Oblique Basis Approach to Nuclear Structure and Reactions

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Perspectives on the modern shell model
and related experimental topics

Sat., Feb. 6, 2010
Overview

• Modeling the interactions b/w nucleons

• Oblique basis approach to the diagonalization problem

• Oblique basis sets - some examples

• Beyond the 2-body interaction

• Oblique (non-orthogonal) basis for particle transfer reactions in heavy nuclei.
Modeling the Interactions: 
Nuclear Shell-Model Hamiltonian

\[ H = \sum_i \varepsilon_i a_i^+ a_i + \sum_{i,j,k,l} V_{ijkl} a_i^+ a_j^+ a_k a_l \]

where \( a_i^+ \) and \( a_i \) are fermion creation and annihilation operators, \( \varepsilon_i \) and \( V_{ijkl} \) are real and \( V_{ijkl} = V_{klij} = -V_{jikl} = -V_{ijlk} \)

Main problems:

- Determining the parameters of the interaction - model fitting using input from experiment
- Doing large model space calculations

Realistic interactions: KB3, GXPF1, FP6D …
Chiral perturbation theory ($\chi$PT) allows for controlled power series expansion

Expansion parameter: $\left(\frac{Q}{\Lambda_{\chi}}\right)^n$, $Q$ – momentum transfer,

$\Lambda_{\chi} \approx 1 \text{ GeV}$, $\chi$ - symmetry breaking scale

NNN - potentials such as Tucson-Melbourne & Urbana

Terms suggested within the Chiral Perturbation Theory

V. Bernard, E. Epelbaum, H. Krebs, and Ulf-G. Meiβner

R. Machleidt, D. R. Entem, nucl-th/0503025
Along the appropriate curve, all $C_D$-$C_E$ points reproduce BE of $^3$H & $^3$He within 0.1 keV.

Along the $C_D$-$C_E$ Curve (average)

BE deviation along the $C_D$-$C_E$ curve

BE deviation is within the accuracy of the kinetic energy for equal mass nucleons $m_n=m_p$.

\[ \delta T = T \frac{\delta m}{m} \approx 26 \text{keV} \left( \approx 37 \times 0.7 \times 10^{-3} \right) \]

$T=3/2$ channel has been neglected in the calculations.

\[ m = (Zm_p + (A-Z)m_n)/A \]

ab-initio no core with QCD derived nuclear interaction

• Pushing the limits using the N[^3]LO,
• May need codes with explicit $m_p$ & $m_n$.

Is the NNN all we need?
Effective Interactions in a Finite Model Space

\[ H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j} V_{ij}(q) \]

1 and 2-body interaction terms

\[ U = e^{iS} \]

Okubo and Lee-Suzuki transformation method

\[ H_{\text{eff}} = U H U^{-1} \]

\[ H_{\text{eff}} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i_1 < i_2} V_{i_1i_2}(q) + \ldots + \sum_{i_1 < \ldots < i_A} V_{i_1 \ldots i_A}(q) \]

1, 2, 3 … up to A-body interaction terms
Effective Hamiltonian in Second Quantized Form

\[ H_{\text{eff}} = \sum_{\alpha} \varepsilon_\alpha a_\alpha^+ a_\alpha + \cdots + \sum_{k=1}^{A} \frac{1}{(k!)^2} \sum_{\alpha_1 \neq \ldots \neq \alpha_k \atop \alpha_{k+1} \neq \ldots \neq \alpha_{2k}} V_{\alpha_1 \ldots \alpha_{2k}} a_\alpha^+ \ldots a_{\alpha_k}^+ a_{\alpha_{k+1}} \ldots a_{\alpha_{2k}} \]


- In principle, **A-body effective Hamiltonians** can be calculated from realistic interactions, but their applications **are yet ahead**!

- Need for exactly solvable models to **understand possible implications of the A-body effective interactions**!
Nuclear Models

• Multi-particle shell model configurations ...
  – Harmonic oscillator single-particle basis ...
  – Configuration mixing (two-body interactions and beyond ...) 
  – We can build our collective states on this or ...

