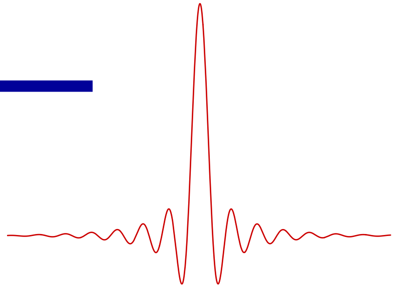
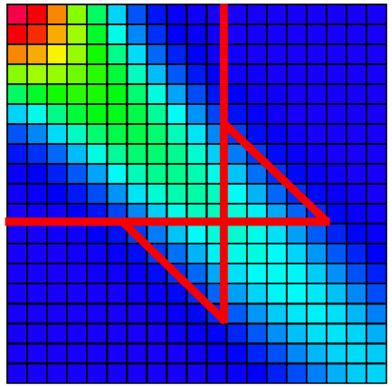
Nuclear Many-Body Continuum States and their Boundary Conditions in a Collective-Coordinate Representation



Outline

- A collective-coordinate for the relative distance
- Boundary conditions in a nonorthogonal basis
- Application to Fermionic Molecular Dynamics



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Introduction

Aim

- ➨ Calculation of resonance parameters and phase shifts
  - Nuclear microscopic many-body model
  - Astrophysical interest: reaction with composite objects

Method

- ➨ Imposition of boundary conditions
- ➨ Use of multiconfiguration calculations

Difficulties

- ➨ Fully antisymmetrized states
- ➨ Nonorthogonal many-body basis

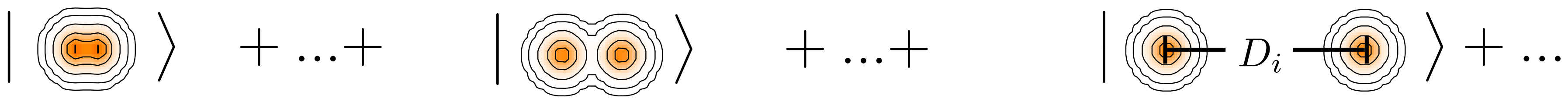
Solutions

- ➨ Collective-coordinate representation
- ➨ Homogeneous linear boundary condition equations

Statement of the Problem

Model Space

- Set of nonorthogonal antisymmetrized many-body states $\{ \left| J^\pi M ; Q_i \right\rangle ; i = 1, 2, \ldots \}$
- Appropriate quantum numbers for asymptotic channels
- Covers Hilbert space related to the process: mean intercluster distance D_i



Eigenvalue Problem

- Trial state $\left| \Psi \right\rangle = \sum_i \Psi_i \left| J^\pi M ; Q_i \right\rangle$
- Many-body Schrödinger equation

$$\underset{\sim}{H} \left| \Psi \right\rangle = Z \left| \Psi \right\rangle$$

- With boundary conditions

Boundary Conditions

- $\left| \Psi \right\rangle$ describes clusters for $r \leq R$
- Match desired asymptotic behaviour

$$\left\langle r \middle| \Psi \right\rangle \overset{r>R}{\propto} \left\langle r \middle| w \right\rangle$$

$$\left\langle r \middle| \Psi \right\rangle ?$$

multiconfiguration calculations

homogeneous linear boundary condition equations

collective-coordinate representation

Modified eigenvalue problem

Collective-Coordinate Representation

Definition of Relative Distance

Size Measure

- Operator $\underset{\sim}{B}$ measures extension of the system

$$\underset{\sim}{B} = \frac{1}{A^2} \sum_{i<j=1}^{A} \left(\underset{\sim}{\vec{x}}(i) - \underset{\sim}{\vec{x}}(j)\right)^2$$

Separation of Relative Motion

- $\underset{\sim}{B}$ decomposes into

$$\underset{\sim}{B} = \underset{\sim}{B}_{rel} + \underset{\sim}{B}_1 + \underset{\sim}{B}_2$$

separate clusters

Asymptotic Interpretation

- Eigenvalues relate to relative distance r

$$\underset{\sim}{B} \left| \beta \right\rangle = \beta \left| \beta \right\rangle \Rightarrow \beta(r) = \frac{A_1 A_2}{A^2} r^2 + \beta_1 + \beta_2$$

