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Matrix elements of physical operators in the beyond mean field calculations

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Contents

1, Motivation

- Full CI (SM)

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

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

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:

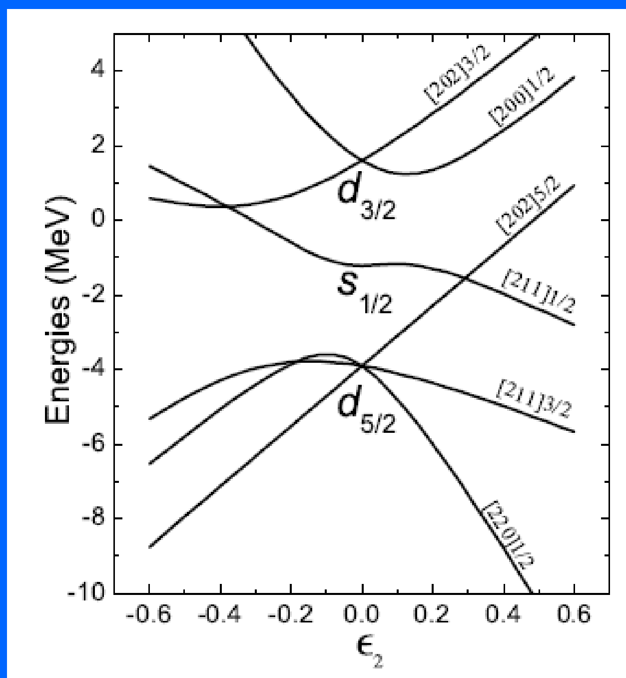
- Simplest way of studying the many-body quantum system.
- Plays central role in understanding the interacting many-body quantum system, and widely used in many fields of physics.

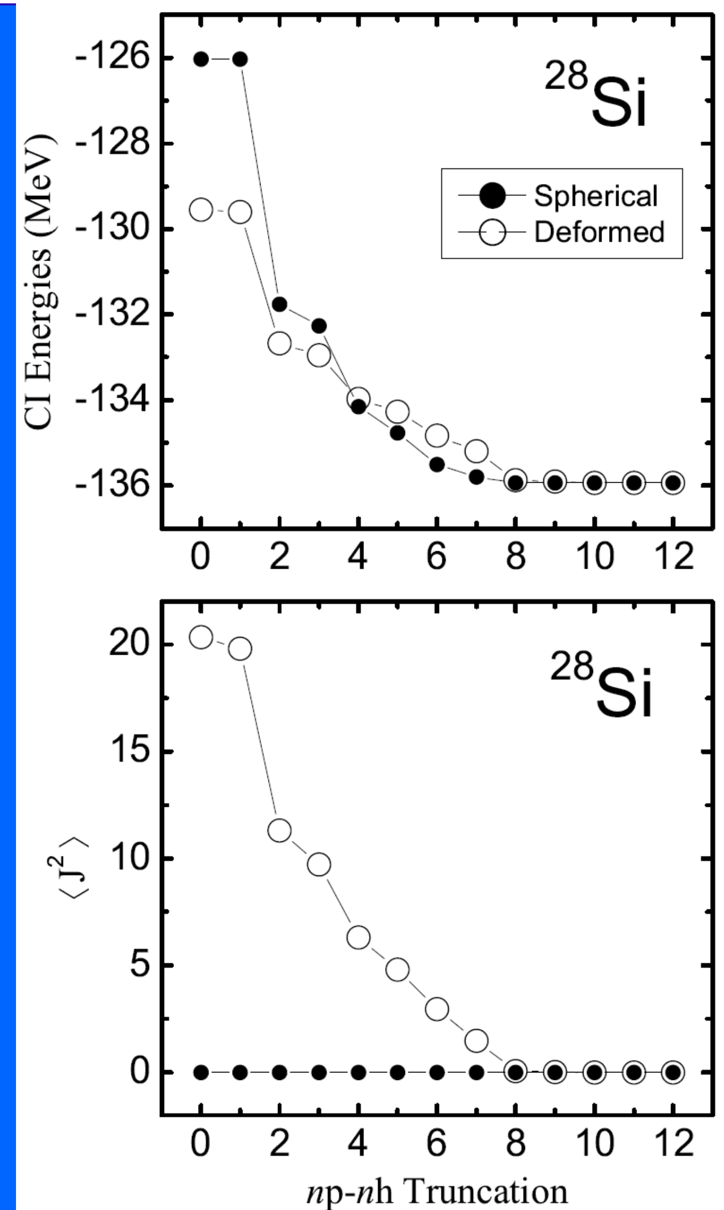
Bad points:

