Resonant and scattering states in the nonlocalized cluster model

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DB and Zhongzhou Ren, PRC 101, 034311 (2020). Hantao Zhang, DB, Zhen Wang, and Zhongzhou Ren, PRC 105, 054317 (2022).

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1

Outline

1 Nuclear clustering

- What's cluster states? Why it is important?
- What's nonlocalized clustering?
- Why resonant and scattering states?
- 2 Theoretical formalism
 - Nonlocalized cluster model
 - \cdots + the *R*-matrix theory
 - \cdots + complex scaling method (CSM)
- 3 The $\alpha + \alpha$ system as a proof of concept
 - The bound-state approximation
 - The *R*-matrix results
 - The CSM results

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Nuclear clustering: Phenomenological viewpoint I

Nuclei are self-bound systems made of protons and neutrons.



 α clusters could be taken as effective building blocks, e.g., ⁸Be $\approx \alpha + \alpha$, ¹²C $\approx \alpha + \alpha + \alpha$, ¹⁶O $\approx \alpha + \alpha + \alpha + \alpha$,

This picture could also be extended to the **heavier** clusters, e.g., ${}^{16}\text{O} \approx \alpha + {}^{12}\text{C}$, ${}^{20}\text{Ne} \approx \alpha + {}^{16}\text{O}$, ${}^{44}\text{Ti} \approx \alpha + {}^{40}\text{Ca}$, \cdots .

Nuclear clustering: Phenomenological viewpoint II

• **Cluster radioactivity**: spontaneous emissions of α particles, ¹⁴C, ²⁰O, ²⁴Ne, · · · from heavy nuclei.



A natural explanation: the emitted cluster first **preforms** inside the **unstable** parent nucleus and then **escapes** via quantum tunneling ⇒ Nuclear clustering in **radioactive** heavy nucleus (任老师团队)

• What about the stable heavy nucleus? Cluster-knockout reaction.



Nuclear clustering: Theoretical viewpoint

Consider a nuclear many-body Schrödinger equation

$$\left(T + \sum_{ij} V_{ij} + \sum_{ijk} V_{ijk}\right) |\Psi\rangle = E |\Psi\rangle,$$

and we want to make **approximations** to the exact wave function $|\Psi\rangle$.



• Which model is better?

 \circ Compare $\langle \mathcal{O} \rangle_{\text{Model}} \equiv \langle \text{Model} | \mathcal{O} | \text{Model} \rangle$ and $\langle \mathcal{O} \rangle_{\Psi} \equiv \langle \Psi | \mathcal{O} | \Psi \rangle$; the closer, the better. Often, systematical improvements can be made upon the good models.

 \circ Cluster state: the cluster configurations are crucial, especially when $(\langle \mathcal{O} \rangle_{CM} - \langle \mathcal{O} \rangle_{\Psi})^2 \ll (\langle \mathcal{O} \rangle_{SM} - \langle \mathcal{O} \rangle_{\Psi})^2.$

It would be nice if there is one model killing all the problems.

Shell model was thought to be a candidate. (Un)Fortunately, life is not that easy!

"Rebellious sons": the Hoyle state, cluster decays from heavy elements



R. Roth et al., PRL 107, 072501 (2011): NCSM + SRG + chiral potentials

Localized Clustering vs Nonlocalized Clustering

How to model a cluster state?

Building blocks: clusters made of nucleons



Nonlocalized cluster model is proposed by 周波, Y. Funaki, H. Horiuchi, 任老师 etc, PRL 110, 262501 (2013), often a better starting point.

Resonant and Scattering States: Phenomenological Viewpoint

Consider the elastic scattering $a + A \rightarrow a + A$. Its cross section is given by \sim

$$\sigma_{\rm el} = \frac{4\pi}{k^2} \sum_{L=0}^{\infty} (2L+1) \sin^2 \delta_L.$$

Naïvely, $k \uparrow, E \uparrow, \sigma_{el} \downarrow$. The presence of resonance invalidates this expectation.



Resonant and Scattering States: Theoretical Viewpoint

Boundary conditions of Schrödinger equations

$$-\frac{\mathrm{d}^2}{\mathrm{d}r^2}\phi(r) + V(r)\phi(r) = k^2\phi(r).$$

V(r) is short-range $\Rightarrow \phi(r) \rightarrow A \exp(-ikr) + B \exp(ikr)$, as $r \rightarrow \infty$.