- Eigenvectors localize in r (localized states)

$$\left\langle \beta \middle| \underset{\sim}{B}^2 \middle| \beta \right\rangle = \left\langle \beta \middle| \underset{\sim}{B} \middle| \beta \right\rangle^2 \Rightarrow \Psi(r(\beta)) := \left\langle \beta(r) \middle| \Psi \right\rangle$$

other contributions integrate out

Limited Hilbert Space

- In model space, $\left| \beta_j \right\rangle = \sum_i \beta_j^{(i)} \left| J^\pi M; Q_i \right\rangle \quad \Longrightarrow$

Asymptotic states must have well separated clusters in ground state

Collective-Coordinate Representation

Definition of Derivative

Velocity operator

- Spatial derivative given by

$$\dot{\underset{\sim}{B}} = \frac{i}{\hbar}[\underset{\sim}{H}, \underset{\sim}{B}]$$

- For example, $\dot{r} \propto d/dr$, $(\dot{r^2}) \propto 1 + 2r\, d/dr$

Asymptotic Decomposition

- Hamiltonian separates relative motion

$$\underset{\sim}{H} = (\underset{\sim}{T}_{rel} + \underset{\sim}{V}_{rel}) + \underset{\sim}{H}_1 + \underset{\sim}{H}_2$$

- $\underset{\sim}{V}_{rel}$ is Coulomb plus centrifugal

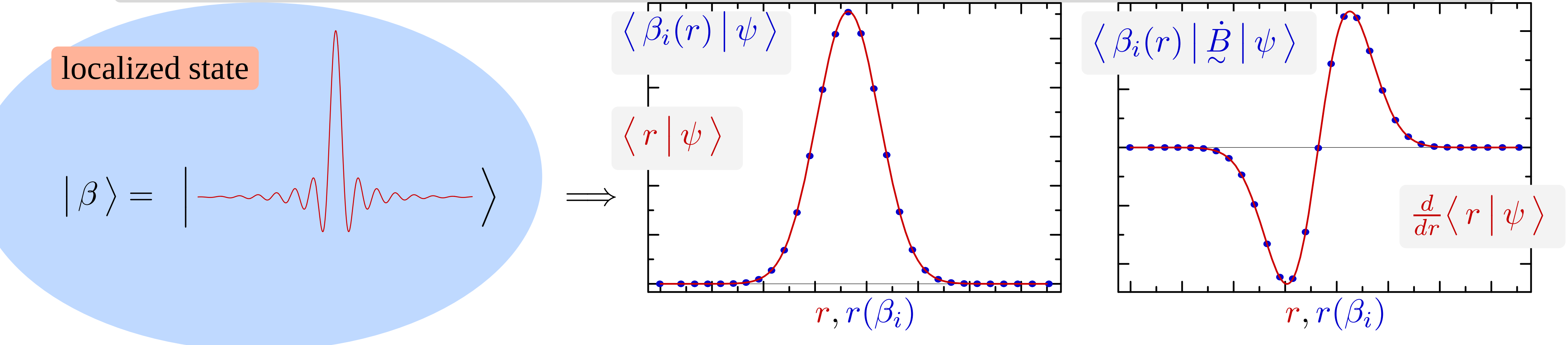
Relative Velocity

- Velocity operator separates relative motion

$$\dot{\underset{\sim}{B}} = \dot{\underset{\sim}{B}}_{rel} + \dot{\underset{\sim}{B}}_1 + \dot{\underset{\sim}{B}}_2$$

- For a basis with frozen clusters in ground state

$$\langle \beta \,|\, \dot{\underset{\sim}{B}}_{rel} \,|\, \Psi \rangle = \langle \beta \,|\, \dot{\underset{\sim}{B}} \,|\, \Psi \rangle \Rightarrow \frac{d}{dr} \langle \beta(r) \,|\, \Psi \rangle$$



Implementation of Boundary Conditions

Homogeneous Linear Equations

Boundary Conditions for a Many-Body System

Collective-Coordinate Representation

$$\left\langle\, \beta(r) \,\middle|\, \Psi \,\right\rangle \overset{r>R}{\propto} \left\langle\, r \,\middle|\, w \,\right\rangle$$

Single Evaluation Point

$$\frac{\left\langle\, \beta(R) \middle| \underset{\sim}{\dot{B}}^{s} \middle| \Psi \right\rangle}{\left\langle\, \beta(R) \,\middle|\, \Psi \,\right\rangle} = \frac{\left\langle R \middle| \underset{\sim}{\dot{B}}^{s} \middle| w \right\rangle}{\left\langle\, R \,\middle|\, w \,\right\rangle}, \quad s = 1, 2, \ldots$$

