Large-scale shell model calculations on E1 spectra of medium-heavy nuclei

Noritaka SHIMIZU
CNS, University of Tokyo

T. Otsuka (Tokyo U.) T. Togashi (CNS, Tokyo),
Y. Utsuno (JAEA/CNS), S. Ebata (MeMe Hokkaido),
and M. Honma (Aizu U.)
Introduction

- Giant Dipole Resonance (GDR) and Pygmy Dipole Resonance (PDR) have been studied intensively by RPA, QRPA, phonon model, ...
  
  e.g. Inakura (2011), Hartmann et al. (2004), ...

- Neutron skin, EoS, symmetry energy
  
  e.g. Reinhard Nazarewics (2012), Klimkiewiz et al. (2007), Colo (2008), ...

- PDR: single-particle excitation vs. collective excitation?

- A few studies by shell model (SM) calc. in medium-heavy nuclei
  
  Schwengner Brown (2010), Sagawa Suzuki (1999), K. Sieja (2013), ...

purpose

Large-scale shell model (LSSM) calculations and Monte Carlo shell model (MCSM) for GDR/PDR in medium-heavy nuclei with including various many-body correlations
A successful example of shell-model calc. (MCSM): Neutron-rich Ni isotopes and shell evolution

Strength function in shell model

• In principle, the shell model is quite useful for describing high excited states.

• $E_1$ excitation causes parity change. 3-major-shell model space ($1\hbar\omega$) is required unlike $M1$ and Gamow-Teller transitions ($0\hbar\omega$ SM).

• In practice, direct diagonalization with the Lanczos method or MCSM cannot be applicable to high excited states because of high level density.

• Methods
  – Lanczos strength function method
    • $E_1$ excitation of Ca isotopes
  – New extension of Monte Carlo shell model for strength function
Model space and effective int. for Ca isotopes

- Model space:
  - full \(sd\)-pf-sdg shell

- \(1\hbar\omega\) truncation:
  - \(0\hbar\omega\) for natural parity state
  - \(1\hbar\omega\) for unnatural parity state
  - Full correlation inside pf-shell

- \((1+3)\hbar\omega\) truncation:
  - \((0+2)\hbar\omega\) for natural parity state
  - \((1+3)\hbar\omega\) for unnatural parity state

- Effective interaction:
  - USD+GXPF1B+VMU
  - Utsuno et al., PTPS 196, 304 (2012)
  - Shell gaps and \(3^-\) states of Ca isotopes

\[ e_A \approx \sqrt{\frac{N}{A} e - \frac{Z}{A} e} \]
Lanczos strength-function method for E1 excitation spectrum

often used for Gamow-Teller transitions

\[ |\varphi_0(1^-) > = O(E1) |0^+ _1> \]

\[ \text{ground state} \]

Lanczos iteration using \( |\varphi_0(1^-)> \) as an initial state. (doorway state)

diagonalize the matrix in the Krylov subspace, \( \{ H^n \varphi_0 >, H^{n-1} \varphi_0 >, \ldots, H^1 \varphi_0 >, \varphi_0 > \} \)

to obtain approximated states \( \{ \phi_0 >, \phi_1 >, \phi_2 >, \ldots, \phi_{n+1} > \} \) in the same way as Lanczos method.

Smoothing with Lorentz distribution
\[ I(x, x_0, \Gamma) = \frac{1}{\pi} \frac{\gamma}{(x - x_0)^2 + \gamma^2} \]

with \( \gamma = \Gamma / 2 \), \( \Gamma = 1.0 \text{MeV} \)

Good distribution obtained in a few hundred Lanczos iterations

Lawson method is used for the removal of contamination of spurious mass motion
Concept of Lanczos strength function method

|\( \varphi_0 \rangle \) \quad \leftarrow \quad |\varphi_0(1^-)\rangle = O(E1) \ |0^+\rangle

\( |\varphi_1\rangle \) \quad \leftarrow \quad |\varphi_1\rangle = H |\varphi_0\rangle

\( |\varphi_2\rangle \) \quad \leftarrow \quad |\varphi_2\rangle = H |\varphi_1\rangle