- **Scattering state**: $k^2 > 0$, $\phi_S(r) \rightarrow \exp(-ikr) + S(k) \exp(ikr)$
- Bound state: $k^2 < 0, \phi_B(r) \rightarrow B \exp(-\kappa r), \kappa = |k|.$
- **Resonant state**: Re k > 0, Im k < 0, $\phi_{R}(r) \rightarrow \exp(ikr) \propto \exp(i\operatorname{Re} kr) \times \exp(-\operatorname{Im} kr)$, blowing up in infinity, $\mathcal{E}_{res} = E - i\Gamma/2 = |\widetilde{E}| \exp(-2i\theta_{R}) \Rightarrow \theta_{R} = \frac{1}{2} \arctan(\frac{\Gamma}{2E}).$

Pole structures of S-matrix



Why the resonant state is important for nuclear clustering?



Bound-state approximation: suitable for resonant cluster states with narrow widths

Pros:

- 1. intuitive physical picture
- 2. bound-state codes reusable

Cons:

 not easy to distinguish between resonant and scattering states, especially for broad resonances
 physical picture sometimes inaccurate

 $\circ~^8\text{Be}(2^+_1)$, a member of the ground-state band of ^8Be , has a large decay width \sim 3 MeV compared to its total energy \sim 1.5 MeV above the 2α threshold.

 \circ $^{12}C(0^+_3)$, which is conjectured to be a breathing mode of the Hoyle state $^{12}C(0^+_2)$, has a large decay width \sim 1.45 MeV compared to its total energy \sim 1.77 MeV above the 3α threshold.

 \Rightarrow A proper treatment of their resonant nature is important.

Goal I

Improving nonlocalized cluster model for resonances.

Why study the scattering states in microscopic cluster models? Main reasons:

1. Scattering states are important ingredients in nuclear reaction theories, e.g., elastic scattering, breakup reaction (CDCC: continuum-discretized coupled channels), etc.

2. Microscopic reaction models are less explored than structural models. The initial and final states naturally contain "clusters" \Rightarrow Microscopic cluster models play a role naturally.

3. Interesting by itself, potential applications in nuclear astrophysics.

Goal II

Studying the nucleus-nucleus elastic scattering in nonlocalized cluster model.

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Nonlocalized Cluster Model

The α -cluster wave function

$$\begin{split} \Phi_{\alpha}(\boldsymbol{R}) &= \frac{1}{\sqrt{4!}} \det\{\varphi_{0s}(\boldsymbol{r}_1 - \boldsymbol{R})\chi_{\sigma_1\tau_1}\cdots\varphi_{0s}(\boldsymbol{r}_4 - \boldsymbol{R})\chi_{\sigma_4\tau_4}\},\\ \varphi_{0s}(\boldsymbol{r}) &= (\pi b^2)^{-3/4} \exp\left[-\frac{\boldsymbol{r}^2}{2b^2}\right]. \end{split}$$

Brink wave function

$$\Phi_{\mathrm{B}}(\boldsymbol{R}) = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{8!}} \det\{\varphi_{0s}(\boldsymbol{r}_{1} - \boldsymbol{R}/2)\chi_{\sigma_{1}\tau_{1}}\cdots\varphi_{0s}(\boldsymbol{r}_{4} - \boldsymbol{R}/2)\chi_{\sigma_{4}\tau_{4}} \\ \times \varphi_{0s}(\boldsymbol{r}_{5} + \boldsymbol{R}/2)\chi_{\sigma_{1}\tau_{1}}\cdots\varphi_{0s}(\boldsymbol{r}_{8} + \boldsymbol{R}/2)\chi_{\sigma_{4}\tau_{4}}\}.$$



