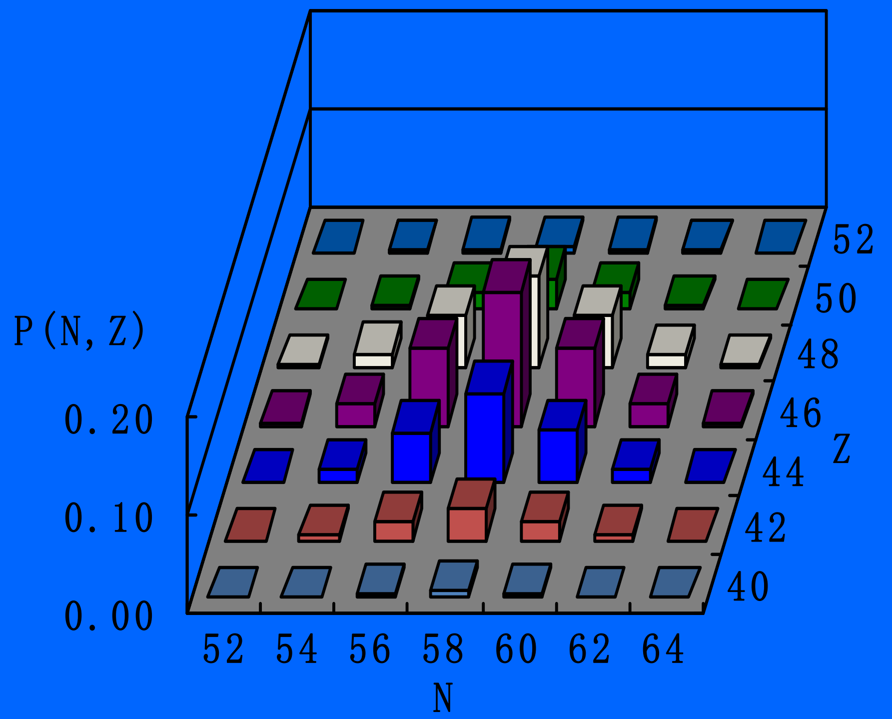
Parity projection operator：

$$P^{\pi} = \frac{1+\pi\hat{P}}{2}, \pi = \pm 1$$

$$\hat{P} P^{\pi} \left| \Phi \right\rangle = \pi P^{\pi} \left| \Phi \right\rangle$$

Particle number projection

$$\hat{P}^N = \frac{1}{2\pi}\int_0^{2\pi} d\phi e^{i(\langle N\rangle - \hat{N})\phi}$$



$$P(N,Z) = \langle \Phi | \hat{P}^N \hat{P}^Z | \Phi \rangle$$

Beyond mean-field methods

- Trial wavefunction for a many-body quantum system:

$$\left|\Psi_{IM}^{NZ\pi}\right\rangle = \sum_{K\kappa} f_{K\kappa}^{I} P_{MK}^{I} P^{\pi} P^{N} P^{Z} \left|\kappa\right\rangle$$

Projected basis

In GCM, the index κ includes the deformation.

- The Hill-Wheeler(HW) equation:

$$\sum_{K'\kappa'} f_{K'\kappa'}^{I} \left\langle \kappa \right| (\hat{H} - E) P_{KK'}^{I} P^{\pi} P^{N} P^{Z} \left| \kappa' \right\rangle = 0$$

Basic matrix elements in the HW euqation

$$\sum_{K'\kappa'} f^{I}_{K'\kappa'} \langle \kappa | (H-E) P^{I}_{KK'} P^{\pi} P^{N} P^{Z} | \kappa' \rangle = 0$$

$$\hat{O} = 1 \text{ or } \hat{H}$$

$$\hat{\mathfrak{R}} = \hat{R}(\Omega) e^{-i\phi_N \hat{N}} e^{-i\phi_Z \hat{Z}}$$

$$\text{or} \quad \hat{P}\hat{R}(\Omega) e^{-i\phi_N \hat{N}} e^{-i\phi_Z \hat{Z}}$$

Basic blocks:

$$\langle \kappa | \hat{O} \hat{\mathfrak{R}} | \kappa' \rangle$$

$$\langle \Phi | \hat{\beta}_{i_1} \hat{\beta}_{i_2} \cdots \hat{\beta}_{i_L} \hat{O} \hat{\mathfrak{R}} \hat{\beta}'^{+}_{j_{L+1}} \hat{\beta}'^{+}_{j_{L+2}} \cdots \hat{\beta}'^{+}_{j_{2n}} | \Phi' \rangle$$

The most fundamental quantity

$$\langle \Phi | \hat{\Re} | \Phi' \rangle = \langle \Phi^a | \Phi^b \rangle$$

- Onishi Formula (Sign is not determined.)

