Clustering and response functions of light nuclei in explicitly correlated Gaussians (ECG)

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Motivation: Unified description of nuclear states with different character e.g. particle-hole excitation, spatially localized clustering
Solving problems relevant to continuum e.g. resonance, response functions

We show our recent works for light nuclei performed in few-body approach:
Spectrum of $^4$He, E1 and spin-dipole responses of $^4$He
(4-body calculation with realistic force)
E1 response of a halo nucleus $^6$He
(6-body calculation with effective central force)
Coexistence of shell-model and clustering states in $^{16}$O
($^{12}$C+n+n+p+p 5-body calculation)

ECG describes correlations and asymptotics properly
Complex scaling method (CSM) converts continuum problems to those of $L^2$ basis

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**ECG basis**

Spherical Gaussian: \[
\exp \left( -\sum_{i<j} \frac{1}{2b^2_{ij}}(r_i - r_j)^2 \right) \rightarrow \exp \left( -\frac{1}{2} \tilde{x} A \tilde{x} \right)
\]

\[\tilde{x} A \tilde{x} = \sum_{i,j} A_{ij} x_i \cdot x_j \quad A_{ij} = A_{ji}\]

N-particle system: \(N-1\) relative coordinates \(\tilde{x} = (x_1, x_2, \ldots, x_{N-1})\)

\[
\begin{pmatrix}
  x_1 \\
  x_2 \\
  \vdots \\
  x_{N-1}
\end{pmatrix}
\]

Non-spherical motion: Global vector \(\tilde{u} \tilde{x} = u_1 x_1 + u_2 x_2 + \ldots + u_{N-1} x_{N-1}\)

(angular part)

\([\mathcal{Y}_L_1(\tilde{u} \tilde{x}) \times \mathcal{Y}_L_2(\tilde{u} \tilde{x})]_{LM}\)

\(\mathcal{Y}_\ell(r) = r^\ell Y_\ell(\hat{r})\)

General form:

\[
\Phi_\alpha = \mathcal{A} \left\{ \exp \left( -\frac{1}{2} \tilde{x} A \tilde{x} \right) \left[ \left[ \mathcal{Y}_{L_1}(\tilde{u} \tilde{x}) \times \mathcal{Y}_{L_2}(\tilde{u} \tilde{x}) \right]_{L} \times \chi^{(\text{Spin})}_{S_1 S_2 S_3 \ldots S} \right]_{J M} \eta^{(\text{Isospin})}_{T_1 T_2 T_3 \ldots T_M} \right\}
\]

Variational parameters: Continuous \(A, u, v\) Discrete \(L_1, L_2, L, S, \ldots\)

\(\pi = +: L=\text{even} (L_1=L, L_2=0), \quad L=\text{odd} (L_1=L, L_2=1)\)

Trial function \[
\Psi = \sum_{\alpha} C_\alpha \Phi_\alpha
\]

\[
H = \sum_{i=1}^{N} T_i - T_{\text{c.m.}} + \sum_{i<j} v_{ij} + \sum_{i<j<k} v_{ijk}
\]
Main features

- Fully microscopic
- No spurious c.m. motion
- Adaptable to arbitrary N-particle system
- Analytic evaluation of matrix elements

**Invariance under a linear coordinate transformation**

\[ y = T x \]

\[ \exp(-\tilde{y} B y) \mathcal{V}_{LM}(\tilde{y} y) = \exp(-\tilde{x} A x) \mathcal{V}_{LM}(\tilde{u} x) \]

\[ A = \tilde{T} B T, \quad u = \tilde{T} v \]

ECG is flexible in describing various correlations and asymptotics in a single scheme

Recent applications of ECG: J. Mitroy et al., RMP 85 (2013)

Basis selection

**Stochastic variational method (SVM)**

Four-nucleon system: $^4$He

Simultaneous description of both $0_1^+$ and $0_2^+$ states that have quite different structure

AV8’ + 3NF
Central, Tensor, LS
Strong short-range repulsion

Energy convergence

The first 1000 bases: $(0 < b_{ij} < 16 \text{ fm})$
Beyond 1000: 3N+N type bases

