Variational Multiparticle-Multihole Configuration Mixing Method

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Plan

I. Introduction (1)

II. Formalism of the variational multiparticle-multihole (mp-mh) configuration mixing method

III. Three applications

Nucleus = A interacting nucleons

(2 ≤ A ≤ 270)

N-N interaction
(QCD not yet usable)

Many-body problem
Numerical solution of exact equations
A ≤ 12-14

Approximations

Bare forces
In medium forces
(Phenomenological)
I. Introduction

N-N potential and Independent Particle Model

• N-N potential

  “molecular potential” + spin-isospin dependence + …

  Nucleonic charge $g$: $g^2/hc \sim 12-14$
  Fine structure constant $\alpha = e^2/hc = 1/137$

• In nuclei

  ✓ Evidence for shell structure
    Magic numbers: 2, 8, 20, 28, 50, 82, 126

  ✓ Independent particle model works: existence of a mean field
Current theoretical nuclear approaches

Shell model
- Inert core + valence space
- Effective interaction between valence nucleons
- Conservation of symmetries
- All correlations taken into account between valence nucleons
  - Description of all excited states

Mean field theories
- No inert core (binding energies)
- Effective force between all nucleons
- Symmetry breaking
- Correlations incorporated step by step
  - Hartree-Fock (HF)
  - Pairing (BCS,HFB)
  - Collective excitations (RPA,GCM)

Variational mp-mh configuration mixing method:
- Attempt to unify the description of correlations beyond HF approximation
Variational mp-mh configuration mixing method

Theoretical point of view

• Gives a unified description of {Pairing + RPA + particle vibration} correlations on top of HF mean field theory
• Respects conservation of particle numbers and Pauli principle
• Treats on the same footing even-even nuclei, odd and odd-odd nuclei
• Can describe both ground states and excited states

Particular interesting physical cases

• K isomers
• Pairing correlations
• Light exotic nuclei
II. Variational mp-mh configuration mixing method

**Trial wave function**

Superposition of Slater Determinants (SD) corresponding to mp-mh excitations upon a given state of HF type

\[
|\Psi> = A_{\pi\nu}^{0p0h} |\Phi_{\pi\nu}>_{0p0h} + \sum_{\alpha\pi\alpha\nu} A_{\alpha\pi\alpha\nu}^{1p1h} |\Phi_{\alpha\pi\alpha\nu}>_{1p1h} + \sum_{\alpha\pi\alpha\nu} A_{\alpha\pi\alpha\nu}^{2p2h} |\Phi_{\alpha\pi\alpha\nu}>_{2p2h} + \ldots
\]

Variational parameters:

**Mixing coefficients**

**Single particle orbitals**
II. Variational mp-mh configuration mixing method

Variational principle

• Functional:

\[ \mathcal{F} = E - \lambda \langle \Psi | \Psi \rangle \]

\( E = \langle \Psi | \hat{H} | \Psi \rangle = \langle \Psi | \hat{K} + \hat{V} | \Psi \rangle \)

• Determination of mixing coefficients:

\[ \frac{\partial \mathcal{F}}{\partial A_{\alpha \pi \alpha \nu}^*} = 0 \]

• Determination of optimized single particle states:

\[ \frac{\partial \mathcal{F}}{\partial \varphi_i^*} = 0 \]
\[ \frac{\partial F}{\partial A^{*}_{\alpha \pi \alpha' \nu}} = 0 \]

\[ \frac{\partial F}{\partial \varphi_{i}^{T*}} = 0 \]

\[ \sum_{\alpha \pi} A_{\alpha \pi \alpha' \pi} (\langle \phi_{\alpha' \pi} | \hat{H}_{\pi}^{\pi} | \phi_{\alpha \pi} \rangle > + \sum_{mn} C_{\pi mn}^{\pi} \langle \phi_{\alpha' \pi} | a_{m}^{\pi} a_{n} | \phi_{\alpha \pi} \rangle >) + \]

\[ \sum_{\alpha' \pi \pi} A_{\alpha' \pi \pi \nu} (\langle \phi_{\pi' \nu} | \hat{H}_{\nu}^{\nu} | \phi_{\alpha' \pi} \rangle > + \sum_{mn} C_{\nu mn}^{\nu} \langle \phi_{\pi' \nu} | a_{m}^{\nu} a_{n} | \phi_{\alpha' \pi} \rangle >) + \]

\[ \sum_{\alpha \pi \pi \nu} A_{\alpha \pi \nu} < \phi_{\alpha' \pi} \phi_{\alpha' \nu} | \hat{V}^{\pi \nu} | \phi_{\alpha \pi} \phi_{\alpha \nu} > = \lambda A_{\alpha' \pi \alpha' \nu} \]