- Symmetries are broken.
- No collective correlation

Configuration Interaction

Spherical basis vs.
deformed basis
with USD interaction





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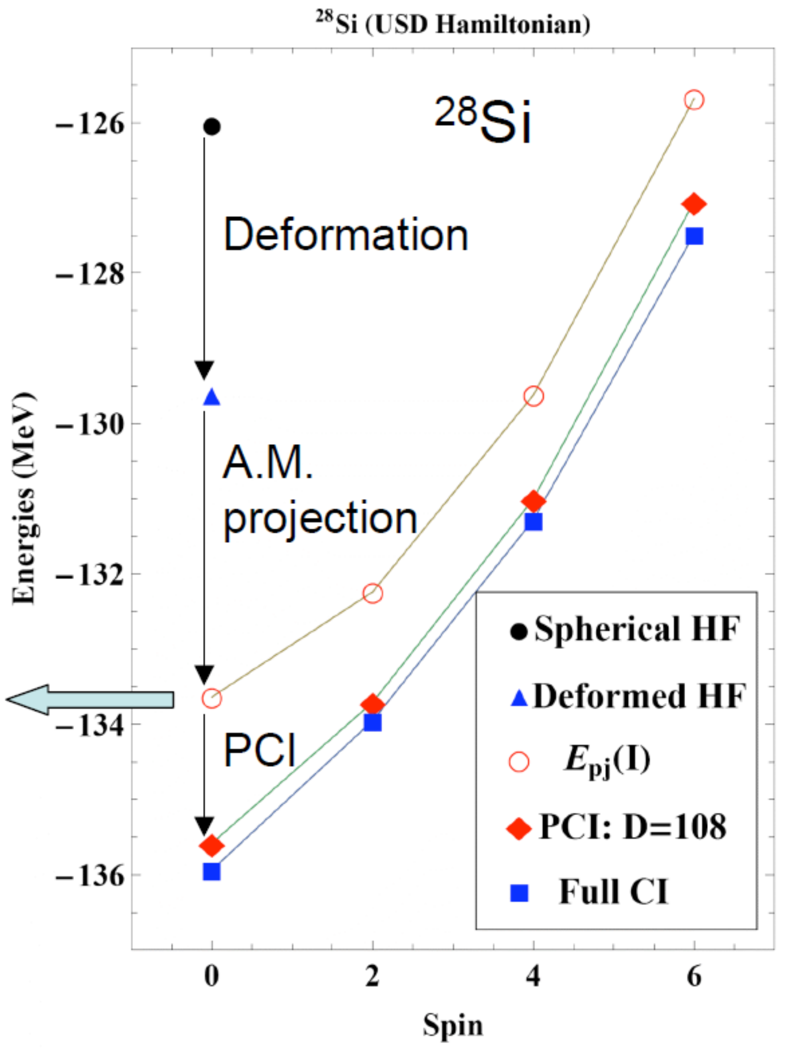
Projected Configuration Interaction(PCI)

Conclusions:

- The projected Energies $E_{pj}(I)$ of a single SD can not reproduce the full CI energies.
- PCI Energies (including np-nh configuration) are very close to the full CI energies.

$$E_{pj}(I) = \frac{\langle \kappa | H P^I_{00} | \kappa \rangle}{\langle \kappa | P^I_{00} | \kappa \rangle}$$



Shell Model dimension:93710

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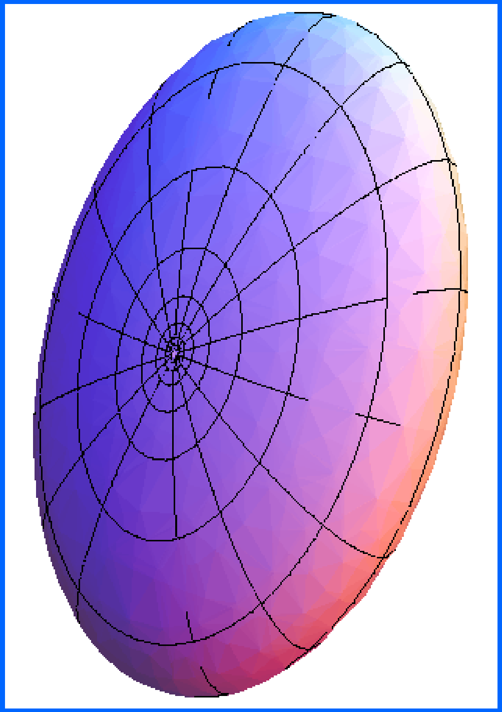
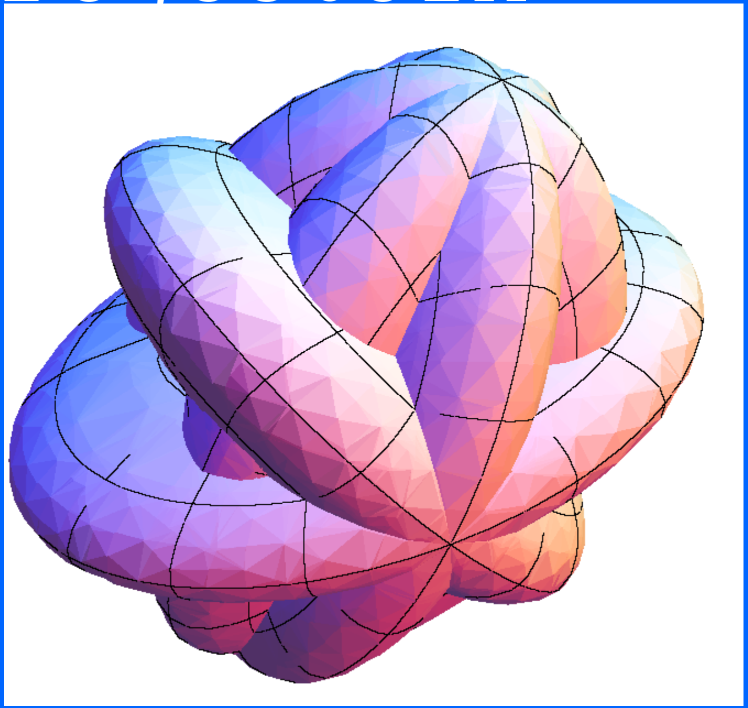
Angular momentum Projectoin