One-body density

$^3$H+p spectroscopic amplitude

Kamada et al., PRC64 (2001)
Spectrum of $^4\text{He}$

Realistic force well reproduces spectrum
Level sequence: $T=0$: $0^-, 2^-, 1^-$
$T=1$: $2^-, 1^-, 0^-, 1^-$

Three lowest negative-parity states have $3N+N$ cluster structure with P-wave relative motion:
Parity-inverted partner of the $0^+_2$ state

Most of the negative parity states are broad resonances

Distribution of HO quanta $Q$

1p-1h is largest for $0^-$ and $2^-$
Large $P_Q$ for high $Q$
Response (strength) function

\[ S(E) = \mathcal{S}_{\mu_f} |\langle \Psi_f | \mathcal{M}_{1\mu} | \Psi_0 \rangle|^2 \delta(E_f - E_0 - E) \]

\[ = -\frac{1}{\pi} \text{Im} \sum_{\mu} \langle \Psi_0 | \mathcal{M}_{1\mu}^\dagger | \mathcal{M}_{1\mu} | \Psi_0 \rangle \frac{1}{E - H + E_0 + i\epsilon} \]

Continuum discretization with CSM

\[ U(\theta) : \quad r_j \rightarrow r_j e^{i\theta}, \quad p_j \rightarrow p_j e^{-i\theta} \]

\[ e^{ik \cdot r} \rightarrow e^{ik \cdot r} (i \cos \theta - \sin \theta) \quad \text{damp at large } r \]

Eigenvalue problem of complex-scaled Hamiltonian \[ H(\theta) = U(\theta) H U^{-1}(\theta) \]

\[ H(\theta) \Psi_{\lambda}^{JM\pi}(\theta) = E_\lambda(\theta) \Psi_{\lambda}^{JM\pi}(\theta) \quad \text{can be solved with } L^2 \text{ basis within suitable } \theta \]

\[ \Psi_{\lambda}^{JM\pi}(\theta) = \sum_i C_i^\lambda(\theta) \Phi_i(x) \]

\[ S(E) = -\frac{1}{\pi} \text{Im} \sum_{\mu} \langle \Psi_0 | \mathcal{M}_{1\mu}^\dagger U^{-1}(\theta) R(\theta) U(\theta) \mathcal{M}_{1\mu} | \Psi_0 \rangle \]

\[ = -\frac{1}{\pi} \sum_{\mu} \text{Im} \frac{\tilde{D}_{\mu}(\theta) D_{\mu}(\theta)}{E - E_\lambda(\theta) + i\epsilon} \]

\[ D_{\mu}(\theta) = \langle (\Psi_{\lambda}^{JM\pi}(\theta))^* | \mathcal{M}_{1\mu}(\theta) | U(\theta) \Psi_0 \rangle \]
The contribution of eigenstate $\lambda$ to $S(E)$
\[ E_\lambda(\theta) = E_c - \frac{i}{2} \Gamma_c \]
\[
\frac{1}{\pi} \frac{1}{(E - E_c)^2 + \frac{1}{4} \Gamma_c^2} \sum_\mu \left[ \frac{1}{2} \Gamma_c \text{Re} \tilde{\mathcal{D}}^{\lambda}_{\mu}(\theta) \mathcal{D}^{\lambda}_{\mu}(\theta) - (E - E_c) \text{Im} \tilde{\mathcal{D}}^{\lambda}_{\mu}(\theta) \mathcal{D}^{\lambda}_{\mu}(\theta) \right]
\]
Lorentz distribution

$\theta$ dependence of $H(\theta)$

kinetic energy
\[ T \rightarrow T e^{-2i\theta} \]

potential energy
- exponential
  \[ e^{-r/\mu} \rightarrow e^{-r(\cos \theta + i \sin \theta)/\mu} \quad \mu \rightarrow \mu/\cos \theta \]
- Gaussian
  \[ e^{-r^2/\mu^2} \rightarrow e^{-r^2(\cos 2\theta + i \sin 2\theta)/\mu^2} \quad \mu \rightarrow \mu/\sqrt{\cos 2\theta} \]

$0 < \theta < 45^\circ$

Continuum energy scales as $k^2 e^{-2i\theta}$

Bound states and resonances should be stable against $\theta$

Useful check

Two-body photoabsorption cross section and radiative capture cross section
\[ \gamma + C \leftrightarrow A + B \]

