Monte Carlo Shell Model calculations on exotic nuclei

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Diagonalization of Hamiltonian matrix

Conventional Shell Model calculation
All Slater determinants

Quantum Monte Carlo Diagonalization method
Important bases are selected

(about 30 dimension)
Our parallel computer

More CPU time for heavier or more exotic nuclei
$^{238}\text{U}$ one eigenstate/day in good accuracy requires 1PFlops

Progress in shell-model calculations and computers

- Dimension of Hamiltonian matrix (publication years of "pioneer" papers)
- Year
- Floating point operations per second

Birth of shell model (Mayer and Jensen)

Conventional Monte Carlo

Lines: $10^5 / 30$ years

More CPU time for heavier or more exotic nuclei

Japanese challenge

Blue Gene
Earth Simulator
Our parallel computer
Basic points of Monte Carlo Shell Model (I)

Two-body interaction can be rewritten as $V = (1/2) \sum_\alpha v_\alpha O_\alpha^2$

$\alpha$: index
$O_\alpha$: one-body operators (rearranged by diagonalization)

Hubberd-Stratonovichi transformation

True eigenstate: $\psi = \sum_\sigma e^{-\beta h(\sigma)} e^{-\beta h(\sigma')} \ldots \psi_0$

imaginary time ($\beta$) evolution by one-body field $h(\sigma)$

One-body operator is introduced as $h(\sigma) = \sum_\alpha s_\alpha \sigma_\alpha v_\alpha O_\alpha$

$\sigma_\alpha$: random number    $\sigma$: set of $\sigma_\alpha$'s
$s_\alpha$: phase
Basic points of Monte Carlo Shell Model (II)

True eigenstate: \( \psi = \sum_{\sigma, \sigma'} \ldots e^{-h(\sigma)} e^{-h(\sigma')} \ldots \psi_0 \)

Use \( \phi (\sigma, \sigma', \ldots) = e^{-\beta h(\sigma)} e^{-\beta h(\sigma')} \ldots \psi_0 \) as a basis for shell-model diagonalization

\( \phi (\sigma, \sigma', \ldots) \) are selected and refined:

(i) Random sampling -> only those lowering energy are kept
(ii) Polished by varying \( \sigma, \sigma', \ldots \) gradually (random noise reduced)
(iii) Symmetry restoration (Angular momentum, parity)

Slater determinants or Cooper-pair type wave functions are used

Usually, 20~50 bases are kept (many more thrown away)
Magnetic moment of $2^+$ level of Xe isotopes

More difficult in computation

\[ A = 128 : 10^{13} \text{ dimension} \]
In the study of structure of neutron-rich exotic unstable nuclei,

Some “surprises” in recent experiments on nuclei with $N \sim 18, 19$:

Extremely low-lying intruder states in

$^{31}\text{Mg} \ (Z=12, \ N=19)$

$^{29}\text{Na} \ (Z=11, \ N=18)$

$^{30}\text{Na} \ (Z=11, \ N=19)$

These have been classified as “normal nuclei”, for instance, in the Island of Inversion picture of Warburton et al.
Island of Inversion: region of intruder ground states

A sharp transition between normal and intruder
Effective single-particle energies in the “SDPF-M” interaction

SPE Gap vs. Correlation Energy (from a viewpoint of spherical shell)

Fully mixed calculations, e.g., Monte Carlo Shell Model, are essential

Otherwise, the gap cannot be investigated precisely

Sensitivity of intruder levels differs between semi-magic and open-shell nuclei.

Gap larger,
Correlation coupling constant larger

Gap smaller,
Correlation coupling constant smaller

The difference in correlation energy is smaller.

Position of intruders is more sensitive to the gap size.

Intruders are likely lower.
Two Gogny(-type) interactions: D1S and GT2

(a) Neutron SPE by D1S (N=20)

(b) Neutron SPE by GT2 (N=20)

Energy [MeV]
Proton number

Talk by Abe
Level scheme of Na isotopes by SDPF-M interaction compared to experiment

FIG. 4. Comparison of the energy levels of $^{27-30}$Na relative to the experimental ground state among the experiment (Exp.) and the shell-model calculations by the SDPF-M and the USD interactions. The $E2$ strength from the ground state is illustrated by the width of the arrow. The experimental $B(E2)$ values of $^{28,30}$Na and the energy levels of $^{27}$Na are taken from Refs. [25] and [36], respectively. For $^{30}$Na, the levels calculated from SDPF-M interaction are grouped into four columns; the first (second) one is $K=2(1)$ rotational band dominated by intruder configurations, the third one represents spherical states which are basically of normal configurations, and negative-parity states are shown in the fourth column.
Electro-magnetic moments and wave functions of Na isotopes

— normal dominant: N=16, 17
— strongly mixed: N=18
— intruder dominant: N=19, 20

Onset of intruder dominance earlier than “island of inversion” picture (at N=20)

Mass systematics in Na isotopes

Figure 4. Two-neutron separation energy, $S_{2n}$ (MeV), as a function of the neutron number, N.