Tohsaki-Horiuchi-Schuck-Röpke (THSR) wave function



Separation of center-of-mass motion

$$\begin{split} \Psi(\beta,\mathbf{T}) &= \Psi_{\rm CM}(\mathbf{X}_{\rm CM}) \times \widehat{\Psi}(\beta,\mathbf{T}), \\ \Psi_{\rm CM}(\mathbf{X}_{\rm CM}) &= \left(\frac{8}{\pi b^2}\right)^{3/4} \exp\left(-\frac{4\mathbf{X}_{\rm CM}^2}{b^2}\right), \\ \widehat{\Psi}(\beta,\mathbf{T}) &= \frac{1}{\sqrt{140}} \mathscr{A}_{12} \left[\Gamma(\boldsymbol{\rho},\beta,\mathbf{T})\widehat{\phi}(\alpha_1)\widehat{\phi}(\alpha_2)\right] \Rightarrow u(\boldsymbol{\rho}), \\ \Gamma(\boldsymbol{\rho},\beta,\mathbf{T}) &= \left(\frac{2}{\pi}\right)^{3/4} \frac{b^{3/2}}{(b^2+2\beta^2)^{3/2}} \exp\left[-\frac{(\boldsymbol{\rho}-\mathbf{T})^2}{b^2+2\beta^2}\right]. \end{split}$$

Angular momentum projection

$$\begin{split} \Psi(\beta, \mathbf{T}) &= \Psi_{\rm CM}(\mathbf{X}_{\rm CM}) \times 4\pi \sum_{LM} \widehat{\Psi}_{LM}(\beta, T) Y_{LM}^*(\Omega_T), \\ \widehat{\Psi}_{LM}(\beta, T) &= \frac{1}{\sqrt{140}} \mathscr{A}_{12} \Gamma_L(\rho, \beta, T) Y_{LM}(\Omega_\rho) \widehat{\phi}(\alpha_1) \widehat{\phi}(\alpha_2) \Rightarrow \frac{u_L(\rho)}{\rho} Y_{LM}(\Omega_\rho), \\ \Gamma_L(\rho, \beta, T) &= \left(\frac{2}{\pi}\right)^{3/4} \frac{b^{3/2}}{(b^2 + 2\beta^2)^{3/2}} \exp\left(-\frac{\rho^2 + T^2}{b^2 + 2\beta^2}\right) \mathbf{i}_L \left(\frac{2\rho T}{b^2 + 2\beta^2}\right). \end{split}$$

Interaction Model

The Hamiltonian is given by

$$H = T - T_{\rm CM} + V_N + V_C,$$

$$T - T_{\rm CM} = -\sum_{i=1}^{A} \frac{1}{2m} \left(\frac{\partial}{\partial \mathbf{r}_i}\right)^2 + \frac{1}{2Am} \left(\frac{\partial}{\partial \mathbf{X}_{\rm CM}}\right)^2$$

Effective nucleon-nucleon interactions are adopted in nonlocalized cluster models, as well as many other microscopic cluster models.

$$V_{N,ij}(r) = \sum_{k=1}^{N_g} V_k \exp\left[-(r/a_k)^2\right] \left(w_k - m_k P_{ij}^{\sigma} P_{ij}^{\tau} + b_k P_{ij}^{\sigma} - h_k P_{ij}^{\tau}\right).$$

Interaction	k	V_k (MeV)	a_k (fm)	w _k	m_k	b_k	h_k
Volkov No. 1	1	-83.34	1.60	1 - M	M	0	0
	2	144.86	0.82	1 - M	M	0	0
Minnesota	1	200	$1/\sqrt{1.487}$	u/2	1 - u/2	0	0
	2	-178	$1/\sqrt{0.639}$	u/4	1/2 - u/4	u/4	1/2 - u/4
	3	-91.85	$1/\sqrt{0.465}$	u/4	1/2 - u/4	-u/4	u/4 - 1/2

Single basis wave function:

• THSR:
$$E_L(\beta) = \min \frac{\langle \widehat{\Psi}_{LM}(\beta) | H_L | \widehat{\Psi}_L M(\beta) \rangle}{\langle \widehat{\Psi}_{LM}(\beta) | \widehat{\Psi}_{LM}(\beta) \rangle}$$
.
• Brink-THSR: $E_L(\beta, T) = \min \frac{\langle \widehat{\Psi}_{LM}(\beta, T) | H_L | \widehat{\Psi}_{LM}(\beta, T) \rangle}{\langle \widehat{\Psi}_{LM}(\beta, T) | \widehat{\Psi}_{LM}(\beta, T) \rangle}$

Multiple basis wave functions:

• THSR:
$$\widetilde{\Psi}_{LM} = \int d\beta f(\beta) \,\widehat{\Psi}_{LM}(\beta).$$

• Brink-THSR: $\widetilde{\Psi}_{LM}(\beta) = \int dT f(T) \,\widehat{\Psi}_{LM}(\beta, T).$

 \Rightarrow variational principle \Rightarrow Hill-Wheeler equation.