Homogeneous Linear Boundary Condition Equations

$$\sum_{j} \left(\left\langle\, \beta(R) \,\middle|\, \underset{\sim}{\dot{B}}^{s} \,\middle|\, J^{\pi} M; Q_j \,\right\rangle - \frac{\left\langle R \middle| \underset{\sim}{\dot{B}}^{s} \middle| w \right\rangle}{\left\langle\, R \,\middle|\, w \,\right\rangle} \left\langle\, \beta(R) \,\middle|\, J^{\pi} M; Q_j \,\right\rangle \right) \Psi_j = 0$$

$$\sum_{j=1} \mathsf{H}_{ij} \Psi_j = Z \sum_{j=1} \mathsf{N}_{ij} \Psi_j$$

$$\Psi_l = \sum_{j=1}^{n} C_{lj}\, \Psi_j, \quad l = n{+}1, n{+}2, \ldots$$

Modified Eigenvalue Problem

- Replace coefficients in eigenvalue problem:

$$\sum_{j=1}^{n} \mathsf{H}_{ij} \Psi_j + \sum_{l=n+1} \mathsf{H}_{il} \Psi_l = Z \left(\sum_{j=1}^{n} \mathsf{N}_{ij} \Psi_j + \sum_{l=n+1} \mathsf{N}_{il} \Psi_l \right) \Longrightarrow$$

$$\sum_{j=1}^{n} \mathsf{H}_{ij}^{BC} \Psi_j = Z \sum_{i=1}^{n} \mathsf{N}_{ij}^{BC} \Psi_j$$

$$Z = E - i\,\frac{\Gamma}{2}$$

Implementation of Boundary Conditions

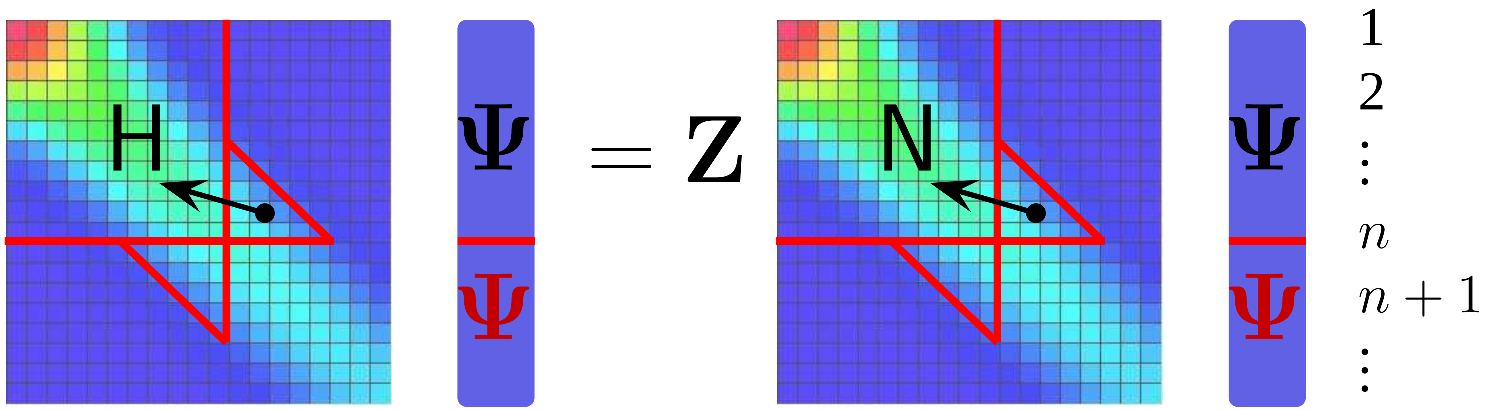
Graphical Interpretation

Limited Hilbert Space

- Solution valid only in a certain region
- Description breaks down near boundaries

Implications of Nonorthogonal Basis

- Overlaps are non-zero
- Matrix elements form a band



Consequences

- Information lost by cut → Embed it by imposing boundary conditions
- Need of several boundary condition equations → match several derivatives

Fermionic Molecular Dynamics
Microscopic Model

FMD Representation

- Many-body state

$$\big|\, Q \,\big\rangle = \underset{\sim}{\mathcal{A}}\Big(\big|\, q_1 \,\big\rangle \otimes \big|\, q_2 \,\big\rangle \otimes \ldots \otimes \big|\, q_A \,\big\rangle\Big)$$