→ self-consistent procedure
→ Renormalization of the HF field

• In the present work: \([h[\rho] \rho] = 0\)
II. Variational mp-mh configuration mixing method

Residual interaction

- **Pairing**

\[
\begin{aligned}
&\langle p_2 \bar{p}_2 | V | p_1 \bar{p}_1 \rangle \\
&\langle h_2 \bar{h}_2 | V | h_1 \bar{h}_1 \rangle \\
&\langle p \bar{p} | V | h \bar{h} \rangle \\
&\langle h \bar{h} | V | p \bar{p} \rangle
\end{aligned}
\]

- **RPA**

\[
\begin{aligned}
&\langle p_1 h_2 | V | h_1 p_2 \rangle \\
&\langle p_1 p_2 | V | h_1 h_2 \rangle \\
&\langle h_1 h_2 | V | p_1 p_2 \rangle
\end{aligned}
\]
II. Variational mp-mh configuration mixing method

- Particle vibration coupling

\[ \langle p_3 p_1 | V | h_1 p_2 \rangle \]
\[ \langle h_2 h_3 | V | h_1 p_1 \rangle \]
Gogny phenomenological effective force \(^{(1)}\)

\[
V_{12} = \sum_{j=1}^{2} e^{-(r_1-r_2)^2/\mu_j^2} \left( W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau \right)
\]

\[
+ t_3 (1 + x_0 P_\sigma) \delta(\vec{r}_1 - \vec{r}_2) \left[ \rho \left( \frac{\vec{r}_1 + \vec{r}_2}{2} \right) \right]^{\alpha}
\]

\[
+ i W_{LS} \nabla_{12} \delta(\vec{r}_1 - \vec{r}_2) \cdot \nabla_{12} (\vec{\sigma}_1 + \vec{\sigma}_2)
\]

\[
+ (1 + 2\tau_{1z})(1 + \tau_{2z}) \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}
\]

- The two ranges (\(\mu_j=1,2 = 0.7\) et 1.2 fm) simulate the “molecular potential”
- Density dependence necessary for saturation
- Spin-orbit necessary for magic numbers

\(\rightarrow\) 14 parameters adjusted on nuclear matter properties and on some stable nuclei

II. Variational mp-mh configuration mixing method

Solution of secular equation

- **Lanczos method**
  - Standard diagonalization method: CPU time increases like $N^3$ ($N$ matrix dimension)
  - Adapted to the search of lowest eigenvalues, numerically efficient
  - Limitating factor for huge matrices: Lanczos vector storage

- **m-scheme** (1)
  - Method applied for axially deformed nuclei
  - Method for coding the Slater Determinant (with good $K$), the operators and storing the non zero matrix elements used in the Lanczos algorithm in shell model-type codes
  - 80% of the work = proton-neutron part

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Calculation schemes

• Possible truncation schemes
  - order of excitation in the wave function (1p1h, 2p2h, ...)
  - size of the single particle state space
  - cut-off energy in mp-mh configurations

• Importance of self-consistency:
  helps to include higher order of HF mp-mh states through “renormalization” of mean-field (ρ built with the correlated wave function)

• Still large matrices ➔ Need for supercomputers ➔ Tera10, CCRT
II. Variational mp-mh configuration mixing method

Dimension of matrices

- $^{16}$O ground state with all correlations (including proton-neutron)
  48 neutron orbitals + 48 proton orbitals

<table>
<thead>
<tr>
<th>mp-mh truncation</th>
<th>1p1h</th>
<th>2p2h</th>
<th>3p3h</th>
<th>4p4h</th>
<th>…</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total dimension</td>
<td>88</td>
<td>31276</td>
<td>5 097411</td>
<td>526 910280</td>
<td>…</td>
</tr>
</tbody>
</table>

- $^{100}$Sn ground state with only pair excitations (without proton-neutron)
  286 neutron orbitals + 286 proton orbitals

<table>
<thead>
<tr>
<th>mp-mh truncation</th>
<th>1 pair</th>
<th>2 pairs</th>
<th>…</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total dimension</td>
<td>13001</td>
<td>62 478001</td>
<td>…</td>
</tr>
</tbody>
</table>