\cdots + the *R*-Matrix Theory

	$\Psi^{ m int}_{ m LM}({ m a}),$	(a)=Ψ _I /da=d¥	$_{LM}^{xt}(a)$ $P_{LM}^{ext}(a)/da$
	$V_N + V_C$ $\Psi^{ ext{int}}_{ ext{LM}}(ho)$		$\frac{V_C}{\Psi_{LM}^{\text{ext}}(\rho) \propto [H_L^{(-)}(\rho) - S_L H_L^{(+)}(\rho)] / \rho \text{ (scattering state)}}{\Psi_{LM}^{\text{ext}}(\rho) \propto H_L^{(+)}(\rho) / \rho \text{ (resonant state)}}$
0	interior region	a	exterior region ρ

υ interior region a exterior region

$$\eta = Z_{\alpha}^{2} e^{2} \sqrt{\frac{\mu}{2E}} \text{ Coulomb-Sommerfeld parameter}$$
$$\widehat{\Psi}_{LM}^{\text{int}}(E) = \int dT f_{L}(T, E) \widehat{\Psi}_{LM}(\beta, T) = \sum_{n} \widetilde{f}_{L}(T_{n}, E) \widehat{\Psi}_{LM}(\beta, T_{n}),$$
$$\widehat{\Psi}_{LM}^{\text{ext}}(E) = \frac{1}{\sqrt{35}} g_{L}^{\text{ext}}(\rho) Y_{LM}(\Omega_{\rho}) \widehat{\phi}(\alpha_{1}) \widehat{\phi}(\alpha_{2}),$$

 $\Rightarrow (H_L + \mathcal{L}(B) - E)\Psi_{IM}^{int} = \mathcal{L}(B)\Psi_{IM}^{ext}$ Bloch-Schrödinger equation $\mathcal{L}(B) = 35 \frac{1}{2\mu a} \delta(\rho - a) \left(\frac{\mathrm{d}}{\mathrm{d}\rho} - B\right)$

Scattering state: B = 0

$$\begin{split} \sum_{n'} [C(0,E)]_{nn'} \widetilde{f}_L(T_{n'},E) &= \langle \widehat{\Psi}_L(\beta,T_n) | \mathcal{L}(0) | \widehat{\Psi}_L^{\text{ext}}(E) \rangle ,\\ [C(0,E)]_{nn'} &= \left(\widehat{\Psi}_L(\beta,T_n) \Big| H_L + \mathcal{L}(0) - E \Big| \widehat{\Psi}_L(\beta,T_{n'}) \right) ,\\ \mathcal{R}_L &= \frac{a}{2\mu} \sum_{nn'} \Gamma_L(a,\beta,T_n) [C(0,E)]_{nn'}^{-1} \Gamma_L(a,\beta,T_{n'}),\\ \mathcal{S}_L &= \frac{\mathcal{H}_L^{(-)}(\eta,ka) - ka \mathcal{H}_L^{(-)'}(\eta,ka) \mathcal{R}_L}{\mathcal{H}_L^{(+)}(\eta,ka) - ka \mathcal{H}_L^{(+)'}(\eta,ka) \mathcal{R}_L}. \end{split}$$

Resonant state: $B = B_* \equiv ka \frac{\mathcal{H}_L^{(+)'}(\eta, ka)}{\mathcal{H}_L^{(+)}(\eta, ka)}$

$$\sum_{n'} \left(\widehat{\Psi}_L(\beta, T_n) | H_L + \mathcal{L}(B_*) | \widehat{\Psi}_L(\beta, T_{n'}) \right) \widetilde{f}_L(T_{n'}, E)$$
$$= E \sum_{n'} \left(\widehat{\Psi}_L(\beta, T_n) | \widehat{\Psi}_L(\beta, T_{n'}) \right) \widetilde{f}_L(T_{n'}, E).$$

self-consistent generalized eigenvalue problem

\cdots + Complex Scaling Method (CSM)