- Single-particle state:

$$\big|\, q_k \,\big\rangle = \big|\, a_k, \vec{b}_k \,\big\rangle \otimes \big|\, \chi_k \,\big\rangle \otimes \big|\, \xi_k \,\big\rangle,$$

  - Coordinate space

$$\big\langle\, \vec{x} \,\big|\, a_k, \vec{b}_k \,\big\rangle = \exp\left\{-\frac{(\vec{x}-\vec{b}_k)^2}{2a_k}\right\}$$

  - Spin space

$$\big|\, \chi_k \,\big\rangle = c_\uparrow \big|\, \uparrow \,\big\rangle + c_\downarrow \big|\, \downarrow \,\big\rangle$$

  - Isospin space

$$\big|\, \xi_k \,\big\rangle \in \left\{\big|\, p \,\big\rangle, \big|\, n \,\big\rangle\right\}$$

Nucleon-Nucleon Interactions

- Effective interactions
  - Volkov, Minnesota
  - Adjusted to considered cases
- Interaction derived from realistic one
  - Argonne: describes NN phase shifts
  - Unitary Correlation Operator Method

Angular Momentum Projection

- Use projection operator

$$\big|\, J^\pi M; Q \,\big\rangle = \underset{\sim}{P}{}^{J^\pi}_{M} \big|\, Q \,\big\rangle$$

Application to FMD

Collective coordinate

$$\underset{\sim}{B} = \frac{1}{A^2}\sum_{i<j=1}^{A}\left(\underset{\sim}{\vec{x}}(i) - \underset{\sim}{\vec{x}}(j)\right)^2$$

Asymptotic behaviour

- Coulomb wave
- Free wave

- Scattering state
- Resonance (Gamov)