$|\Phi\rangle$

A intrinsic state



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

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

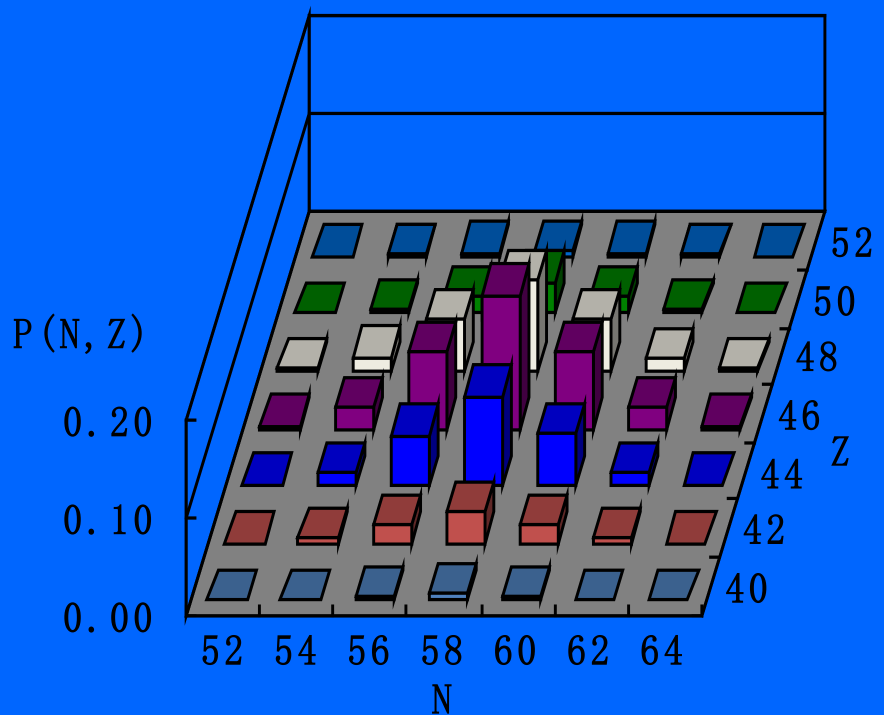
Parity projection operator:

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

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

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

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

Basic blocks:

$$\langle \kappa | \hat{O} \hat{\Re} | \kappa' \rangle$$

$$\boxed{\begin{aligned} &\hat{O} = 1 \text{ or } \hat{H} \\ &\hat{\Re} = \hat{R}(\Omega) e^{-i\phi_N \hat{N}} e^{-i\phi_Z \hat{Z}} \\ &\text{or} \quad \hat{P}\hat{R}(\Omega) e^{-i\phi_N \hat{N}} e^{-i\phi_Z \hat{Z}} \end{aligned}}$$

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

More General form of Matrix Element

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

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

$$\langle \Phi^{a} | \hat{z}_1 \hat{z}_2 \cdots \hat{z}_L \hat{O} \hat{z}_{L+1} \hat{z}_{L+2} \cdots \hat{z}_{2n} | \Phi^{b} \rangle$$

$$\boxed{\hat{z}_i = \sum_j (A^a_{ij} \hat{\beta}^a_j + B^a_{ij} \hat{\beta}^{a+}_j) = \sum_j (A^b_{ij} \hat{\beta}^b_j + B^b_{ij} \hat{\beta}^{b+}_j)}$$

$$\text{For } \hat{O} = 1, \quad I_0 = \left\langle \Phi^a \left| \hat{z}_1 \hat{z}_2 \cdots\cdots \hat{z}_{2n} \right| \Phi^b \right\rangle$$

$$\text{For } \hat{O} = \hat{T} = \sum_{ij=1}^{M} T_{ij} \hat{c}_i^+ \hat{c}_j,$$

$$I_1 = \sum_{ij=1}^{M} T_{ij} \left\langle \Phi^a \left| \hat{z}_1 \hat{z}_2 \cdots \hat{z}_L \hat{c}_i^+ c_j \hat{z}_{L+1} \cdots \hat{z}_{2n} \right| \Phi^b \right\rangle$$

Our Motivation

$$\text{For } \hat{O} = \hat{V} = \sum_{ij=1}^{M} V_{ijkl} \hat{c}_i^+ \hat{c}_j^+ \hat{c}_l \hat{c}_k ,$$

$$I_2 = \sum_{ijkl=1}^{M} V_{ijkl} \left\langle \Phi^a \middle| \hat{z}_1 \hat{z}_2 \cdots \hat{z}_L \hat{c}_i^+ \hat{c}_j^+ \hat{c}_l \hat{c}_k \hat{z}_{L+1} \cdots \hat{z}_{2n} \middle| \Phi^b \right\rangle$$

I_2 needs to be evaluated quickly! But unfortunately:

1, e.g. M =100, then there will be 10^8 terms summing up to obtain only one single I_2 matrix element.

2, Moreover, I_2 is the kernel of the multi-dimensional integration when projection is performed.