Complex scaling transformation

$$\mathbf{r} \to \mathbf{r} \exp(i\theta), \qquad \psi(\mathbf{r}) \to \exp(i3\theta/2) \,\phi(\mathbf{r} \exp(i\theta)).$$

$$\Rightarrow \text{similarity transformation } S(\theta) = \prod_{j} [\exp(3i\theta/2) \exp(i\theta\mathbf{r}_{j} \cdot \nabla_{j})],$$

$$H \to S(\theta) H S(\theta)^{-1}, \quad \Psi \to S(\theta) \Psi.$$

The Schrödinger equation:

$$-\frac{d^2}{dr^2}\phi(r) + V(r)\phi(r) = k^2\phi(r)$$

$$\Rightarrow -\exp(-2i\theta)\frac{d^2}{dr^2}\phi_\theta(r) + V(r\exp(i\theta))\phi_\theta(r) = k^2\phi_\theta(r).$$

Square integrable eigensolutions:

 $\begin{aligned} &\circ \text{Bound state: } \phi_{\text{B}}(r) \propto \exp(-\kappa r) \to \phi_{\text{B}}^{\theta}(r) \propto \exp(-\kappa r \exp(i\theta)) \\ &\circ \text{Resonant state: } \phi_{\text{R}}(r) \propto \exp(i|k| \exp(-i\theta_{\text{R}})r) \Rightarrow \\ &\phi_{\text{R}}^{\theta}(r) \propto \exp(i|k|r \exp(-i\theta_{\text{R}} + i\theta)); \text{ when } \theta > \theta_{\text{R}}, \phi_{\text{R}}^{\theta}(r) \to 0 \text{ as } r \to \infty. \\ &\circ \text{Scattering state: } \phi_{\text{R}}(r) \propto A \exp(-ikr) + B \exp(ikr) \Rightarrow \\ &\phi_{\text{R}}^{\theta}(r) \propto A \exp(-ikr \exp(i\theta)) + B \exp(ikr \exp(i\theta)); \text{ when } k \to k \exp(-i\theta), \\ &\text{square integrable, discretized energy.} \end{aligned}$

22



⇐ ABC theorem by Aguilar, Combes, and Balslev.

$$\circ H \to H_{\theta} = \exp(-2i\theta)(T - T_{\rm CM}) + \sum_{i < j} \left[V_N(r_{ij} \exp(i\theta)) + V_C(r_{ij} \exp(i\theta)) \right],$$

 \circ The complex scaled $\alpha\text{-cluster}$ wave function

$$\Phi^{\theta}_{\alpha}(\boldsymbol{R}) = \frac{1}{\sqrt{4!}} \det\{\varphi^{\theta}_{0s}(\boldsymbol{r}_1 - \boldsymbol{R})\chi_{\sigma_1\tau_1}\cdots\varphi^{\theta}_{0s}(\boldsymbol{r}_4 - \boldsymbol{R})\chi_{\sigma_4\tau_4}\},$$

$$\varphi^{\theta}_{0s}(\boldsymbol{r}) = (\pi b^2 \exp(-2i\theta))^{-3/4} \exp\left[-\frac{\boldsymbol{r}^2}{2b^2 \exp(-2i\theta)}\right].$$
 23

• Complex scaled Brink wave function

$$\begin{split} \Phi_{\mathrm{B}}^{\theta}(\boldsymbol{R}) &= \frac{1}{\sqrt{2}} \frac{1}{\sqrt{8!}} \mathrm{det} \{ \varphi_{0s}^{\theta}(\boldsymbol{r}_{1} - \boldsymbol{R}/2) \chi_{\sigma_{1}\tau_{1}} \cdots \varphi_{0s}^{\theta}(\boldsymbol{r}_{4} - \boldsymbol{R}/2) \chi_{\sigma_{4}\tau_{4}} \\ &\times \varphi_{0s}^{\theta}(\boldsymbol{r}_{5} + \boldsymbol{R}/2) \chi_{\sigma_{1}\tau_{1}} \cdots \varphi_{0s}^{\theta}(\boldsymbol{r}_{8} + \boldsymbol{R}/2) \chi_{\sigma_{4}\tau_{4}} \}. \end{split}$$