Detailed balance
\[ \sigma_\gamma^{AB}(E_\gamma) = \frac{k^2(2J_A + 1)(2J_B + 1)}{2k_\gamma^2(2J_0 + 1)} \sigma_{\text{cap}}^{AB}(E_{\text{in}}) \quad E_{\text{in}} = E_\gamma - E_{\text{th}} \]

$\sigma_{\text{cap}}^{AB}$ can be calculated in a standard reaction theory: serve as a test of CSM
Photoabsorption of $^4$He

$$\sigma_\gamma(E_\gamma) = \frac{4\pi^2}{\hbar c} E_\gamma \left(\frac{1}{3}S(E_\gamma)\right)$$

Physics motivation:
Experimental discrepancy in low-energy $\sigma_\gamma$ E1 sum rule

Basis functions for E1 excitation:
sum rule, 2- and 3-body decay channels
(cluster model)

$$\Psi_{f}^{\text{sp}} = A\left[\Phi_{0}^{(4)}(i)\chi_{1}(r_{1} - x_{4})\right]_{1M}$$
Important for sum rule

$$\Psi_{f}^{3\text{N}+\text{N}} = A\left[\Phi_{J_{3}}^{(3)}(i) \exp\left(-a_{3}x_{3}^{2}\right)\chi_{1}(x_{3})\chi_{2}^{(4)}\right]_{1M}$$

$$\Psi_{f}^{d+p+n} = A\left[\Phi_{J_{3}}^{(dN)}(i) \exp\left(-a_{3}x_{3}^{2}\right)\chi_{0}(x_{3})\chi_{2}^{(4)}\right]_{1M}$$

$$\Phi_{J_{3}}^{(dN)}(i) = \left[\Psi_{J_{2}}^{(2)}(i) \exp\left(-a_{2}x_{2}^{2}\right)\chi_{1}(x_{2})\chi_{2}^{(3)}\right]_{J_{3}}$$

coordinates acted by E1 operator

AV8’ + 3NF
Comparison with experiment

θ dependence

Check of CSM

(Microscopic R-matrix calculation)
Sum rule

\[ m_k(E_{\text{max}}) = \int_0^{E_{\text{max}}} E_\gamma \sigma_\gamma(E_\gamma) \, dE_\gamma \]

NEWSR \[ m_{-1}(\infty) = G \left( Z^2 \langle r_p^2 \rangle - \frac{Z(Z-1)}{2} \langle r_{pp}^2 \rangle \right) \]

EWSR \[ m_0(\infty) = G \frac{3N Z \hbar^2}{2Am_N}(1 + K) \]

Enhancement factor \[ K = \sum_q K_q \quad V_{2\text{NF}} = \sum_q V_q \]

\[ K_q = \frac{2Am_N}{3NZ\hbar^2 e^2} \frac{1}{2} \sum_\mu \langle \Psi_0 | [\mathcal{M}_{1\mu}^\dagger, [V_q, \mathcal{M}_{1\mu}]] | \Psi_0 \rangle \]

<table>
<thead>
<tr>
<th>( q )</th>
<th>( \langle V_q \rangle )</th>
<th>( K_q )</th>
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<tr>
<td>1</td>
<td>17.39</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>( \sigma_i \cdot \sigma_j )</td>
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</tr>
<tr>
<td>3</td>
<td>( \tau_i \cdot \tau_j )</td>
<td>-5.22</td>
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<td>4</td>
<td>( \sigma_i \cdot \sigma_j \tau_i \cdot \tau_j )</td>
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<td>( \tau_i \cdot \tau_j )</td>
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<td>5</td>
<td>( S_{ij} )</td>
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<tr>
<td>6</td>
<td>( S_{ij} \tau_i \cdot \tau_j )</td>
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<tr>
<td>( (L \cdot S)_{ij} )</td>
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<td>(0.667 )</td>
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<td>7</td>
<td>( (L \cdot S)_{ij} \tau_i \cdot \tau_j )</td>
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<tr>
<td>Total</td>
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Major contribution by one-pion exc. force
Spin-dipole excitations of $^4$He