\ldots

\( |\varphi_n\rangle \) \quad \leftarrow \quad |\varphi_k\rangle : \text{basis vectors huge in } M\text{-scheme}

10^{10} \text{ dim. } \Rightarrow 80\text{GB} / \text{a vector}

1 \leq k \leq n, \ n \sim 300
Convergence of strength distribution

$|\varphi_0 (1^-) > = O(E1)|0^+ >$

\[ \Gamma = 1 \text{MeV} \]

1 iter.

\[ \sigma \text{[mb]} \]

\[ Ex. \text{[MeV]} \]

\[ 0 \quad 5 \quad 10 \quad 15 \quad 20 \quad 25 \quad 30 \quad 35 \quad 40 \]

100 iter.

\[ \sigma \text{[mb]} \]

\[ Ex. \text{[MeV]} \]

\[ 0 \quad 5 \quad 10 \quad 15 \quad 20 \quad 25 \quad 30 \quad 35 \quad 40 \]

300 iter.

\[ \sigma \text{[mb]} \]

\[ Ex. \text{[MeV]} \]

\[ 0 \quad 5 \quad 10 \quad 15 \quad 20 \quad 25 \quad 30 \quad 35 \quad 40 \]

1,000 iter.

\[ \sigma \text{[mb]} \]

\[ Ex. \text{[MeV]} \]

\[ 0 \quad 5 \quad 10 \quad 15 \quad 20 \quad 25 \quad 30 \quad 35 \quad 40 \]
E1 excitation of Ca isotopes in LSSM

NS, Y. Utsuno, S. Ebata, T. Otsuka, M. Honma and T. Mizusaki, in preparation

1hw/3hw sd-pf-sdg shell calculations for negative-parity states of Ca isotope to describe E1 excitations

SM calc. well reproduce exp.
GDP peak position and width

- GDR \((1+3)\hbar\omega\) essential
- Ex. < 15MeV \(1\hbar\omega\) enough

“Lanczos strength function method”

Photoabsorption cross section \(^{48}\text{Ca} 1\hbar\omega\)

1hw : upto 1hw excitation in sd-pr-sdg shell
\(4.1\times10^6\) M-scheme dim.

at PC

(1+3)hw: up to 3hw excitation in sd-pf-sdg shell
\(1.2\times10^{10}\) M-scheme dim.

at supercomputer
photoabsorption cross section of Ca isotopes including odd nuclei

Low-energy region \((1\hbar\omega)\)

\(\sigma\) (mb)

Ex. (MeV)

\(\sigma\) (mb)

Ex. (MeV)

SM calc. well reproduce exp. GDP peak position and width

- GDR \((1+3)\hbar\omega\) essential
- Ex. < 15MeV \(1\hbar\omega\) enough

RPA: Cb-TDHF by S. Ebata, 5fm 3D sphere, 1fm mesh
$rY^{(1)}$ matrix element for neutron

$$B(E1) = \left( e_{t_z} \sum_{i,j} \langle \text{g.s.} \left| rY^{(1)}(i,j,tz) \right| 1^- \rangle \right)^2$$

stretched orbital pairs contribute
GDR: constructive
PDR: destructive

PDR state

|PDR⟩ ... large B(E1) state in low energy

$$\langle \text{g.s.} \left| rY^{(1)}(i,j) \right| \text{PDR}⟩$$

$$|\text{SR}⟩ = \frac{1}{N} rY^{(1)}|\text{g.s.}⟩$$

$$\langle \text{g.s.} \left| rY^{(1)}(i,j) \right| \text{SR}⟩$$

Sum rule state (GDR)
$rY^{(1)}$ matrix element for proton

$$B(E1) = \left( e_{tz} \sum_{i,j} \langle \text{g.s.} \| rY^{(1)}(i, j, tz) \| 1^- \rangle \right)^2$$

