# **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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# 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
	- $\blacksquare \cdots$  + the *R*-matrix theory
	- $\blacksquare$   $\cdots$   $\vdash$  complex scaling method (CSM)
- **3** The  $\alpha + \alpha$  system as a proof of concept
	- The bound-state approximation
	- The *R*-matrix results
	- $\blacksquare$  The CSM results

## **4** Summary

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## **4** Summary

# Nuclear clustering: Phenomenological viewpoint I

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



 $\alpha$  **clusters** could be taken as effective building blocks, e.g.,  ${}^{8}$ Be  $\approx \alpha + \alpha$ ,  ${}^{12}C \approx \alpha + \alpha + \alpha$ ,  ${}^{16}O \approx \alpha + \alpha + \alpha + \alpha$ ,  $\cdots$ .

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, <sup>14</sup>C,  $^{20}$ O,  $^{24}$ Ne,  $\cdots$  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 *|*Ψ*⟩*.



#### *◦* **Which model is better?**

**◦** Compare  $\langle O \rangle$ <sub>Model</sub>  $\equiv$   $\langle$ Model| $O$ |Model $\rangle$  and  $\langle O \rangle$ <sub>Ψ</sub>  $\equiv$   $\langle \Psi | O | \Psi \rangle$ ; the closer, the better. Often, systematical improvements can be made upon the good models.

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

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. **8**

### Resonant and Scattering States: Phenomenological Viewpoint

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

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

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**:  $\text{Re} k > 0$ ,  $\text{Im} k < 0$ ,  $\phi_R(r) \to \exp(ikr) \propto \exp(ik\epsilon k r)$ *×* exp(*−*Im *k r*), blowing up in infinity,  $\mathcal{E}_{\text{res}} = E - i\Gamma/2 = |\tilde{E}| \exp(-2i\theta_{\text{R}}) \Rightarrow \theta_{\text{R}} = \frac{1}{2} \arctan(\frac{\Gamma}{2E}).$

**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:**

1. not easy to **distinguish between resonant and scattering states**, especially for broad resonances 2. physical picture sometimes inaccurate

<sup>o</sup> <sup>8</sup>Be(2<sup>+</sup>), a member of the ground-state band of <sup>8</sup>Be, has a large decay width *∼* 3 MeV compared to its total energy *∼* 1.5 MeV above the 2*α* threshold.

*◦* <sup>12</sup>C(0<sup>+</sup> 3 ), which is conjectured to be **a breathing mode of the Hoyle state** <sup>12</sup>C(0<sup>+</sup><sub>2</sub>), has a large decay width  $\sim$  1.45 MeV compared to its total energy *∼* 1.77 MeV above the 3*α* threshold.

*⇒* 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: continuumdiscretized coupled channels), etc.

2. Microscopic reaction models are less explored than structural models. The initial and final states naturally contain "clusters" *⇒* 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**

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

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

### **Brink wave function**

$$
\Phi_{\mathbf{B}}(\boldsymbol{R}) = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{8!}} \det \{ \varphi_{0s}(\mathbf{r}_1 - \mathbf{R}/2) \chi_{\sigma_1 \tau_1} \cdots \varphi_{0s}(\mathbf{r}_4 - \mathbf{R}/2) \chi_{\sigma_4 \tau_4} \times \varphi_{0s}(\mathbf{r}_5 + \mathbf{R}/2) \chi_{\sigma_1 \tau_1} \cdots \varphi_{0s}(\mathbf{r}_8 + \mathbf{R}/2) \chi_{\sigma_4 \tau_4} \}.
$$



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



### **Separation of center-of-mass motion**

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

### **Angular momentum projection**

$$
\Psi(\beta, \mathbf{T}) = \Psi_{\text{CM}}(\mathbf{X}_{\text{CM}}) \times 4\pi \sum_{LM} \widehat{\Psi}_{LM}(\beta, T) Y_{LM}^*(\Omega_T),
$$
  

$$
\widehat{\Psi}_{LM}(\beta, T) = \frac{1}{\sqrt{140}} \mathcal{A}_{12} \Gamma_L(\rho, \beta, T) Y_{LM}(\Omega_\rho) \widehat{\phi}(\alpha_1) \widehat{\phi}(\alpha_2) \Rightarrow \frac{u_L(\rho)}{\rho} Y_{LM}(\Omega_\rho),
$$
  

$$
\Gamma_L(\rho, \beta, T) = \left(\frac{2}{\pi}\right)^{3/4} \frac{b^{3/2}}{(b^2 + 2\beta^2)^{3/2}} \exp\left(-\frac{\rho^2 + T^2}{b^2 + 2\beta^2}\right) i_L \left(\frac{2\rho T}{b^2 + 2\beta^2}\right).
$$

## Interaction Model

The Hamiltonian is given by

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

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

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

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



*.*

### **Single basis wave function**:

$$
\circ \text{ THEN: } E_L(\beta) = \min \frac{\langle \widehat{\Psi}_{LM}(\beta) | H_L | \widehat{\Psi}_L M(\beta) \rangle}{\langle \widehat{\Psi}_{LM}(\beta) | \widehat{\Psi}_{LM}(\beta) \rangle}.
$$
  