Overlaps

$$I_0 = \left\langle \Phi^a \middle| \hat{z}_1 \hat{z}_2 \cdots\cdots \hat{z}_{2n} \middle| \Phi^b \right\rangle$$

The generalized Wick's Theorem

[1] R. Balian, E. Brezin, Nuovo Cimento B 64 (1969) 37.

$$\left\langle \hat{z}_1 \hat{z}_2 \hat{z}_3 \hat{z}_4 \right\rangle = \left\langle \hat{z}_1 \hat{z}_2 \right\rangle \left\langle \hat{z}_3 \hat{z}_4 \right\rangle - \left\langle \hat{z}_1 \hat{z}_3 \right\rangle \left\langle \hat{z}_2 \hat{z}_4 \right\rangle + \left\langle \hat{z}_1 \hat{z}_4 \right\rangle \left\langle \hat{z}_2 \hat{z}_3 \right\rangle$$

(2n-1)!! terms

Pfaffian:

[2]M. Oi, T. Mizusaki, Phys. Lett. B 707 (2012) 305.
[3]T. Mizusaki, M. Oi, Phys. Lett. B 715 (2012) 219.
[4]B. Avez, M. Bender, Phys. Rev. C 85 (2012) 034325.
[5]G.F. Bertsch, L.M. Robledo, Phys. Rev. Lett. 108 (2012) 042505.
[6]T. Mizusaki, M. Oi, Fang-Qi Chen, Yang Sun, Phys. Lett. B 725 (2013) 175.

Pfaffian

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

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

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

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

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

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

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

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

Overlaps

$$\left\langle - \middle| \hat{z}_1 \hat{z}_2 \cdots\cdots \hat{z}_{2n} \middle| - \right\rangle = \mathrm{pf}(S)$$

$$S_{ij} = \begin{cases} \left\langle - \middle| \hat{z}_i \hat{z}_j \middle| - \right\rangle & i < j \\ -S_{ji} & i > j \end{cases}$$

[Taken from G.F. Bertsch, L.M. Robledo, Phys. Rev. Lett. 108 (2012) 042505]

The above formula can be generalizes as:

$$I_0 = \left\langle \Phi^a \middle| \hat{z}_1 \hat{z}_2 \cdots\cdots \hat{z}_{2n} \middle| \Phi^b \right\rangle = \left\langle \Phi^a \middle| \Phi^b \right\rangle \mathrm{pf}(\mathrm{S})$$

Hu, Gao , Chen. Physics Letters B 734 (2014) 162

$$\mathrm{S}_{ij} = \begin{cases} \dfrac{\left\langle \Phi^a \middle| \hat{z}_i \hat{z}_j \middle| \Phi^b \right\rangle}{\left\langle \Phi^a \middle| \Phi^b \right\rangle} & i < j \\ -\mathrm{S}_{ji} & i > j \end{cases}$$

$$\left\langle \Phi^a \middle| \Phi^b \right\rangle \neq 0$$

Pfaffian	**~(2n)^3**
GWT	~(2n-1)!!

Explicit forms of $s_{ij}(i<j)$

$$\hat{z}_i = \sum_j (A^a_{ij}\hat{\beta}^a_j + B^a_{ij}\hat{\beta}^{a+}_j)$$

$$= \sum_j (A^b_{ij}\hat{\beta}^b_j + B^b_{ij}\hat{\beta}^{b+}_j)$$

$$\begin{pmatrix} \hat{\beta}^b \\ \hat{\beta}^{b+} \end{pmatrix} = \begin{pmatrix} \mathrm{X} & \mathrm{Y} \\ \mathrm{Y}* & \mathrm{X}* \end{pmatrix} \begin{pmatrix} \hat{\beta}^a \\ \hat{\beta}^{a+} \end{pmatrix}$$

$$\hat{\beta}^b = \mathrm{X}\hat{\beta}^a + \mathrm{Y}\hat{\beta}^{a+}$$

$$\hat{\beta}^a = \mathrm{X}^{-1}\hat{\beta}^b - \mathrm{X}^{-1}\mathrm{Y}\hat{\beta}^{a+}$$

$$\begin{pmatrix} A^a & B^a \end{pmatrix} = \begin{pmatrix} A^b & B^b \end{pmatrix} \begin{pmatrix} \mathrm{X} & \mathrm{Y} \\ \mathrm{Y}* & \mathrm{X}* \end{pmatrix}$$

$$\left\langle \Phi^a \middle| \hat{z}_i \hat{z}_j \middle| \Phi^b \right\rangle$$

$$= \sum_{i_1 j_1} A^a_{ii_1} B^b_{jj_1} \left\langle \Phi^a \middle| \hat{\beta}^a_{i_1} \hat{\beta}^{b+}_{j_1} \middle| \Phi^b \right\rangle$$

$$= \sum_{i_1 i_2 j_1} A^a_{ii_1} \mathrm{X}^{-1}_{i_1 i_2} B^b_{jj_1} \left\langle \Phi^a \middle| \hat{\beta}^b_{i_2} \hat{\beta}^{b+}_{j_1} \middle| \Phi^b \right\rangle$$

$$= \sum_{i_1 i_2 j_1} A^a_{ii_1} \mathrm{X}^{-1}_{i_1 i_2} B^b_{jj_1} \delta_{i_2 j_1} \left\langle \Phi^a \middle| \Phi^b \right\rangle$$

$$= [A^a \mathrm{X}^{-1} B^{bT}]_{ij} \left\langle \Phi^a \middle| \Phi^b \right\rangle$$

$$\boxed{\mathrm{S}_{ij} = \frac{\left\langle \Phi^a \middle| z_i z_j \middle| \Phi^b \right\rangle}{\left\langle \Phi^a \middle| \Phi^b \right\rangle} = \begin{cases} [A^a B^{aT} + A^a \mathrm{X}^{-1} \mathrm{Y} A^{aT}]_{ij} \\ [A^a \mathrm{X}^{-1} B^{bT}]_{ij} \\ [A^b B^{bT} + B^b \mathrm{Y}* \mathrm{X}^{-1} B^{bT}]_{ij} \end{cases}}$$