Basis

Frozen state approximation:
clusters in their ground state

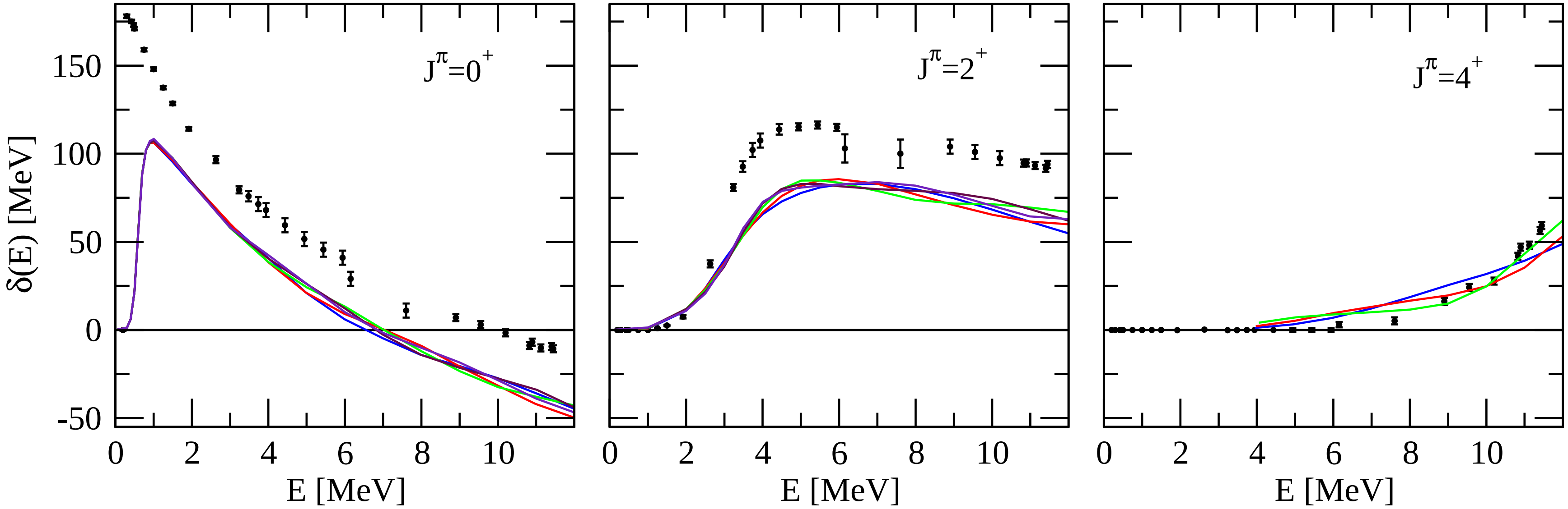
Resonances in ^{8}Be

		$J^\pi = 0^+$		$J^\pi = 2^+$		$J^\pi = 4^+$	
		E [MeV]	Γ [MeV]	E [MeV]	Γ [MeV]	E [MeV]	Γ [MeV]
	Experiment	0.09204(5)	5.57(25) 10^{-6}	3.12(1)	1.513(15)	11.44(15)	≈ 3.5
Volkov (α-α)	CLD	0.60	0.25	3.07	2.38	11.60	6.99
	CSM	0.59	0.24	3.07	2.39	11.60	7.04
	Phase Shift	0.60	0.25	3.07	2.38	11.60	7.00
	FMD (Gamov)	0.59	0.25	3.08	2.39	11.59	6.94
AV18-based	FMD (Gamov)	0.273(3)	0.0130(5)	2.71(2)	2.38(2)	-	-