SD operator

$$\sum_{i=1}^{N} [\rho_i \times \sigma_i]_{\lambda\mu} T_i^p$$

$$\rho_i = r_i - x_N$$

$$T_i^p = \begin{cases} 
1 & \text{Isoscalar (IS)} \\
t_z(i) & \text{Isovector (IV0)} \\
t_{\pm}(i) & \text{Charge-exc. (IV$\pm$)} \quad (^4\text{H}, ^4\text{Li})
\end{cases}$$

$\lambda=0,1,2$ (multipolarity)

Good correspondence between the peak energy and the resonance energy

SD resonance is narrower than E1 resonance
Resonance parameters

<table>
<thead>
<tr>
<th>$J^\pi T$</th>
<th>$E_R$</th>
<th>Exp.</th>
<th>$\Gamma$</th>
<th>Exp.</th>
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<td></td>
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<td>$S(E)$</td>
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<td>0$^-$0</td>
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<td>13.24</td>
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</table>

$E(\theta)$: Stable eigenvalues of $H(\theta)$

$S(E)$: Peaks of strength function

B.A.: Bound-state approximation

Almost no data that can be compared to theoretical SD strength functions

Charge-exc. reaction $^4\text{He}({^7}\text{Li}, {^7}\text{Be}\gamma)$

Spin-nonflip parts $\rightarrow$ E1

Spin-flip parts $\rightarrow$ SD

Nakayama et al., PRC76 (2007)
Electric dipole excitations of halo nuclei

$^6\text{He}$

$\alpha+n+n$ three-body model is fairly good

E1 response of $^6\text{He}$ has so far been studied within the three-body model

E1 strength is calculated in 6-body model that makes it possible to treat **both low- and high-lying strengths**

Minnesota potential fitted to $S_{2n}$ is used ($u=1.05$)

$^6\text{He}$ ground state in six-body model
good convergence in a small dimension

Comparison of B(E1) for $^4\text{He}$

Minnesota

AV8'}
Calculation is continuum discretization taking into account 3-body decay channels of $\alpha+n+n$ and $t+d+n$. Basis dimension used for $J^{\pi}=1^{-}$ ($T=1, 2, 3$) continuum is about 14,000.
Smearing with Lorenzians

\[
\frac{dB(E1,E)}{dE} = \sum_{\nu} N(E_\nu, \Gamma)L(E, E_\nu, \Gamma)B(E1, \nu)
\]

\[L(E, E_\nu, \Gamma) = \frac{\Gamma}{2\pi} \frac{1}{(E - E_\nu)^2 + (\Gamma/2)^2}\]

SDM vs GDR

\[\Gamma = 0.75 - 2.0\,\text{MeV}\]

Aumann et al., PRC59 (1999)

\[u = 1.05\] reproducing \(S_{2n}\) leads to the enhancement of low-lying strength (SDM)

Larger \(u\) leads to stronger binding of neutrons:

SDM shrinks but GDR survives

A few peaks exists between SDM and GDR

SDM peak is much larger than GDR peak

Proton-proton rms distance of the discretized continuum states

\[\tau_{pp}/\tau_{\text{pp}}(\text{He})\]

Sudden rise at about 25 MeV
Proton and neutron transition densities

$$\rho_{p/n}^{\text{tr}}(E_v, r) = \langle \Psi_1(E_v) \| \sum_{i \in p/n} \mathcal{V}_1(r_i - x_6) \delta(|r_i - x_6| - r) \| \Psi_0 \rangle$$

Below 25 MeV:
In-phase oscillation inside the $^4$He core
Out-of-phase oscillation near the surface
Growing oscillations of halo neutrons with E

Completely out-of-phase at GDR
E1 NEWSR

\[ \sum_{\nu} B(E1, \nu) = e^2 \left( Z^2 \langle r_p^2 \rangle - \frac{Z(Z-1)}{2} \langle r_{ppl}^2 \rangle \right) \quad 7.21 \, e^2 \text{ fm}^2 \]

Full model accounts for 99.9% of NEWSR

Cluster sum rule (CSR) \hspace{1cm} \text{Alhassid, Gai, Bertsch, PRL 49 (1982)}

\[ B(E1; NEWCSR) = e^2 \left( \frac{2Z}{A} \right)^2 \langle R^2 \rangle \quad 5.44 \, e^2 \text{ fm}^2 \]