### PDR state

| PDR $\rangle$ ... large B(E1) state in low energy

$$\langle \text{g.s.} \| rY^{(1)}(i, j) \| \text{PDR} \rangle$$

- 50Ca
- 52Ca
- 54Ca
- 56Ca
- 58Ca
- 60Ca

### Sum rule state (GDR)

| SR $\rangle = \frac{1}{N} rY^{(1)} | \text{g.s.} \rangle$

$$\langle \text{g.s.} \| rY^{(1)}(i, j) \| \text{SR} \rangle$$

- 50Ca
- 52Ca
- 54Ca
- 56Ca
- 58Ca
- 60Ca

**Graphs**

- **PDR state**
  - $|0d_{5/2} \rightarrow 0f_{7/2}\rangle$
  - $|0d_{3/2} \rightarrow 0f_{5/2}\rangle$
  - $|1s_{1/2} \rightarrow 1p_{3/2}\rangle$

- **Sum rule state (GDR)**
  - $|0d_{5/2} \rightarrow 0f_{7/2}\rangle$
  - $|0d_{3/2} \rightarrow 0f_{5/2}\rangle$
  - $|1s_{1/2} \rightarrow 1p_{3/2}\rangle$
Beyond $3\hbar\omega$ truncation and toward heavier region by Monte Carlo shell model (MCSM)
Very brief outline of MCSM

- Efficient description of nuclear many-body states based on the basic picture of nuclear structure
  = intrinsic state + rotation + superposition

\[
|\Psi^{IM\pi}(N_b)\rangle = \sum_{d=1}^{N_b} f^{(d)} \sum_{K=-I}^{I} g^{(d)}_K \hat{P}_{\pi} \hat{P}_{MK} |\varphi(D^{(d)})\rangle
\]

MCSM basis dimension \( \approx 100 \)

Wave function = \( f^{(1)} + f^{(2)} + f^{(3)} + \ldots \)

\( D^{(d)} \) : determined stochastically and variationally
Nℏω configuration with N>3?

B(E1) sum rule

by Monte Carlo shell model

- $^{48}\text{Ca}$ B(E1) sum rule ($e^2\text{fm}^2$)
  - $1\hbar\omega$ \ldots 16.5
  - $(1+3)\hbar\omega$ \ldots 13.6
  - MCSM 50dim \ldots 10.1

- $^{51}\text{V}$ B(E1) sum rule
  - $1\hbar\omega$ \ldots 18.1
  - $(1+3)\hbar\omega$ \ldots NA
  - MCSM 50dim \ldots 12.4

Many-body correlations suppress B(E1) rule
Monte Carlo shell model for E1 spectrum

Photo-absorption cross section of $^{48}\text{Ca}$

$1\hbar\omega$: up to $1\hbar\omega$ excitation in $sd$-$pf$-$sdg$ shell

$4.1 \times 10^6$ M-scheme dim.

at PC

$(1+3)\hbar\omega$: up to $3\hbar\omega$ excitation in $sd$-$pf$-$sdg$ shell

$1.2 \times 10^{10}$ M-scheme dim.

at supercomputer

$79\text{Se} (1+3)\hbar\omega$: $1.2 \times 10^{14}$ dim.

far beyond the current capability of Lanczos method

Monte Carlo shell model for E1 spectrum
Concept to describe \( E1 \) spectrum with MCSM

\[
E1 = \sqrt{\frac{3}{4\pi}} \sum_{i=1}^{A} e_{i} \vec{r}_{i}
\]

\( e_i = N / A \) (proton),

\( -Z / A \) (neutron)

We introduce an exponential of one-body operator.

\[
\exp(i\varepsilon \cdot E1) \equiv \exp(i\varepsilon \cdot \sum_{i=1}^{A} e_{i}(x_{i} + y_{i} + z_{i}))
\]

We consider the following type of states:

\[
\left| \phi_{i}^{E1} \right> = \exp(i\varepsilon \cdot E1)\left| \phi_{i}^{g.s.} \right>
\]

Although this was a good idea, it is still too naïve to use this kind of states as the basis vectors for \( E1 \) spectrum.
Decomposition of $\exp(i\varepsilon \cdot E1)$ operator

The $E1$ operator is decomposed so as to treat transitions between different sets of orbits separately:

$\exp(i\varepsilon \cdot E1(0f_{7/2} \rightarrow 0g_{9/2}))$, $\exp(i\varepsilon \cdot E1(0g_{9/2} \rightarrow 0h_{11/2}))$, ...