The case of $\left|\Phi^b\right\rangle = \hat{\Re}\left|\Phi^a\right\rangle = \hat{\Re}\left|\Phi\right\rangle$

$$\mathrm{S}_{ij} = \begin{cases} \dfrac{\langle\Phi|\hat{\beta}_i\hat{\beta}_j\hat{\Re}|\Phi\rangle}{\langle\Phi|\hat{\Re}|\Phi\rangle} = [\mathrm{X}^{-1}\mathrm{Y}]_{ij} \equiv B_{ij} \\ \dfrac{\langle\Phi|\hat{\beta}_i\hat{\Re}\hat{\beta}_j^{+}|\Phi\rangle}{\langle\Phi|\hat{\Re}|\Phi\rangle} = [\mathrm{X}^{-1}]_{ij} \equiv C_{ij} \\ \dfrac{\langle\Phi|\hat{\Re}\hat{\beta}_i^{+}\hat{\beta}_j^{+}|\Phi\rangle}{\langle\Phi|\hat{\Re}|\Phi\rangle} = [\mathrm{Y}^{*}\mathrm{X}^{-1}]_{ij} \equiv A_{ij} \end{cases}$$

$$\begin{pmatrix} \hat{\beta}^{b} \\ \hat{\beta}^{b+} \end{pmatrix} = \hat{\Re}\begin{pmatrix} \hat{\beta}^{a} \\ \hat{\beta}^{a+} \end{pmatrix}\hat{\Re}^{-1}$$

$$= \begin{pmatrix} \mathrm{X} & \mathrm{Y} \\ \mathrm{Y}^{*} & \mathrm{X}^{*} \end{pmatrix}\begin{pmatrix} \hat{\beta}^{a} \\ \hat{\beta}^{a+} \end{pmatrix}$$

$$\langle\Phi|\hat{\beta}_{i_1}\hat{\beta}_{i_2}\cdots\hat{\beta}_{i_n}\hat{\Re}\hat{\beta}_{j_1}^{+}\hat{\beta}_{j_2}^{+}\cdots\hat{\beta}_{j_{n'}}^{+}|\Phi\rangle = \langle\Phi|\hat{\Re}|\Phi\rangle\,\mathrm{pf}\begin{pmatrix} \mathrm{B} & \mathrm{C} \\ -C^{T} & A \end{pmatrix}$$

[T. Mizusaki, M. Oi, Fang-Qi Chen, Yang Sun, Phys. Lett. B 725 (2013) 175.]

Matrix elements of operators

$$I_0 = \left\langle \Phi^a \middle| \hat{z}_1 \hat{z}_2 \cdots\cdots \hat{z}_{2n} \middle| \Phi^b \right\rangle = \left\langle \Phi^a \middle| \Phi^b \right\rangle \mathrm{pf}(S)$$

$$I_1 = \sum_{ij} T_{ij} \left\langle \Phi^a \middle| \hat{z}_1 \hat{z}_2 \cdots \hat{z}_L \hat{c}_i^+ c_j \hat{z}_{L+1} \cdots \hat{z}_{2n} \middle| \Phi^b \right\rangle$$

$$I_2 = \sum_{ijkl} V_{ijkl} \left\langle \Phi^a \middle| \hat{z}_1 \hat{z}_2 \cdots \hat{z}_L \hat{c}_i^+ \hat{c}_j^+ \hat{c}_l \hat{c}_k \hat{z}_{L+1} \cdots \hat{z}_{2n} \middle| \Phi^b \right\rangle$$

$$X\{i,j\}, X\{i,j,l,k\}, X\{i_1,i_2,\cdots,i_{2n}\}$$

$$X\{i,j\}=X\{j,i\}=\begin{array}{cc} & \begin{array}{ccccc} & i & & j & \end{array} \\ \begin{array}{c} \\ i \\ \\ j \\ \\ \end{array} & \begin{bmatrix} & \vdots & & \vdots & \\ \cdots & \cdot & \cdots & \cdot & \cdots \\ & \vdots & & \vdots & \\ \cdots & \cdot & \cdots & \cdot & \cdots \\ & \vdots & & \vdots & \end{bmatrix} \end{array}, (i<j)$$

$$\alpha_{ij}=\begin{cases} 1 & i<j \\ -1 & i>j \end{cases}$$

$$\alpha_{ijlk}=\alpha_{ij}\alpha_{il}\alpha_{ik}\alpha_{jl}\alpha_{jk}\alpha_{lk}$$

Pfaffian version of Laplace expansion

Journal of Combinatorial Theory, Series A **88**, 136–157 (1999)

Pfaffian expansion with respect to the i_0-th row

$$\mathrm{pf}(X) = \sum_{i=1, i\neq i_0}^{m} (-1)^{i_0+i-1} \alpha_{i_0,i} X_{i_0 i} \mathrm{pf}(X\{i_0, i\})$$

Pfaffian expansion with respect to the i_0-th and j_0-th rows

$(j_0 = i_0 + 1)$

$$\begin{aligned} \mathrm{pf}(X) &= X_{i_0 j_0} \mathrm{pf}(X\{i_0, j_0\}) \\ &+ \sum_{i,j} (-1)^{i+j} \alpha_{ij} X_{i_0 i} X_{j_0 j} \mathrm{pf}(X\{i_0, j_0, i, j\}) \end{aligned}$$