(75% of NWESR)

Maximum excitation energy that exhausts CSR

\[ \sum_{\nu=1}^{\nu_{\text{max}}} B(E1, \nu) \quad E_{\nu_{\text{max}}} = 26.8 \text{ MeV} \]

SDM and GDR are well separated
E1 strength below 25 MeV is understood with $\alpha$+n+n 3-body structure
SDM consists of T=1 states while GDR of T=2 states
Neutron-dripline nucleus
Borromean as $^{20}\text{C}+\text{n}+\text{n}$ system (S-wave 2n halo)
Very large matter radius from reaction cross section; $5.4 \pm 0.9$ fm
Tanaka et al., PRL104 (2010)

Very small but poorly known $S_{2n}$: $-0.14 \pm 0.46$ MeV
Gaudefroy et al., PRL109 (2012)

The aim is to study both the ground state properties and low-lying E1 strength without assuming the $^{20}\text{C}$ core
Mean-field approach with Skyrme energy density functionals
Random-phase approximation

Difficult to reproduce 3-body structure
SIII central part is weakened to reproduce the dripline features

$f_0=0.884$: $\varepsilon_F=-0.5$ MeV
rms matter radius=3.89 fm
rms radius of $2s_{1/2}$ orbit=7.20 fm
$2s_{1/2}$ and $1d_{5/2}$ orbits are nearly degenerate
($S_{2n}$ negative: $^{22}\text{C}$ spherical, $^{20}\text{C}$ oblate)
E1 strength

Large low-lying strength comparable to that of GDR
‘Giant’ low-lying resonance (much larger than usual PDR)
EWS occupies 6 and 15% of TRK sum at $E_{\text{exc}}=5$ and 10 MeV, respectively
EWS exceeds EWCSR at $E_{\text{exc}}=3.3$ MeV
$1d_{5/2}$ orbit excitation is important

$S(E1) [e^2 fm^2/MeV]$ $E.W.S. [%TRK/MeV]$

Excitation Energy [MeV]

FIG. 6. (Color online) Calculated $^{22}$C dipole strength function distributions for separation energies $S_{2n} = 50, 100, 200,$ and 400 keV (upper to lower curves). The insert compares dipole strength distributions for $S_{2n} = 10$ keV (upper line) and 50 keV (lower line).

Low-lying strength is very sensitive to $S_{2n}$
The effect of core excitation makes difference beyond $E_{\text{exc}} > 2$ MeV

$S_{2n}=0.4$ MeV $E_T$ (MeV)

$^{20}$C+n+n 3-body model
Ershov, Vaagen, Zhukov, PRC86 (2012)
GDR peak: out-of-phase inner oscillation with oscillating extended neutron tail
Low-lying peaks: SDM like pattern
Neutron density extends to 25 fm

Comparison of E1 strength between $^6$He and $^{22}$C
The pattern of the strength is similar, but the origin of the strength between low-lying resonance and GDR is not the same:
- halo-neutron excitation in $^6$He
- both halo-neutron and 1d$_{5/2}$ orbit excitations in $^{22}$C
(may depend on the degeneracy of orbits near Fermi surface)
\[ ^{12}\text{C} + n + n + p + p \text{ calculation for } 0^+ \text{ states in } ^{16}\text{O} \]

\[ ^{16}\text{O} \text{ is doubly magic} \]
\[ \text{The first excited state is } 0^+ \text{ at 6.05 MeV} \]
\[ \text{Contradiction to the shell-model filling of single particle orbits} \]
\[ \text{Multiparticle-multihole (esp. 4p-4h) configurations in deformation} \]
\[ \text{Shape coexistence} \]

\[ \text{Several recent attempts:} \]
\[ \text{Configuration mixing of Slater determinants} \]
\[ \text{Bender, Heenen NPA713 (2003)} \]
\[ \text{Shinohara et al., PRC74 (2006)} \]

\[ \text{Large-scale calculations: NCSM} \]
\[ \text{Maris et al., PRC79 (2009)} \]
\[ \text{CCT} \]
\[ \text{Wloch et al., PRL94 (2005)} \]