• Group theory models - group chain so(3)=G_i⊂⋯⊂G_j; 
  – Elliott’s SU(3), Symplectic model, Interacting Boson Model (IBM) ...
  – Lie algebra based models are good because:
    • Guaranteed to be exactly solvable...
    • Well defined extension of the operators in product spaces:
      Co-product \( \Delta(X)=X_1 \otimes Y_2 + Y_1 \otimes X_2 \) (often \( Y=1 \))
      \( L_{\text{system}} = L_1 + L_2 + L_3 + \ldots \)

• Geometric models - liquid drop model \( R(\theta,\varphi)=R_0(1+\alpha^{\lambda\mu}Y_{\lambda\mu}(\theta,\varphi)) \) ...
  – \((\beta,\gamma)\) shape parameters ↔ \((\lambda,\mu)\) su(3) irreps.
## Group Theory Models

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<tr>
<th>rank</th>
<th>$A_n$, $su(n+1)$</th>
<th>$B_n$, $so(2n+1)$</th>
<th>$C_n$, $sp(2n)$</th>
<th>$D_n$, $so(2n)$</th>
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<td>$sp(2)$ ~ $su(2)$</td>
<td>$so(2)$ ~ $u(1)$</td>
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<td>2</td>
<td>$su(3)$ Elliott</td>
<td>$so(5)$ pn-pairing</td>
<td>$sp(4)$ ~ $so(5)$</td>
<td>$so(4)$ ~ $su(2)$</td>
</tr>
<tr>
<td>3</td>
<td>$su(4)$ Wigner</td>
<td>$so(7)$ ⊂ $so(8)$</td>
<td>$sp(6)$ Rowe &amp; Rosensteel</td>
<td>$so(6)$ ~ $su(4)$</td>
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<tr>
<td>4</td>
<td>$su(5)$</td>
<td>$so(9)$</td>
<td>$sp(8)$</td>
<td>$so(8)$ Evans, FDSM</td>
</tr>
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</table>
The Challenge ...

Nuclei display unique characteristics:

- Single-particle Features
- Pairing Correlations
- Deformation/Rotations
We usually understand a problem when it is:

- **exactly solvable** (symmetry at play)
- **perturbative** regime

Two or more different sets of basis states could be employed to understand the problem …
Important Exactly Solvable 2-body Nuclear Interactions

- **Quadrupole-Quadrupole** interaction, Elliott’s SU(3) model:

\[ \hat{H} = \varepsilon N - \frac{\chi}{2} \mathbf{Q} \cdot \mathbf{Q} \]

- **Pairing interaction**:

\[ \hat{H} = \sum_{\alpha} \varepsilon_{\alpha} (a_{\alpha\uparrow}^{\dagger}a_{\alpha\uparrow} + a_{\alpha\downarrow}^{\dagger}a_{\alpha\downarrow}) - G \sum_{\alpha\beta} a_{\alpha\uparrow}^{\dagger}a_{\alpha\downarrow}^{\dagger}a_{\beta\downarrow}a_{\beta\uparrow} \]
SU(3) Symmetry Breaking in the pf-shell nuclei

Realistic spin-orbit \((l\cdot s)\) single particle energy splitting!

Turn off the s.p.e. spin-orbit splitting!

Coherent state structure in \(^{48}\text{Cr}\) using Kuo-Brown-3 interaction.

Eigenvalue Problem in an Oblique Basis

- Spherical basis states $e_i$
- SU(3) basis states $E_\alpha$
- Overlap matrix $\hat{g}$

\[
\hat{g} = \begin{pmatrix}
\langle e_i | e_j \rangle & \langle e_i | E_\beta \rangle \\
\langle E_\alpha | e_j \rangle & \langle E_\alpha | E_\beta \rangle
\end{pmatrix} = \begin{pmatrix}
1 & \mu \\
\mu^* & 1
\end{pmatrix}
\]

- The eigenvalue problem

\[
H\psi = E\psi \quad \Rightarrow \quad \hat{H} \cdot \hat{\psi} = E \hat{g} \cdot \hat{\psi}
\]
Example of an Oblique Basis Calculation: $^{24}$Mg

We use the Wildenthal USD interaction and denote the spherical basis by SM(#) where # is the number of nucleons outside the $d_{5/2}$ shell, the SU(3) basis consists of the leading irrep (8,4) and the next to the leading irrep, (9,2).