Pfaffian version of Laplace expansion

Pfaffian expansion with respect to i_0-th, j_0-th, k_0-th and l_0-th rows

$j_0 = i_0 + 1,\ k_0 = j_0 + 1,\ l_0 = k_0 + 1$

$$
\begin{aligned}
\mathrm{pf}(X) &= Y_{i_0 j_0 k_0 l_0}\,\mathrm{pf}(X\{i_0, j_0, k_0, l_0\}) \\
&+ \sum_{i,j} (-1)^{i+j} \alpha_{ij} Z^{ij}_{i_0 j_0 k_0 l_0}\,\mathrm{pf}(X\{i_0, j_0, k_0, l_0, i, j\}) \\
&+ \sum_{i,j,k,l} \{(-1)^{i+j+k+l} \alpha_{ijkl} W^{ijkl}_{i_0 j_0 k_0 l_0} \\
&\qquad \times \mathrm{pf}(X\{i_0, j_0, k_0, l_0, i, j, k, l\})\}
\end{aligned}
$$

$$
Y_{i_0 j_0 k_0 l_0} = X_{i_0 j_0} X_{k_0 l_0} - X_{i_0 k_0} X_{j_0 l_0} + X_{i_0 l_0} X_{j_0 k_0}
$$

$$
\begin{aligned}
Z^{ij}_{i_0 j_0 k_0 l_0} &= X_{i_0 j_0} X_{k_0 i} X_{l_0 j} - X_{i_0 k_0} X_{j_0 i} X_{l_0 j} \\
&+ X_{i_0 l_0} X_{j_0 i} X_{k_0 j} + X_{j_0 k_0} X_{i_0 i} X_{l_0 j} \\
&- X_{j_0 l_0} X_{i_0 i} X_{k_0 j} + X_{k_0 l_0} X_{i_0 i} X_{j_0 j}
\end{aligned}
$$

$$
W^{ijkl}_{i_0 j_0 k_0 l_0} = X_{i_0 i} X_{j_0 j} X_{k_0 k} X_{l_0 l}
$$

Pfaffian version of Lewis Carroll formula

M. Ishikawa, M. Wakayama, Adv. Stud. Pure Math. 28 (2000) 133.

T. Mizusaki, M. Oi, Phys. Lett. B 715 (2012) 219

$$\mathrm{pf}(X\{i,j\}) = \alpha_{ij}(-1)^{i+j} X_{ij}^{-1}\mathrm{pf}(X)$$

$$\begin{aligned}\mathrm{pf}(X\{i,j,k,l\}) \quad &= \quad (-1)^{i+j+k+l}\alpha_{ijkl}\mathrm{pf}(X) \times \\ &\quad\ (X_{ij}^{-1}X_{kl}^{-1} - X_{ik}^{-1}X_{jl}^{-1} + X_{il}^{-1}X_{jk}^{-1})\end{aligned}$$

Basic quantities for

$$T_0 = \sum_{\mu\nu}^{N} T_{\mu\nu}\mathbb{C}^{(0)}_{\mu\nu}$$

$$\mathbb{T}_{ij} = \sum_{\mu\nu}^{N} T_{\mu\nu}\mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(-)}_{\nu j}$$

$$\mathbb{S}^{(+)}_{\mu k} = \begin{cases} -\frac{\langle\Phi^a|\hat{z}_k\hat{c}^\dagger_\mu|\Phi^b\rangle}{\langle\Phi^a|\Phi^b\rangle}, & 1 \le k \le L \\ \frac{\langle\Phi^a|\hat{c}^\dagger_\mu\hat{z}_k|\Phi^b\rangle}{\langle\Phi^a|\Phi^b\rangle}, & L+1 \le k \le 2n \end{cases}$$

$$\mathbb{S}^{(-)}_{\mu k} = \begin{cases} -\frac{\langle\Phi^a|\hat{z}_k\hat{c}_\mu|\Phi^b\rangle}{\langle\Phi^a|\Phi^b\rangle}, & 1 \le k \le L \\ \frac{\langle\Phi^a|\hat{c}_\mu\hat{z}_k|\Phi^b\rangle}{\langle\Phi^a|\Phi^b\rangle}, & L+1 \le k \le 2n \end{cases}$$

$$\mathbb{C}^{(+)}_{\mu\nu} = \frac{\langle\Phi^a|\hat{c}^\dagger_\mu\hat{c}^\dagger_\nu|\Phi^b\rangle}{\langle\Phi^a|\Phi^b\rangle},$$

$$\mathbb{C}^{(0)}_{\mu\nu} = \frac{\langle\Phi^a|\hat{c}^\dagger_\mu\hat{c}_\nu|\Phi^b\rangle}{\langle\Phi^a|\Phi^b\rangle},$$

$$\mathbb{C}^{(-)}_{\mu\nu} = \frac{\langle\Phi^a|\hat{c}_\mu\hat{c}_\nu|\Phi^b\rangle}{\langle\Phi^a|\Phi^b\rangle}.$$

$$V_0 = \frac{\langle\Phi^a|\hat{V}|\Phi^b\rangle}{\langle\Phi^a|\Phi^b\rangle} = \frac{1}{4}\sum_{\mu\nu\delta\gamma} V_{\mu\nu\gamma\delta}\mathbb{C}_{\mu\nu\delta\gamma}$$