Number of non zero matrix elements : 5 759 422500
Number of words stored : 17 833 473518
III. First application – K isomers in $^{178}$Hf

- **4 isomeric states**

- **Model assumptions**
  - mean field build with the zero range interaction Skyrme SIII
  - residual interaction: contact interaction
  - valence space: ±5 MeV around the Fermi level
  - neutron and proton are treated separately
  - no self-consistency

- **$0^+$ ground state of $^{178}$Hf**
  - axially deformed nucleus
  - weak level density - weak pairing regime

III. First application – K isomers in $^{178}$Hf

**Neutrons**

$9/2^+ \quad \lambda \quad 7/2^- \quad 5/2^-

**Protons**

$5/2^+ \quad 9/2^- \quad 7/2^+

<table>
<thead>
<tr>
<th>Neutron</th>
<th>Proton</th>
</tr>
</thead>
<tbody>
<tr>
<td>HF</td>
<td>HF</td>
</tr>
<tr>
<td>1 pair (&gt;1%)</td>
<td>1 pair (&gt;1%)</td>
</tr>
<tr>
<td>$0^+$</td>
<td>$16^+$</td>
</tr>
<tr>
<td>68</td>
<td>91</td>
</tr>
<tr>
<td>21</td>
<td>3</td>
</tr>
<tr>
<td>54</td>
<td>68</td>
</tr>
<tr>
<td>36</td>
<td>24</td>
</tr>
</tbody>
</table>

**Isomers**

<table>
<thead>
<tr>
<th>Isomers</th>
<th>mp-mh</th>
<th>Exp.</th>
<th>$\varepsilon_{ph}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$16^+$</td>
<td>2.59</td>
<td>2.45</td>
<td>1.484</td>
</tr>
<tr>
<td>$8^-$</td>
<td>1.17 (n)</td>
<td>1.15</td>
<td>0.637 (0.846)</td>
</tr>
<tr>
<td>$6^+$</td>
<td>1.41 (n)</td>
<td>1.54</td>
<td>1.278 (1.565)</td>
</tr>
<tr>
<td>$14^-$</td>
<td>2.83</td>
<td>2.57</td>
<td>2.120</td>
</tr>
</tbody>
</table>

(in %)

(in MeV)

- Quenching of correlations in isomeric states
- Importance of the configuration mixing (effect on energies)
Second application – Richardson exact solution for the Pairing hamiltonian

**Pairing hamiltonian**

\[ \hat{H} = \sum_f 2\epsilon_f \hat{N}_f - g \sum_{ff'} b_f^+ b_{f'}^+ \]

\[ \hat{N}_f = \frac{1}{2}(a_f^+ a_f + a_{f'}^+ a_{f'}) \]

\[ b_f^+ = a_f^+ a_f^+ \]

\[ [b_f^+, b_{f'}^+] = \delta_{ff'} (1 - 2\hat{N}_f) \]

**Exact solution** \(^{(1)}\)

- Similarity between the many-fermion-pair system with pairing forces and the many-boson system with one-body forces

- Exact wave function: mp-mh wave function including all the configurations built as pair excitations

- Exact solution obtained from a coupled system of algebraic equations deduced from variational principle

Test of the importance of the different terms in the mp-mh wave function expansion (2p2h, 4p4h ...)

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(1) R.W. Richardson, Phys.Rev. 141 (1966) 949
III. Second application – Richardson model

Picket fence model

- System of $2N$ particles in $2N$ equispaced and doubly-degenerated levels
- System of identical fermions
- Constant pairing interaction strength
- Prototype of axially deformed nuclei
Ground state Correlation energy (1)

\[ E_{\text{corr}} = E(g \neq 0) - E(g = 0) \]

\[ \Delta E_{\text{corr}} = E_{\text{corr}}^{(\text{exact})} - E_{\text{corr}}^{(\text{mp-mh})} \]

Truncation in mp-mh order of excitation

Truncation in excitation energy

III. Second application – Richardson model

Ground state occupation probabilities

$V_n^2$ vs $n$ for $2N=16$, $g=0.66$

- $2p2h$
- $4p4h$
- $6p6h$
- Exact
III. Third application – Pairing in $^{116}$Sn

Third application-Pairing in $^{116}$Sn with Gogny force (1)

- $^{116}$Sn : spherical nucleus with $Z=50$ and $N=66$

- Mean field and residual parts of Hamiltonian calculated with the D1S Gogny force

- Wave function built only with pair excitations (excluding pn pairs)