Strength distribution is too concentrated.

Peaks corresponding to different orbital combinations appear.

Ref. T. Otsuka, T. Togashi, N. Shimizu et al.
**E1 excitation spectrum** can be calculated by MCSM

**Ground state:**

\[
|\Psi\rangle = \sum_{k=1}^{N_{\text{MCSM}}} f_k P^{J,\pi} \varphi_k
\]

Basis vector of the ground state (Slater determinant)

**Basis vectors for E1 spectrum** \((a,b,c,d, \ldots : \text{orbits})\)

\[
\exp(i\varepsilon \cdot E1(a \rightarrow b))|\varphi_k\rangle, \exp(i\varepsilon \cdot E1(c \rightarrow d))|\varphi_k\rangle, \ldots (k = 1,2,\ldots)
\]

**Additional bases for fine tuning:**

variation for energy average by the conjugate gradient

\[
|\varphi_k (E1(a \rightarrow b))^\text{Var}\rangle, |\varphi_k (E1(c \rightarrow d))^\text{Var}\rangle, \ldots
\]

**Diagonalization with these basis vectors after projection to 1-**

**Excitation spectrum up to certain fine structure**

E1 spectrum with \(~3000\) levels connected somehow to the g.s. (confirmed by E1 sum rule)
Overview of description of $E1$ spectrum with MCSM

Step 1. The ground state is solved by MCSM.

$$|\Psi(\text{g.s.})\rangle = \sum_i f_i |\varphi_i^{\text{g.s.}}\rangle$$

Step 2. Basis vectors for $E1$ spectrum are generated by acting

$$\exp(i\epsilon \cdot E1(a \rightarrow b)), \exp(i\epsilon \cdot E1(c \rightarrow d)), \ldots$$
on basis vectors of the ground state.

Step 3. More basis vectors are generated by the variation for the basis
vectors of step 2. Diagonalize H by all basis vectors.

$$\exp(i\epsilon \cdot E1(a \rightarrow b))|\varphi_i^{\text{g.s.}}\rangle, \exp(i\epsilon \cdot E1(c \rightarrow d))|\varphi_i^{\text{g.s.}}\rangle, \ldots$$

Step 4. Low-energy $E1$ excited states are solved independently
by “normal” MCSM and are added to the spectrum.

Photo absorption cross section is calculated

$$\sigma(E) [\text{fm}^2] = \frac{16\pi^3}{9} \frac{e^2}{\hbar c} \sum_{J_n^f} \frac{1}{\pi} \frac{\gamma}{(E - Ex(J_n^f))^2 + \gamma^2} \cdot Ex(J_n^f) \cdot B(E1; J^i \rightarrow J_n^f).$$

Excitation energy of n-th $E1$ excited state

Lorentzian width: $\gamma = \Gamma/2$ (adjusted parameter)
Concept of MCSM strength function

with keeping Slater-det. form

\[ |\Phi_{g.s.}\rangle = \sum_i f_i P^{J\pi} |\varphi_i\rangle \]

\[ |\varphi_{0,k}\rangle \]
\[ |\varphi_{0,k}^{\text{Var}}\rangle \]
\[ |\varphi_{0,k}^{\text{VarVar}}\rangle \]
\[ |\varphi_{0,l}\rangle \]
\[ |\varphi_{0,l}^{\text{Var}}\rangle \]
\[ |\varphi_{0,l}^{\text{VarVar}}\rangle \]

Var: variation by 2-step conjugate gradient

\[ |\varphi_{1,k}\rangle = e^{i\varepsilon O_k} |\varphi_1\rangle \]

\[ O_k = E1(a \rightarrow b) \]
Concept of Lanczos strength function method

"Sum rule" state

\[ |\varphi_0\rangle = O(E1) |0^+_1\rangle \]

\[ |\varphi_1\rangle = H|\varphi_0\rangle \]

\[ |\varphi_2\rangle = H|\varphi_1\rangle \]

\[ \vdots \]

\[ |\varphi_n\rangle \]

\[ |\varphi_k\rangle : \text{basis vectors} \]

huge in \( M \)-scheme

\[ 10^{10} \text{ dim.} \Rightarrow 80\text{GB} \]

\[ 1 \leq k \leq n, \ n \sim 300 \]
E1 excitation described by Monte Carlo shell model