$$\mathbb{V}^{(1)}_{ij} = \frac{1}{4}\sum_{\mu\nu\delta\gamma} V_{\mu\nu\gamma\delta}\mathbb{D}^{ij}_{\mu\nu\delta\gamma},$$

$$\mathbb{V}^{(2)}_{ijkl} = \frac{1}{4}\sum_{\mu\nu\delta\gamma} V_{\mu\nu\gamma\delta}\mathbb{E}^{ijkl}_{\mu\nu\delta\gamma},$$

$$\begin{aligned} \mathbb{C}_{\mu\nu\delta\gamma} &= \mathbb{C}^{(+)}_{\mu\nu}\mathbb{C}^{(-)}_{\delta\gamma} - \mathbb{C}^{(0)}_{\mu\delta}\mathbb{C}^{(0)}_{\nu\gamma} + \mathbb{C}^{(0)}_{\mu\gamma}\mathbb{C}^{(0)}_{\nu\delta}, \\ \mathbb{D}^{ij}_{\mu\nu\delta\gamma} &= \mathbb{C}^{(+)}_{\mu\nu}\mathbb{S}^{(-)}_{\delta i}\mathbb{S}^{(-)}_{\gamma j} - \mathbb{C}^{(0)}_{\mu\delta}\mathbb{S}^{(+)}_{\nu i}\mathbb{S}^{(-)}_{\gamma j} \\ &+ \mathbb{C}^{(0)}_{\mu\gamma}\mathbb{S}^{(+)}_{\nu i}\mathbb{S}^{(-)}_{\delta j} + \mathbb{C}^{(0)}_{\nu\delta}\mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(-)}_{\gamma j} \\ &- \mathbb{C}^{(0)}_{\nu\gamma}\mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(-)}_{\delta j} + \mathbb{C}^{(-)}_{\delta\gamma}\mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\nu j}, \\ \mathbb{E}^{ijkl}_{\mu\nu\delta\gamma} &= \mathbb{S}^{(+)}_{\mu i}\mathbb{S}^{(+)}_{\nu j}\mathbb{S}^{(-)}_{\delta k}\mathbb{S}^{(-)}_{\gamma l}. \end{aligned}$$

$$\mathsf{S}_{ij} = \begin{cases} \frac{\langle\Phi^a|\hat{z}_i\hat{z}_j|\Phi^b\rangle}{\langle\Phi^a|\Phi^b\rangle} & i < j \\ -\mathsf{S}_{ji} & i > j \end{cases}$$

Our compact formula for one-body operator

$$I_1 = \left[T_0 - \mathrm{Tr}\left(\mathbb{T}\mathbb{S}^{-1}\right)\right]\mathrm{pf}(\mathbb{S})\langle\Phi^a|\Phi^b\rangle,$$

$$T_0 = \sum_{\mu\nu}^{N} T_{\mu\nu}\mathbb{C}_{\mu\nu}^{(0)}$$

$$\mathbb{T}_{ij} = \sum_{\mu\nu}^{N} T_{\mu\nu}\mathbb{S}_{\mu i}^{(+)}\mathbb{S}_{\nu j}^{(-)}$$

$$I_1 = \sum_{ij=1}^{M} T_{ij}\left\langle \Phi^a \left| \hat{z}_1\hat{z}_2\cdots\hat{z}_L\hat{c}_i^{+}c_j\hat{z}_{L+1}\cdots\hat{z}_{2n}\right| \Phi^b \right\rangle$$

Our compact formula for two-body operator

$$I_2 = \langle \Phi^a | \Phi^b \rangle \, \mathrm{pf}(\mathbb{S}) \Bigg[V_0 - \mathrm{Tr}\left(\mathbb{V}^{(1)} \mathbb{S}^{-1}\right) + \sum_{i,j,k,l=1}^{2n} \mathbb{V}^{(2)}_{ijkl} \left(\mathbb{S}^{-1}_{ij} \mathbb{S}^{-1}_{kl} - \mathbb{S}^{-1}_{ik} \mathbb{S}^{-1}_{jl} + \mathbb{S}^{-1}_{il} \mathbb{S}^{-1}_{jk} \right) \Bigg].$$

$$V_0 = \frac{\langle \Phi^a | \hat{V} | \Phi^b \rangle}{\langle \Phi^a | \Phi^b \rangle} = \frac{1}{4} \sum_{\mu\nu\delta\gamma} V_{\mu\nu\gamma\delta} \mathbb{C}_{\mu\nu\delta\gamma}$$

$$\mathbb{V}^{(1)}_{ij} = \frac{1}{4} \sum_{\mu\nu\delta\gamma} V_{\mu\nu\gamma\delta} \mathbb{D}^{ij}_{\mu\nu\delta\gamma},$$

$$\mathbb{V}^{(2)}_{ijkl} = \frac{1}{4} \sum_{\mu\nu\delta\gamma} V_{\mu\nu\gamma\delta} \mathbb{E}^{ijkl}_{\mu\nu\delta\gamma},$$

$$I_2 = \sum_{ijkl=1}^{M} V_{ijkl} \left\langle \Phi^a \left| \hat{z}_1 \hat{z}_2 \cdots \hat{z}_L \hat{c}^+_i \hat{c}^+_j \hat{c}_l \hat{c}_k \hat{z}_{L+1} \cdots \hat{z}_{2n} \right| \Phi^b \right\rangle$$