- Correlation energy : $E_{\text{cor}} = \langle \Psi | \hat{H}[\rho] | \Psi \rangle - \langle HF | \hat{H}[\rho] | HF \rangle$

III. Third application – Pairing in $^{116}$Sn

$^{116}\text{Sn}$ - Correlation energy

![Graph showing correlation energy vs. number of neutron single particle levels]

- $E_{corr}$ = \begin{align*}
\text{mp-mh} & : 5.441 \text{ MeV} \\
\text{BCS} & : 3.364 \text{ MeV} \\
\text{difference} & : 2.077 \text{ MeV}
\end{align*}

$E_{corr}$ = BCS - 3.364 MeV

→ need for 4p4h

Binding energy in $^{116}\text{Sn}$

- Exp : 988.683 MeV
- HF : 981.462 MeV
- BCS : 984.826 MeV
- mp-mh : 986.903 MeV

2p2h : 4.474 MeV
4p4h : 0.967 MeV
III. Third application – Pairing in $^{116}$Sn

$^{100}$Sn - Correlation energy

Fixed proton valence space (286 levels)

$-E_{\text{corr}} = \begin{cases} 
\text{mp-mh} & 3.672 \text{ MeV} \\
\text{BCS} & 0.000 \text{ MeV} \\
\text{difference} & 3.672 \text{ MeV}
\end{cases}$

$2p2h : 3.397 \text{ MeV}$
$4p4h : 0.275 \text{ MeV}$

→ 4p4h less important in $^{100}$Sn
### III. Third application – Pairing in $^{116}$Sn

**Correlated Wave Functions**

<table>
<thead>
<tr>
<th>(%)</th>
<th>HF</th>
<th>(1 pair)$_\nu$</th>
<th>(1 pair)$_\pi$</th>
<th>(2 pairs)$_\nu$</th>
<th>(1 pair)$<em>\nu$ (1 pair)$</em>\pi$</th>
<th>(2 pairs)$_\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{116}$Sn</td>
<td>65.38</td>
<td>26.04</td>
<td>4.50</td>
<td>2.68</td>
<td>1.23</td>
<td>0.17</td>
</tr>
<tr>
<td>$^{100}$Sn</td>
<td>90.85</td>
<td>5.02</td>
<td>3.70</td>
<td>0.16</td>
<td>0.18</td>
<td>0.09</td>
</tr>
</tbody>
</table>

75 components $> 0.05\%$ $\rightarrow$ 23.2%

- 2 configurations 2p2h built with 1d$_{3/2}$: 8.2%
- 6 configurations 2p2h built with 0h$_{11/2}$: 2.5%
- 67 configurations: 12.5% ($0.05\% < x < 0.3\%$)
  (number of configurations: ~70 millions)

0.05% $< 37$ components $< 0.1\%$
(number of configurations: 63 millions)
III. Third application – Pairing in $^{116}\text{Sn}$

Single particle level spectrum

Protons

$\beta$

Neutrons

BCS-D1S Bruyères-le-Châtel
III. Third application – Pairing in $^{116}\text{Sn}$

Single particle states occupation probabilities

$^{116}\text{Sn}$

- Proton single particle levels
- Neutron single particle levels

$^{100}\text{Sn}$

No impact of correlations on occupancies!
III. Third application – Pairing in $^{116}$Sn

Preliminary results - Self-consistency effect - $^{116}$Sn

• Correlation energy

<table>
<thead>
<tr>
<th></th>
<th>1 pair</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non self-consistent</td>
<td>4.474</td>
</tr>
<tr>
<td>Approximate Self-consistent</td>
<td>5.065</td>
</tr>
</tbody>
</table>

Energy gain

• Correlated wave function

<table>
<thead>
<tr>
<th></th>
<th>HF</th>
<th>1 pair</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non self-consistent</td>
<td>87.29</td>
<td>12.71</td>
</tr>
<tr>
<td>Approximate Self-consistent</td>
<td>82.60</td>
<td>17.40</td>
</tr>
</tbody>
</table>
Summary

- Self-consistent mp-mh approach unifies the description of important correlations beyond mean field in nuclei (Pairing, RPA, Particle vibration)
  
  ✓ Now tractable for medium-heavy nuclei with present computers (pairing hamiltonian)

- First applications to nuclear superfluidity quite encouraging

- Future ones: collective vibrations, exotic light nuclei

- Requires re-definition of effective N-N interaction in pn channels (under way)