Benchmark test

Lanczos calc. (exact)

M-scheme dimension 3,844,499

Monte Carlo shell model (MCSM)

600 MCSM basis vectors

\[ |\Psi\rangle = \sum_{k=1}^{N_{MCSM}} f_k P^J \pi |\varphi_k\rangle \]

\[ |\varphi_k\rangle = \prod_{\alpha=1}^{N} \left( \sum_{i=1}^{N_{sp}} c_i \ D_{i\alpha}^{(k)} \right) |\rangle \]

\( ^{18}\text{O} \) with p-sd shell psdwb int.
Photoabsorption cross section of $^{88}$Sr, $^{90}$Sr

- Model space:
  pf - sdg - pfh($0h_{11/2}$, $1f_{7/2}$, $2p_{3/2}$) shell
  (3 major shell)

- Effective Hamiltonian: $V_{MU}$ (+ M3Y LS)
  (central force scaled by 0.55)
  *Y. Utsuno et al., PRC86, 051301(R) (2012)

- The number of basis:
  1000 basis vectors are used to describe $E1$ spectrum.

M-scheme dimension of Hamiltonian matrix for $^{90}$Sr is $8.2 \times 10^{14}$ with truncation of 3hw excitation.

---

Cross section (mb)

**Photoabsorption cross section $\sigma_{abs}$ of $^{88}$Sr ($Z=38$, $N=50$), $^{90}$Sr ($Z=38$, $N=52$)**

<table>
<thead>
<tr>
<th>Cross section (mb)</th>
<th>Lorentzian width $\Gamma_{LLFP}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>88Sr (stable nucleus)</td>
<td>$\sigma_{abs} = \sigma(\gamma, \gamma')$</td>
</tr>
<tr>
<td>$^{88}$Sr($\gamma$,n) EXP data</td>
<td>B(E1) sum: 24.97</td>
</tr>
<tr>
<td></td>
<td>Sum rule : 26.94</td>
</tr>
</tbody>
</table>

| $^{90}$Sr (Long-lived fission product (LLFP)) | B(E1) sum: 25.14 |
|  | Sum rule : 28.47 |

http://cdfe.sinp.msu.ru/saladin/gdrmain.html
Results of Se (Z=34) isotopes

- Model space:
  \textit{sd - pf - sdx - 0h}_{11/2} \\
  ( 4 major shell )

- Effective Hamiltonian: *SDPF-MU (sd-pf) + V_{MU} (others) \\
  (central force scaled by 0.35)

*Y. Utsuno et.al., PRC86, 051301(R) (2012)

Photoabsorption cross section $\sigma_{\text{abs}}$ of $^{76}\text{Se}$ (N=42), $^{78}\text{Se}$ (N=44), $^{79}\text{Se}$ (N=45)

Cross section (mb)

![Graphs showing photoabsorption cross section for $^{76}\text{Se}$, $^{78}\text{Se}$, and $^{79}\text{Se}$]

Lorentzian width $\Gamma = 2.0\text{MeV}$


300 bases are used to describe $E1$ spectrum as preliminary calculation.
Summary

• Lanczos strength function in LSSM
  – E1 of Ca isotopes with LSSM
    • GDR \((1+3)\hbar\omega\) essential, higher \(\hbar\omega\) configuration
    • PDR \(1\hbar\omega\) enough
    • odd nuclei are feasible : Ca isotopes, \(^{51}\text{V}\)
  – PDR enhancement in \(^{52}\text{Ca}-^{60}\text{Ca}\)
    • PDR is on the tail of GDR
    • \(rY^{(1)}\) reduced matrix elements

• Monte Carlo shell model for strength function
  – construct \(J^\pi\)-projected subspace spanned by \(E1\)-excited Slater determinants
  – feasibility tested, odd nuclei are feasible
  – undergoing application to systematic studies and LLFP nuclides