N.Onishi,S.Yoshida,*Nucl.Phys.*80(1966)367.

- Solving the sign problem

K.Neergård,E.Wüst,Nucl.Phys.A402(1983)311.
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F.Dönau,Phys.Rev.C58(1998)872.
M.Bender,Paul-HenriHeenen,Phys.Rev.C78(2008)024309.
K.Hara,A.Hayashi,P.Ring,Nucl.Phys.A385(1982)14.
M.Oi,N.Tajima,Phys.Lett.B606(2005)43.

Pfaffian

$$(1,2,\cdots,2n) \xrightarrow{\text{Perm}} (i_1,i_2,\cdots,i_{2n})$$

$$\mathrm{pf}(R) = \frac{1}{2^n}\frac{1}{n!}\sum_{\text{Perm}} \epsilon(\mathrm{P}) r_{i_1 i_2} r_{i_3 i_4}\cdots r_{i_{2n-1} i_{2n}}$$

$$\mathrm{pf}\begin{bmatrix} 0 & r_{12} \\ -r_{12} & 0 \end{bmatrix} = r_{12}$$

$$\det[r_{11}] = r_{11}$$

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

$$= r_{12}r_{34} - r_{13}r_{24} + r_{14}r_{23}$$

$$\det\begin{bmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{bmatrix}$$

$$= r_{11}r_{22} - r_{12}r_{21}$$

Robledo's formula

[Phys.Rev.C79(2009)021302(R)]

$$\left\langle \Phi^a \middle| \Phi^b \right\rangle = (-1)^{N(N+1)} \mathrm{pf}(M)$$

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

$$M = \begin{pmatrix} M^b & -I \\ I & M^{a*} \end{pmatrix} = \begin{pmatrix} (V^b U^{b-1})^* & -I \\ I & V^b U^{a-1} \end{pmatrix}$$

Technical aspects of the evaluation of the overlap of Hartree- Fock- Bogoliubov wave functions

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

- Two extreme cases:

(1)Full occupied orbits

(2)Full emptied orbits

- Using different reference vacuum instead of the true vacuum

Another formula by Bertsch and Robledo

Phys.Rev.Lett.108(2012)042505.

$$|\Phi\rangle = \frac{1}{n}\hat{\beta}_1\hat{\beta}_2\cdots\hat{\beta}_M|-\rangle$$

$$n = \prod_{i=1}^{M/2} v_i$$

$$\langle\Phi|\hat{\Re}|\Phi'\rangle = \frac{(-1)^{M/2}}{nn'}\mathrm{pf}(\mathbf{M})$$

$$\mathbf{M} = \begin{pmatrix} V^T U & V^T D V'^* \\ -V'^+ D^T V & U'^+ V'^* \end{pmatrix}$$

$$D_{ij} = \langle i|\hat{\Re}|j\rangle$$

The Bloch–Messiah theorem

One has to carefully treat the singularity of the U V matrix caused by the full ocuppied or full emptied levels.

$$U = D\bar{U}C$$

$$V = D^*\bar{V}C$$

$$\begin{pmatrix} u_i & 0 \\ 0 & u_i \end{pmatrix} \qquad \begin{pmatrix} 0 & v_i \\ -v_i & 0 \end{pmatrix}$$

P. Ring, P.Schuck,
The Nuclear Many-Body Problem

Singularity of U,V matrices

$$u_i^2 + v_i^2 = 1$$

$u_i = 0, v_i = 1$ Fully Occupied, no U^{-1}

$u_i = 1, v_i = 0$ Fully empty, no V^{-1}

$u_i = 10^{-8}, v_i = 1$ Fully Occupied, but U^{-1} exists

$u_i = 1, v_i = 10^{-8}$ Fully Empty, but V^{-1} exists

Our new formula

Gao/Hu/Chen
Physics Letters B 732 (2014) 360–363

$$\left|\Phi\right\rangle = \frac{1}{n}\hat{\beta}_1\hat{\beta}_2\cdots\hat{\beta}_M\left|-\right\rangle$$

$$\left\langle\Phi\middle|\hat{\mathfrak{R}}\middle|\Phi'\right\rangle = (-1)^{M/2} S n n' \operatorname{pf}(\mathbf{W})$$

$$S = \det D^{*}\det D'\det C\det C'^{*}$$

Extremely tiny

$$\mathbf{W} = \begin{pmatrix} [U'V'^{-1}]^{+} & -D^{T} \\ D & UV^{-1} \end{pmatrix}$$

$$n = \prod_{i=1}^{M/2} v_i$$

A testing example

Deformed BCS vacuum for ^{226}Th

Standard Nilsson parameters,(kappa,mu)