<table>
<thead>
<tr>
<th>Model Space</th>
<th>SU3 (8,4)</th>
<th>SU3+ (8,4)&amp; (9,2)</th>
<th>GT100</th>
<th>SM(0)</th>
<th>SM(1)</th>
<th>SM(2)</th>
<th>SM(4)</th>
<th>Full</th>
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<td>Dimension (m-scheme)</td>
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<td>128</td>
<td>500</td>
<td>29</td>
<td>449</td>
<td>2829</td>
<td>18290</td>
<td>28503</td>
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<tr>
<td>%</td>
<td>0.08</td>
<td>0.45</td>
<td>1.75</td>
<td>0.10</td>
<td>1.57</td>
<td>9.92</td>
<td>64.17</td>
<td>100</td>
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Visualizing the SU(3) space with respect to the SM space using the naturally induced basis in the SU(3) space.
Overlaps With The Exact Eigenvectors For 24Mg

Three-Mode Systems

J-Pair Modes

<p>| | | |</p>
<table>
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<td>$G_{pp}$</td>
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<td>$G_{nn}$</td>
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</tr>
<tr>
<td>$S_{pp}$</td>
<td>$S_{pn}$</td>
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</tr>
</tbody>
</table>

Closed Shell Core

$pp$, $pn$, $nn$

Oblique basis using states constructed from physically significant S and D pairs.

Three-Mode Systems

Full shell-model calculations to obtain the spectrum of near closed shell nuclei.
Evaluation Steps

Matrix elements ($\mathcal{H}$ and $\mathcal{g}$)

$\mathcal{H}$ and $\mathcal{g}$

$g = U U^T$ (Cholesky)

Eigenstates ($\text{Lanczos}$)

$\langle \psi_1 | O | \psi_2 \rangle$ and $\langle \mathcal{E}_1 | O | \mathcal{E}_2 \rangle$

$m$-scheme

$\varepsilon_L$ and $\langle j_1 j_2 J' | \mathcal{V} | j_3 j_4 J'' \rangle$
Algebraic Models

- **Standard pairing** is actually an SU(2) RG-model.

- **Proton-neutron T=1 pairing** is SO(5) RG-model.

- **Generalized Richardson-Gaudin models** are new interesting set of exactly solvable algebraic models.

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<td>$so(4) \sim su(2)\oplus su(2)$</td>
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The Pairing Problem

\[ \hat{H} = \sum_j \varepsilon_j n_j - \sum_{jj'} c_{jj'} A_j^+ A_{j'}^-, \]

\[ A_j^+ = \sum_{m>0} (-)^{j-m} a_{jm}^+ a_{j-m}^+. \]

Exactly solvable cases:

- **Constant pairing** \( c_{jj'} = G \) with non-degenerate single particle energies \( \varepsilon_j \neq \varepsilon_{j'} \). R. W. Richardson, *Phys. Lett.* 5, 82 (1963).

- **Separable pairing** \( c_{jj'} = c_j \delta_{jj'} \) with degenerate single particle energies \( \varepsilon_j = \varepsilon_{j'} \). F. Pan, J. P. Draayer, W. E. Ormand, *Phys. Lett.* B 422, 1 (1998).

- \( T=1 \) proton-neutron pairing as Richardson-Gaudin model with non-degenerate single particle energies. J. Dukelsky, V.G. Gueorguiev, P. Van Isacker (PRL 96, 072503(2006)).

Extended Pairing Model

\[ H_{\text{eff}} = \sum_{\alpha} \varepsilon_{\alpha} a_\alpha^+ a_\alpha + \cdots + \sum_{k=1}^{A} \frac{1}{(k!)^2} \sum_{\alpha_1 \neq \cdots \neq \alpha_k, \alpha_{k+1} \neq \cdots \neq \alpha_{2k}} V_{\alpha_1 \ldots \alpha_{2k}} a_{\alpha_1}^+ \cdots a_{\alpha_k}^+ a_{\alpha_{k+1}} \cdots a_{\alpha_{2k}} \]

- **Nilsson single particle energies** \( \varepsilon_{jm} \) play the role of **1-body effective Hamiltonian** that takes into account the nuclear deformation due to the Q·Q interaction.