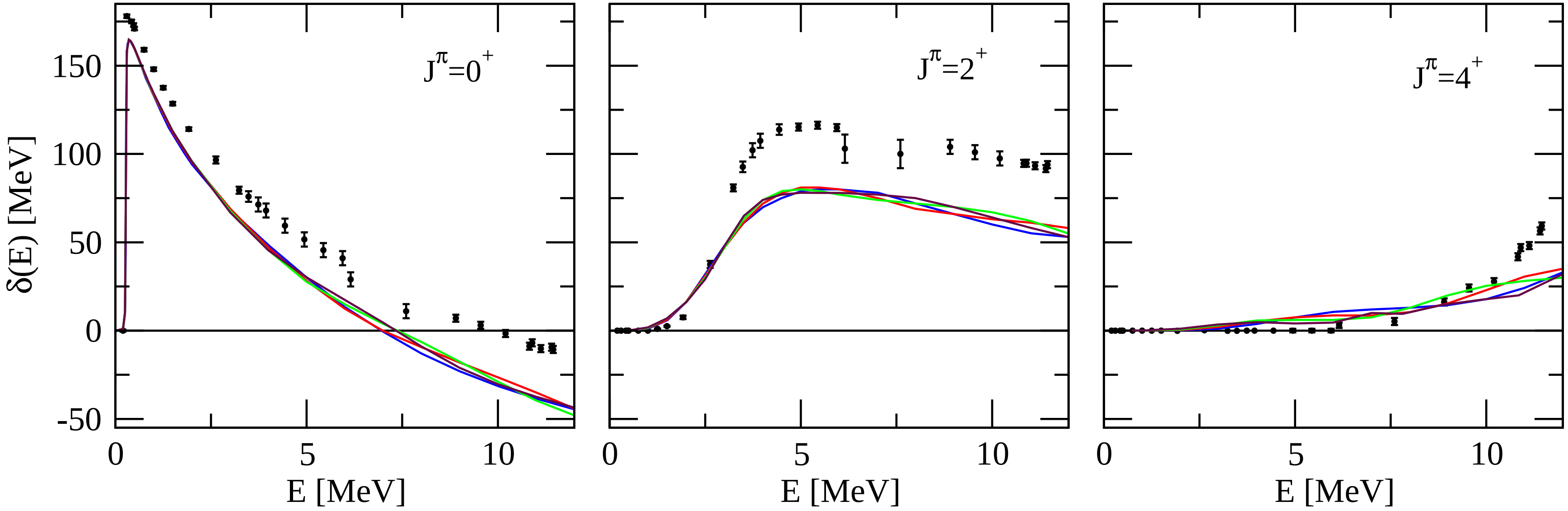
Application to FMD

Phase shifts in ^{8}Be

Volkov



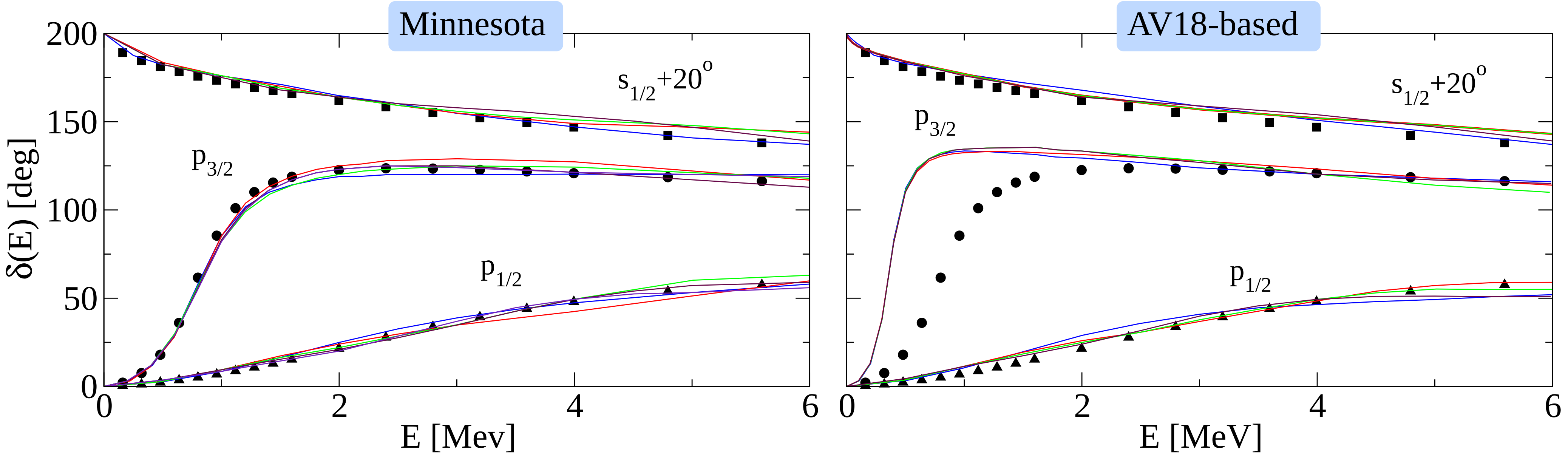
AV18-based



Application to FMD

Resonances in ^{5}He

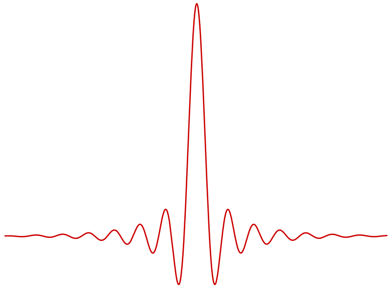
		$J^\pi = 3/2^-$		$J^\pi = 1/2^-$	
		E [MeV]	Γ [MeV]	E [MeV]	Γ [MeV]
	Experiment	0.798	0.648	2.07	5.57
Minnesota (n-α)	CLD	0.78	0.64	2.01	5.42
	Phase Shift	0.78	0.64	1.98	5.45
	S-Matrix, RGM	0.76	0.63	1.89	5.20
	FMD (Gamov)	0.79	0.68	2.20	5.38
AV18-based	FMD (Gamov)	0.37	0.23	1.6	4.9

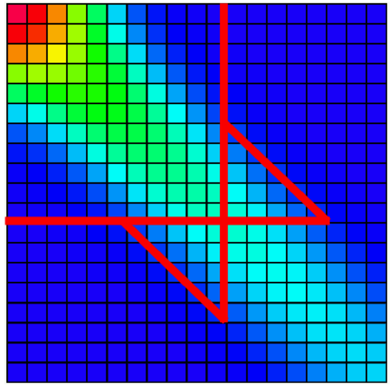


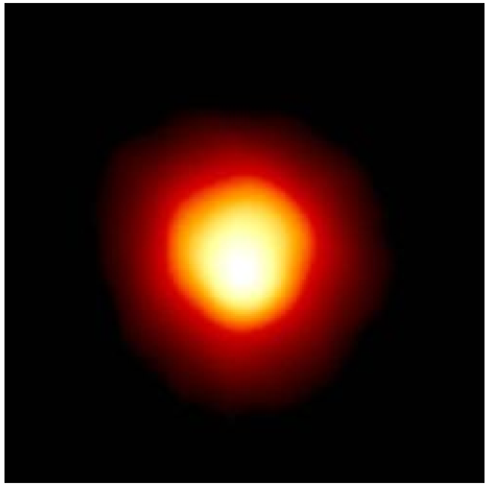
Summary & Outlook

Summary

- Implementation of boundary conditions in a many-body microscopic problem
  - ✔ *Collective-Coordinate Representation*
  - ✔ *Homogeneous Linear Boundary Condition Equations*
- Calculation of resonances and phase shifts
  - ✔ Validity confirmed by comparison to previous works
  - ✔ First results in FMD using a realistic interaction for ^{8}Be and ^{5}He







Outlook

- Improve model space
  - Use improved single-particle states
  - Include polarization effects in the many-body configurations
- Application to nuclei of astrophysical interest
- Coupled channels and A(a,b)B reactions
- Nucleus-nucleus potentials in the Collective-Coordinate Representation