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

### **Multiple basis wave functions**:

\n- \n
$$
\text{THSR: } \widetilde{\Psi}_{LM} = \int d\beta f(\beta) \, \widehat{\Psi}_{LM}(\beta).
$$
\n
\n- \n
$$
\text{Brink-THSR: } \widetilde{\Psi}_{LM}(\beta) = \int dTf(T) \, \widehat{\Psi}_{LM}(\beta, T).
$$
\n
\n- \n
$$
\Rightarrow \text{variational principle} \Rightarrow \text{Hill-Wheeler equation.}
$$
\n
\n

## $\cdots$  + the *R*-Matrix Theory



**Scattering state:**  $B = 0$ 

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

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

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

self-consistent generalized eigenvalue problem

# *· · ·* + Complex Scaling Method (CSM)

### **Complex scaling transformation**

 $\mathbf{r} \to \mathbf{r} \exp(i\theta), \qquad \psi(\mathbf{r}) \to \exp(i3\theta/2) \phi(\mathbf{r} \exp(i\theta)).$  $\Rightarrow$  similarity transformation  $S(\theta) = \prod [\exp(3i\theta/2) \exp(i\theta \mathbf{r}_j \cdot \nabla_j)],$ *j*  $H \to S(\theta)HS(\theta)^{-1}, \quad \Psi \to S(\theta)\Psi.$ 

**The Schrödinger equation**:

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

### **Square integrable eigensolutions:**

*◦* Bound state: *ϕ*B(*r*) *∝* exp(*−κr*) *→ ϕ θ* B (*r*) *∝* exp(*−κr* exp(*iθ*)) *◦* Resonant state: *ϕ*R(*r*) *∝* exp(*i|k|* exp(*−iθ*R)*r*) *⇒*  $\phi_R^{\theta}(r) \propto \exp(i|k| r \exp(-i\theta_R + i\theta))$ ; when  $\theta > \theta_R$ ,  $\phi_R^{\theta}(r) \to 0$  as  $r \to \infty$ . *◦* Scattering state: *ϕ*R(*r*) *∝ A* exp(*−ikr*) + *B* exp(*ikr*) *⇒*  $\phi_{R}^{\theta}(r) \propto A \exp(-ikr \exp(i\theta)) + B \exp(ikr \exp(i\theta))$ ; when  $k \to k \exp(-i\theta)$ , square integrable, discretized energy. **22** 



*⇐* **ABC theorem** by **A**guilar, **C**ombes, and **B**alslev.

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

*◦* **The complex scaled** *α***-cluster wave function**

$$
\Phi_{\alpha}^{\theta}(\boldsymbol{R}) = \frac{1}{\sqrt{4!}} \det \{ \varphi_{0s}^{\theta}(r_1 - \boldsymbol{R}) \chi_{\sigma_1 \tau_1} \cdots \varphi_{0s}^{\theta}(r_4 - \boldsymbol{R}) \chi_{\sigma_4 \tau_4} \},
$$
  

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

*◦* **Complex scaled Brink wave function**

$$
\Phi_{\mathbf{B}}^{\theta}(\boldsymbol{R}) = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{8!}} \det \{ \varphi_{0s}^{\theta}(r_1 - \boldsymbol{R}/2) \chi_{\sigma_1 \tau_1} \cdots \varphi_{0s}^{\theta}(r_4 - \boldsymbol{R}/2) \chi_{\sigma_4 \tau_4} \times \varphi_{0s}^{\theta}(r_5 + \boldsymbol{R}/2) \chi_{\sigma_1 \tau_1} \cdots \varphi_{0s}^{\theta}(r_8 + \boldsymbol{R}/2) \chi_{\sigma_4 \tau_4} \}.
$$

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

$$
H_{\theta} \rightarrow H,
$$
  
\n
$$
\varphi_{0s}^{\theta}(r_1 - R/2) \rightarrow \exp(-i3\theta/2)\varphi_{0s}^{\theta}(r \exp(-i\theta) \mp R/2),
$$
  
\n
$$
= (\pi b^2)^{-3/4} \exp\left[-\frac{(r - R \exp(i\theta))^2}{2b^2}\right].
$$

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

*◦* **Complex scaled THSR wave function**

$$
\Psi(\beta) \to \Psi_{\theta}(\beta) \equiv \mathcal{N} \int d^3 R \exp\left(-\frac{\mathbf{R}^2}{2\beta^2}\right) \Phi_{\text{B}}(\mathbf{R} \exp(i\theta))
$$

$$
= \mathcal{N}' \int d^3 R \exp\left(-\frac{\mathbf{R}^2}{2[\beta \exp(i\theta)]^2}\right) \Phi_{\text{B}}(\mathbf{R}).
$$

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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  ${}^{8}$ Be 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.



The energy surfaces for the  $0^+$ ,  $2^+$ , and  $4^+$  states of  ${}^{8}$ Be given by a single Brink-THSR wave function. **<sup>28</sup>**

# The *R*-Matrix Results

## <sup>8</sup>**Be**

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



**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  $\beta$  takes the values of 0 fm, 0.5 fm, and 1 fm. The channel radius is given by  $a = 7.0 \text{ fm.}$  **30** 

# 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. **31** 

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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 <sup>8</sup>Be and the *α* + *α* elastic scattering are taken to validate the hybrid models, well consistent with other methods.