- **Simplifying assumption**: equal coupling between different configurations:
  \[ V_{\alpha_1 \alpha_2} = V_{\alpha_1 \alpha_2 \alpha_3 \alpha_4} = V_{\alpha_1 \ldots \alpha_{2A}} = G \]

- The **RESULT** is **Exactly solvable Hamiltonian**:

\[ \hat{H} = \sum_i \varepsilon_i n_i - G \sum_{ij} b_i^+ b_j - G \sum_{k=2}^{A} \frac{1}{(k!)^2} \sum_{i_1 \neq \cdots \neq i_{2k}} b_{i_1}^+ \cdots b_{i_k}^+ b_{i_{k+1}} \cdots b_{i_{2k}}, \quad b_i^+ = a_{i \uparrow}^+ a_{i \downarrow}^+ \]

5 pairs in 10 levels

$e_1 = 1.179$
$e_2 = 2.650$
$e_3 = 3.162$
$e_4 = 4.588$
$e_5 = 5.006$
$e_6 = 6.969$
$e_7 = 7.262$
$e_8 = 8.687$
$e_9 = 9.899$
$e_{10} = 10.20$
• Nilsson levels using nuclear deformation \textit{(Audi & Wapstra (1995))}.
• Pauli blocking for odd A nuclei.
• Set the scale of the single particle energies from near closed shell system… \textit{(Nilsson BE is 3/4 E filling, Ring & Schuck)}

BE Relative to the $^{208}$Pb core
Extended Pairing

- Has nice and interesting systematic behavior!
- The Extended Pairing model gives reasonable results...
- Many-body interactions beyond two- & three-body!

Other problems that can benefit from Non-Orthogonal Basis
Transfer Reactions for Deformed Nuclei Using Sturmian Basis

- **States for axially deformed nuclei:**
  - Bohr-Mottelson rotor model for deformed nuclei;
  - Rotor plus particle/hole system; \( \Psi_\Omega = \psi_v \Phi_k^{core} \), \( E_\Omega = E_k^{core} + \varepsilon_v \);
  - Deformed Woods-Saxon potential for the single particle states.

- **Transfer reactions on deformed nuclei:**
  - Distorted Wave Born Approximation (DWBA) within the Optical Model Potential (OMP) theory:
    \[
    d\sigma(J_iK_i \to J_fK_f;\nu) = \sum_{ij} \sum_{n} (a_v \nu_v c_{nij}^\nu)^2 d\sigma_{nlj}^{DW} ;
    \]
    \( a_v \) - Coriolis band mixing amplitude, 
    \( \nu_v \) - BCS occupation number, 
    \( \psi_v = c_{nij}^\nu \varphi_{nij} \) - all \( \varphi_{nij} \) have the same energy \( \varepsilon_v \)!

Sturmian Basis provides proper wave function tails...


V. G. Gueorguiev, P. D. Kunz, J. E. Escher, and F. S. Dietrich (nucl-th/07062002)
The circle indicates the region of agreement between the linear and the exact numerical treatment.

### Table: Neutron Separation

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<th>( \nu )</th>
<th>( \epsilon_{\nu} ) [MeV]</th>
<th>( J^\pi )</th>
<th>( \nu )</th>
<th>( \epsilon_{\nu} ) [MeV]</th>
<th>( J^\pi )</th>
<th>( \nu )</th>
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Norm convergence as function of the model space.

\[ \psi_v = c_v^{nlj} \phi_{nlj} \quad \text{all } \phi_{nlj} \text{ have the same energy } \varepsilon_v. \]
Model space convergence of the Sturmian basis

![Graph showing the model space convergence of the Sturmian basis.](#)
Excited States in $^{156}$Gd

$\sigma(J^\pi,E)$ for $^{157}$Gd($^3$He,$^4$He)$^{156}$Gd

V. G. Gueorguiev, P. D. Kunz, J. E. Escher, and F. S. Dietrich (nucl-th/07062002)
\begin{align*}
\rho_\lambda(E) &= \frac{1}{2\pi} \frac{4\Gamma}{4(E - E_\nu)^2 + \Gamma^2} \\
\sigma(E) &= \sum_\lambda \rho_\lambda(E)\sigma_\lambda, \quad \Gamma = a + bE.
\end{align*}
Summary

• QCD derived effective interactions and effective O-L-S methods suggest A-body interactions terms …

• The oblique basis build on the essential modes can help in the understanding of heavy nuclei.

• In studies of nuclear reactions non-orthogonal basis may resolve the tail problem inherited in the HO wave function.