Quadrupole deformation ε_2=0.2

N_N=4-8. i.e., 290 s.p.states,96 active neutrons

N_Z=3-7. i.e., 220 s.p. states,70 active protons

$$n_N^2 = \prod_{i=1}^{M/2} v_{N,i}^2 = (10^{-16})^{\frac{290-96}{2}} = 10^{-1552}$$

$$n_Z^2 = \prod_{i=1}^{M/2} v_{Z,i}^2 = (10^{-16})^{\frac{220-70}{2}} = 10^{-1200}$$

$$x = y \times (10^{-200})^k$$

Numerical test

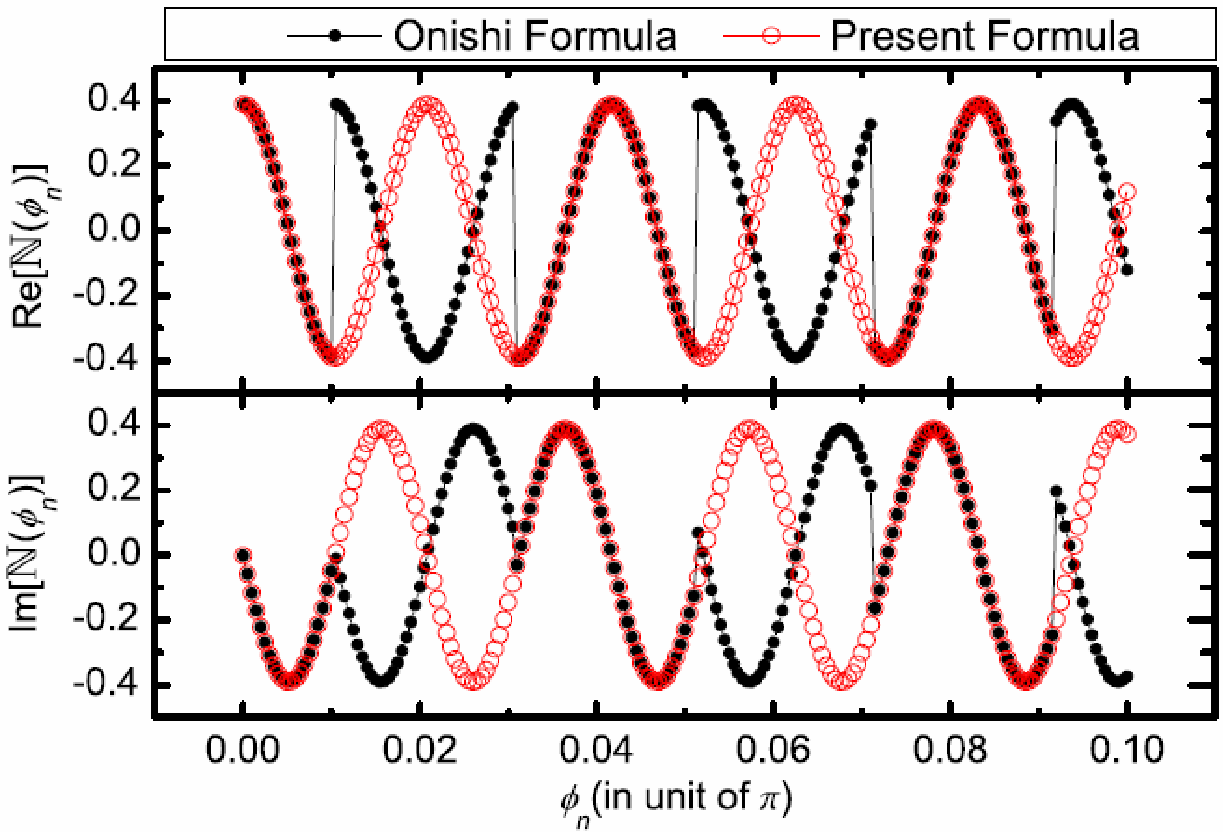

Fig. 1. (Color online.) Overlaps of the ground state neutron slater determinant for ^{226}Th as functions of ϕ_n with Euler angles $\alpha = \gamma = 0°$, $\beta = 10°$, calculated with present formula [Eq. (18)] and the Onishi formula [Eq. (24) with '+' sign]. $\mathrm{Re}[\mathbb{N}(\phi_n)]$ and $\mathrm{Im}[\mathbb{N}(\phi_n)]$ are the real and imaginary parts of the overlap.

$$R = \left| \frac{\mathbb{N}_{\mathrm{Onishi}}(\phi_n)}{\mathbb{N}_{\mathrm{pf}}(\phi_n)} - 1 \right|.$$

$<10^{-13}$

Summary

1, Change $u_i\ v_i=0$ to $u_i\ v_i=10^{-8}$ to avoid the singularity of U,V.

2, Present a new overlap formula between arbitrary HFB vacuum states.

3, Numerical test has been made for the reliability of our formula.

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Thank you!