\[ \text{Semi-microscopic } ^{12}\text{C} + \alpha \text{ 2-cluster model} \]
\[ \text{Suzuki, PTP55,56 (1976)} \]
\[ \text{Rotation of } ^{12}\text{C} \text{ and Pauli constraint for two-cluster relative motion} \]
\[ \text{All } T=0 \text{ levels below } E_{\text{exc}}=15 \text{ MeV but 10.96(0^-) are reproduced} \]
\[ \text{Electric transitions and } \alpha \text{-decay widths} \]

\[ \text{The aim is to understand the coexisting mechanism by performing 5-body calculation without assuming a preformed } \alpha \text{-cluster} \]
\[ ^{12}\text{C} \text{ is assumed to remain in its ground state} \]
\[ 4\text{-nucleon dynamics is solved by excluding the occupied orbits in } ^{12}\text{C} \]
\[ H = T_v + T_{cv} + V_v + V_{cv} \]

- **Intrinsic kinetic energy of four valence nucleons**
  \[ T_v = \sum_{i=1}^{4} T_i - T_{c.m.} \]

- **Kinetic energy between c-v**
  \[ T_{cv} \]

- **Potential energy among valence nucleons**
  \[ V_v = \sum_{i<j} v_{ij} \]

- **Potential energy between c-v**
  \[ V_{cv} = \sum_{i=1}^{4} U_i \]

Minnesota potential, Woods-Saxon potential to fit $^{13}\text{C}$ (1/2$^-$, 1/2$^+$, 5/2$^+$)

**Pauli constraint**: \[ \Gamma_i |\Psi \rangle = 0 \]

Projection operator onto 0$s_{1/2}$ and 0$p_{3/2}$ HO orbits

Add a pseudo potential $\lambda \sum_{i=1}^{4} \Gamma_i$ to Hamiltonian

$\lambda$ is taken very large

**Basis functions**

\[ \mathcal{A}\{ e^{-\frac{1}{2} \vec{x}^2} [ \mathcal{Y}_L(\hat{u}_1 \vec{x} \mathcal{Y}_L(\hat{u}_2 \vec{x})]_L \chi_L]_{00} \eta_{TM_T} \} \]

$\lambda=0,1,2; \ T=0$

Calculation reproduces the two 0$^+$ states in agreement with experiment

Slow convergence because many bases are needed to eliminate the forbidden states
Energy contents of four nucleons in the $0_2^+$ state are similar to that of $\alpha$-particle.
Summary

We have applied ECG to bound and continuum problems
Two $0^+$ states in both $^4$He and $^{16}$O
Photoabsorption cross section of $^4$He with CSM
(cluster concept is useful to construct basis functions for decay channels)
E1 response of $^6$He
Resonances of A=4 systems analyzed with help of response functions

The pseudopotential for eliminating Pauli-forbidden orbits makes convergence very slow: other way to accelerate convergence is desired

Future challenges

Non-inert core plus 4-nucleon approach
$^{12}$C($0^+, 2^+$)+n+n+p+p
1- states (7.12, 9.58) and 2+ (6.92) state
E1 and E2 radiative capture reactions $^{12}$C($\alpha, \gamma$)$^{16}$O at Helium burning stage
Isospin impurity has to be taken into account for E1
$^{208}$Pb($0^+, 3^-$)+n+n+p+p
$\alpha$-decay width and enhanced E1 transitions in $^{212}$Po

Varga, Lovas, Liotta, PRL 69 (1992); NPA 550 (1992)
Astier et al., PRL 104 (2010)
Collaborators and References:

ECG with realistic forces:

$^4$He:
  W. Horiuchi, Y.S., PRC 78 (2008), PRC 87 (2013), FBS 54 (2013),
  PRC 90 (2014)

$^6$He:
  D. Mikami, W. Horiuchi, Y.S., PRC 89 (2014)

$^{16}$O:
  W. Horiuchi, Y.S., PRC 89 (2014)

$^{22}$C:
Enhanced E1 transitions in $^{212}$Po

$^{208}$Pb($^{18}$O, $^{14}$C)

Astier et al. (2010)

Negative parity states at low excitation!

$B(E1) \sim 10^{-3}$ W.u.

Different centers of mass and charge