Doing the substitution $\mathbf{r} \rightarrow \mathbf{r} \exp(-i\theta)$ in the matrix elements

$$\begin{split} H_{\theta} &\to H, \\ \varphi_{0s}^{\theta}(\mathbf{r}_{1} - \mathbf{R}/2) &\to \exp(-i3\theta/2)\varphi_{0s}^{\theta}(\mathbf{r}\exp(-i\theta) \mp \mathbf{R}/2), \\ &= (\pi b^{2})^{-3/4}\exp\left[-\frac{(\mathbf{r} - \mathbf{R}\exp(i\theta))^{2}}{2b^{2}}\right]. \end{split}$$

Therefore, the complex scaling transformation can be done by replacing $\Phi_{\rm B}(\mathbf{R}) \rightarrow \Phi_{\rm B}^{\theta}(\mathbf{R}) \equiv \Phi_{\rm B}^{\theta}(\mathbf{R} \exp(i\theta))$, while keeping the Hamiltonian not transformed.

• Complex scaled THSR wave function

$$\begin{split} \Psi(\beta) &\to \Psi_{\theta}(\beta) \equiv \mathcal{N} \int \mathrm{d}^{3}R \exp\left(-\frac{\boldsymbol{R}^{2}}{2\beta^{2}}\right) \Phi_{\mathrm{B}}(\boldsymbol{R}\exp(i\theta)) \\ &= \mathcal{N}' \int \mathrm{d}^{3}R \exp\left(-\frac{\boldsymbol{R}^{2}}{2[\beta\exp(i\theta)]^{2}}\right) \Phi_{\mathrm{B}}(\boldsymbol{R}). \end{split}$$

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The $\alpha + \alpha$ System

Triple- α process in stars



The $\alpha + \alpha$ scattering is the background process.

The Bound-State Approximation



The energy curves for the 0^+ , 2^+ , and 4^+ states of ⁸Be given by a single Brink-THSR wave function, with the parameter β being 0 fm, 1 fm, 2 fm, and 3 fm. For $\beta = 0$ fm, the Brink-THSR wave function is reduced to the Brink wave function.**27**



The energy surfaces for the 0^+ , 2^+ , and 4^+ states of ⁸Be given by a single Brink-THSR wave function.

The R-Matrix Results

⁸Be

Iteration solutions of the Bloch-Schrödinger equation for the low-lying resonant states of ⁸Be.

Iterations	L = 0	L=2	L = 4	
1	0.1	3	20-2.5i	
2	$0.09622 - 8.1197 \times 10^{-6} i$	2.9692 - 0.5601i	11.6042 - 1.1359i	
3	$0.09700 - 4.1253 \times 10^{-6} i$	2.8748 - 0.6641i	11.3162 - 2.2401i	
12	$0.09687 - 5.0984 \times 10^{-6} i$	2.8190 - 0.6636i	11.8490 - 2.2588i	
13	$0.09687 - 5.0984 \times 10^{-6} i$	2.8190 - 0.6636i	11.8460 - 2.2579i	
14			11.8459 - 2.2599i	
20			11.8466 - 2.2594i	
21			11.8466 - 2.2594i	

The $\alpha + \alpha$ scattering



The phase shifts for the $\alpha + \alpha$ elastic scattering in the *S*, *D*, and *G* waves against the total energy of the $\alpha + \alpha$ system in the CM frame. The parameter β takes the values of 0 fm, 0.5 fm, and 1 fm. The channel radius is given by a = 7.0 fm.

The CSM Results



Complex energy spectrum for the 4^+ state with THSR wave functions. The blue square, red circle, and orange triangle correspond to $\theta = 20^\circ, 23^\circ, 26^\circ$ respectively.

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• Nonlocalized cluster model is a microscopic model for nuclear cluster physics based on the picture of nonlocalized clustering.

• Hybridize nonlocalized cluster model with the *R*-matrix theory and CSM to study resonant and scattering states.

 \circ The spectrum properties of ^8Be and the $\alpha+\alpha$ elastic scattering are taken to validate the hybrid models, well consistent with other methods.