- Single Particle Energy (MeV)
- Intrinsic gain

USD
SDPF-M
Exp.
FIG. 2 (color online). Proposed level scheme for $^{29}$Na populated following the $\beta^-$ decay of $^{29}$Ne. The absolute $\beta$-decay branching to each level per 100 decays is indicated along with the calculated log$ft$ values. Shown on the right are shell model calculations with the USD and SDPF-M interactions.
FIG. 3. Partial experimental level scheme of $^{31}\text{Mg}$, with new spin/parity assignments, compared to various shell-model calculations (see text for details). The magnetic moments of theoretical levels are mentioned on the right (units $\mu_N$).
FIG. 9: Proposed level scheme of $^{28}$Ne. The results of different shell model calculations [7, 22] are included in the right part of the figure. The energy of the first excited state observed in Coulomb excitation experiment is taken from Ref. [20]. The spin 4 assignment to the 3008 keV state is taken from Ref. [21].
By now, we know...

Island of Inversion: region of intruder ground states

A sharp transition between normal and intruder
The shell model (MCSM) results have been obtained by the SDPF-M interaction for the full-$sd + f_{7/2} + p_{3/2}$ space.

The effective gap between the $sd$ and $pf$ shells

Intruder low-lying states even with modest deformation

\begin{itemize}
  \item $\sim 3\text{MeV}$
  \item $\sim 6\text{MeV}$
\end{itemize}
In many calculations, the gap is rather constant (5 ~ 6 MeV), and the inversion between normal and intruder ground states is basically due to different deformation energies.

Such description may not explain recent data.

The gap (i) can be quite small, (ii) depends on N and Z, (iii) can vary, even if the nucleus is still far from the drip line.

What causes such changes of shell structure.
Tensor Interaction

\[ V_T = (\tau_1 \tau_2) \left( [\sigma_1 \sigma_2]^{(2)} Y^{(2)}(\Omega) \right) Z(r) \]

- \( \pi \) meson: primary source
- Deuteron: binding, S-D coupling, Q-moment
- \( \rho \) meson (\( \sim \pi + \pi \)): minor (\( \sim 1/4 \)) cancellation

Ref: Osterfeld, Rev. Mod. Phys. 64, 491 (92)
The atomic nucleus is bound due to meson exchange. (Yukawa 1935)

Multiple pion exchanges $\rightarrow$ nuclear binding
But multiple processes are rather characterless

Where can we see one pion exchange?
One pion exchange $\sim$ Tensor force

First-order tensor force effect in spectroscopy
$\rightarrow$ manifestation of pions in nuclei
Intuitive Picture

wave function of relative motion

spin of nucleon

large relative momentum

small relative momentum

deuteron $\iff$ attractive

Monopole Interaction due to Tensor Interaction

Identity for tensor monopole interaction

\[(2j_> + 1) v_{m,T}^{(j' j_>)} + (2j_< + 1) v_{m,T}^{(j' j_<)} = 0\]

\[v_{m,T}: \text{monopole strength for isospin } T\]

Tensor interaction is the primary origin of the $p-n$ $j_\sigma - j_\tau$ coupling.

```
proton neutron 
```

\[
\begin{align*}
\sigma \tau \\
\text{central}
\end{align*}
\]
Systematic variation of neutron effective single-particle energies due to the tensor interaction ($\pi + \rho$ meson)

**Federman-Pittel effect**

- Repulsion between $g_{9/2}$ and $h_{11/2}$
- Widening between $h_{11/2}$ and $g_{7/2}$, not a spin-orbit partner

**Lines**: $\pi + \rho$ meson

**Points**: Corresponding experimental level

- Protons in $g_{9/2}$ shown relative to $d_{5/2}$

**N=51 isotones**

- Neutron single particle levels
- Proton number vs. energy (MeV)
- Overlap of radial wave functions is emphasized -

they can simultaneously fill the $l_g^{9/2}$ proton and $l_g^{7/2}$ neutron orbitals. The strong overlap of these spin-orbit-partner orbitals can lead to important $n$-$p$ correlations in this region and thus to deformation.

At this point it is useful to generalize our earlier remarks as to when strong $n$-$p$ correlations should occur. As noted earlier, the crucial criterion is that the neutrons and protons occupy orbitals with good overlap. It was pointed out long ago [8] that the overlap between two orbitals $(n_N l_N j_N)$ and $(n_P l_P j_P)$ is maximum if $n_N = n_P$ and $l_N \approx l_P$. So far, we have focussed on cases in which $n_N = n_P$ and $l_N = l_P$, although we have emphasized that $j_N$ need not be the same as $j_P$. 
Summary

N=20 gap varies and can be small for Ne-Na-Mg (independently of the distance to the drip line)

$^{31}\text{Mg}, ^{29}\text{Na}, ^{30}\text{Na}$ and many others

"Island of Inversion" is bigger and has wide reefs

Shell evolution due to tensor interactions

- drives $j_>$ or $j_<$ levels in a specific and robust way
  
  intuitive picture $\rightarrow$ many cases expected from p-shell to superheavies

- is the dominant origin of shell evolution

  - N=20 gap also largely due to the tensor force

  - Federman-Pittel mechanism ($g9/2$-$g7/2,h11/2$)

- Installation of tensor effect into mean field models (GT2)
  
  $\rightarrow$ Abe
Central forces:

Complex origins

Multiple meson exchange,
hard core (quarks, QCD may be needed)
3-body forces

Present form of Gogny interaction
good also because of full spin-isospin channels

Tensor force:

Simpler origin
dominated by one pion exchange (of course $\rho$, higher order ...)

Config. dependent effects $\rightarrow$ Density Functional form $\ldots$?
Mean field formalism needed?

$\leftrightarrow$ Chiral Perturbation
Collaborators

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