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Computational time

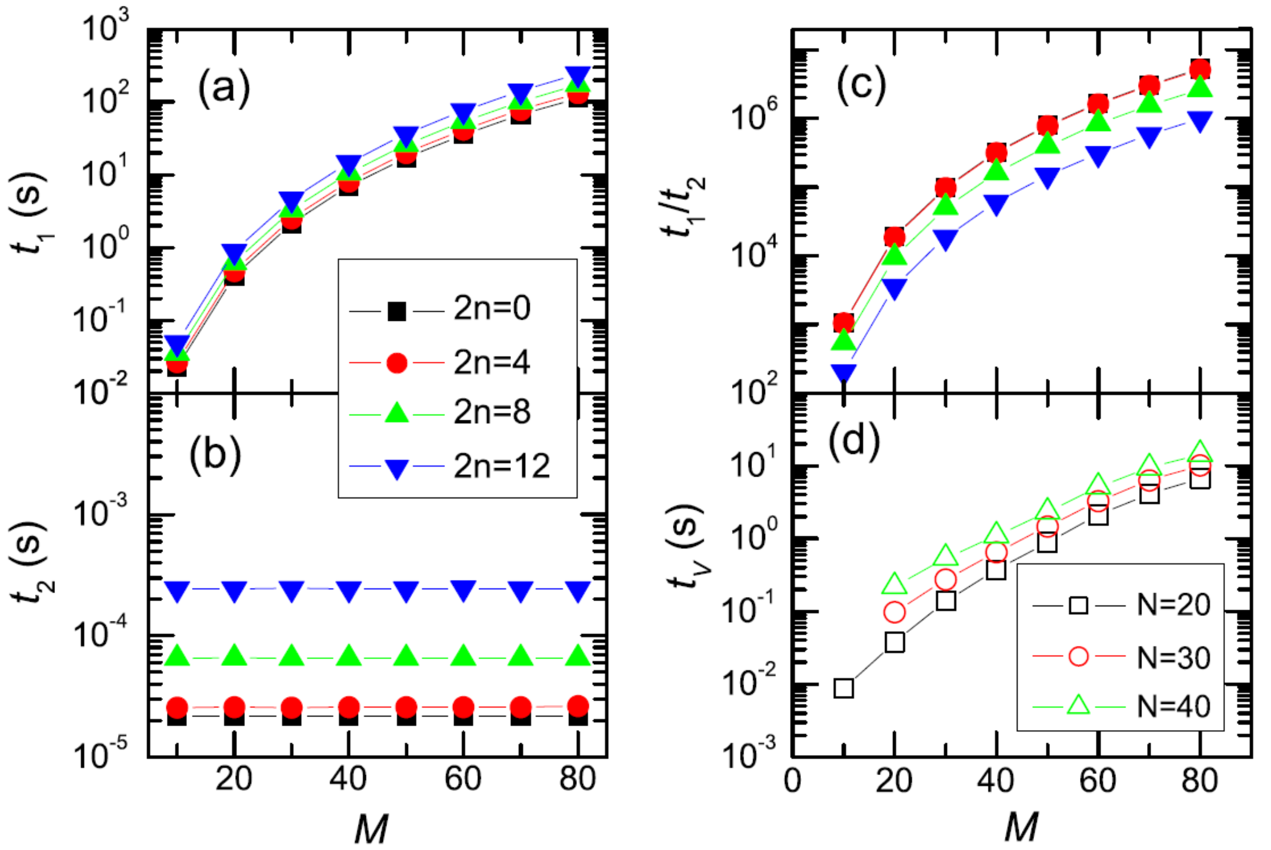

Fig. 1. (Color online.) (a) CPU time, t_1, for the conventional method, as a function of M and $2n$; (b) CPU time, t_2, for Eq. (31), as a function of M and $2n$; (c) Ratio of t_1 to t_2; (d) Total CPU time, t_V, for V_0, $\mathbb{V}^{(1)}$ and $\mathbb{V}^{(2)}$, N is the dimension of $\mathbb{V}^{(1)}$ and $\mathbb{V}^{(2)}$ with $1 \le i, j, k, l \le N$.

$$R = \frac{t_{old}}{t_{new}} = \frac{L^2 t_1}{t_V + L^2 t_2}$$

If L=100,M=80

$$R \approx 10^5$$

Forthcoming Challenge

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

$$\left\langle \kappa \middle| \hat{O} P^{I}_{KK'} P^{N} P^{Z} \middle| \kappa' \right\rangle$$
$$= \frac{2I+1}{32\pi^4} \int d\varphi_N \int d\varphi_Z \int d\Omega D(\Omega) e^{iN\varphi_N} e^{iN\varphi_Z} \left\langle \kappa \middle| \hat{O} \hat{\Re}(\Omega, \varphi_N, \varphi_Z) \middle| \kappa' \right\rangle$$

How to implement the five dimensional integration efficiently?

Conclusion

We present new formulae for the matrix elements of one-body and two-body physical operators, which are applicable to arbitrary Hartree–Fock–Bogoliubov wave functions, including those for multi-quasiparticle excitations.

The testing calculations show that our formulae may substantially reduce the computational time by several orders of magnitude when applied to many-body quantum system in a large Fock space.

For more details and the testing Fortran code see:
Hu, Gao , Chen, *Physics Letters B 734 (2014) 162*

Collabrators

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Thank you for your attention!