Microscopic Nuclear Structure and Reaction Calculations in the FMD Approach



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Overview

Effective Nucleon-Nucleon interaction:

Unitary Correlation Operator Method

Short-range Central and Tensor Correlations

Many-Body Method:

Fermionic Molecular Dynamics

- Model
- Nuclear Structure Applications

Reactions:

³He(α , γ)⁷Be radiative capture

- ⁷Be Bound States and Scattering Phase Shifts
- S-Factor

Unitary Correlation Operator Method Nuclear Force

Argonne V18 (T=0)

spins aligned parallel or perpendicular to the relative distance vector



- strong repulsive core: nucleons can not get closer than ≈ 0.5 fm
- central correlations

- strong dependence on the orientation of the spins due to the tensor force
- tensor correlations

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tensor correlations

the nuclear force will induce strong short-range correlations in the nuclear wave function

• Unitary Correlation Operator Method

Realistic Effective Interaction





central correlator C_r shifts density out of the repulsive core tensor correlator C_{Ω} aligns density with spin orientation

Neff and Feldmeier, Nucl. Phys. A713 (2003) 311

• Unitary Correlation Operator Method

Realistic Effective Interaction











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 $\langle T \rangle$

 $\langle H \rangle$

 $\langle V \rangle$



Fermionic

Slater determinant

$$\boldsymbol{Q} \rangle = \mathcal{A}\left(\left| \boldsymbol{q}_1 \right\rangle \otimes \cdots \otimes \left| \boldsymbol{q}_A \right\rangle \right)$$

• antisymmetrized A-body state

FMD Fermionic Molecular Dynamics

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Molecular

single-particle states

$$\langle \mathbf{x} | q \rangle = \exp \left\{ -\frac{(\mathbf{x} - \mathbf{b})^2}{2\alpha} \right\} \otimes | \chi^{\uparrow}, \chi^{\downarrow} \rangle \otimes | \xi \rangle$$

- Gaussian wave-packets in phase-space (complex parameter b encodes mean position and mean momentum), spin is free, isospin is fixed
- width α is an independent variational parameter for each wave packet

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Antisymmetrization

FMD PAV, VAP and Multiconfiguration

Projection After Variation (PAV)

- intrinsic state may break symmetries of Hamiltonian
- restore inversion, translational and rotational symmetry by projection on parity, linear and angular momentum

$$\mathop{\mathbb{P}}_{\sim}^{\pi} = \frac{1}{2}(1 + \pi \prod)$$

$$P_{MK}^{J} = \frac{2J+1}{8\pi^2} \int d^3 \Omega D_{MK}^{J}^{*}(\Omega) R(\Omega)$$

$$\mathcal{P}^{\mathbf{P}} = \frac{1}{(2\pi)^3} \int d^3 X \exp\{-i(\mathbf{P} - \mathbf{P}) \cdot \mathbf{X}\}$$

FMD

PAV, VAP and Multiconfiguration

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Variation After Projection (VAP)

- effect of projection can be large
- full Variation after Angular Momentum and Parity Projection (VAP) for light nuclei
- perform VAP in GCM sense by applying constraints on radius, dipole moment, quadrupole moment or octupole moment and minimizing the energy in the projected energy surface for heavier nuclei

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Multiconfiguration Calculations

• **diagonalize** Hamiltonian in a set of projected intrinsic states

$$\left\{ \left| \, \mathbf{Q}^{(a)} \, \right\rangle \,, \quad a = 1, \ldots, N \right\}$$

$$\underset{\sim}{P^{\pi}}=\frac{1}{2}(1+\pi\underset{\sim}{\Pi})$$

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$$\sum_{K'b} \langle \mathbf{Q}^{(\alpha)} | \underbrace{HP}_{KK'}^{J^{\pi}} \underbrace{P^{\mathbf{P}=0}}_{KK'} | \mathbf{Q}^{(b)} \rangle \cdot c_{K'b}^{\alpha} = E^{J^{\pi}\alpha} \sum_{K'b} \langle \mathbf{Q}^{(\alpha)} | \underbrace{P}_{KK'}^{J^{\pi}} \underbrace{P^{\mathbf{P}=0}}_{KK'} | \mathbf{Q}^{(b)} \rangle \cdot c_{K'b}^{\alpha}$$

Example: Neon Isotopes



Separation Energies



nuclear structure details responsible for peculiar behaviour of charge radii

Geithner, Neff, et. al., Phys. Rev. Lett. 101 (2008) 252502



Thomas Neff — NIC XI, 07/19/10

³He(*α*, γ)⁷Be **Models**

Potential models

- ⁴He and ³He are point-like particles
- interacting via an effective nucleus-nucleus potential fitted to bound state properties and phase shifts

Microscopic Cluster Models

- antisymmetrized wave function built with ⁴He and ³He clusters
- polarization effects sometimes included by adding other channels like ⁶Li plus proton
- interacting via an effective nucleon-nucleon potential, adjusted to describe bound state properties and phase shifts

Fermionic Molecular Dynamics

- antisymmetrized wave function built with ⁴He and ³He FMD clusters
- FMD wave functions obtained in variation after angular momentum projection on 1/2⁻, 3/2⁻, 5/2⁻, 7/2⁻ and 1/2⁺, 3/2⁺ and 5/2⁺ with radius constraint in the interaction region to include polarization effects
- interacting via realistic UCOM interaction that reproduces the nucleon-nucleon phase shifts

³He(α, γ)⁷Be **Bound and Scattering States**



dashed lines - frozen configurations only, solid lines - FMD configurations in interaction region included

Bound states

	Experiment	FMD
E _{3/2-}	-1.59 MeV	-1.50 MeV
E _{1/2-}	-1.15 MeV	-1.49 MeV
r _{charge}	2.647(17) fm	2.67 fm

- Scattering phase shifts well described, polarization effects important
- splitting between 3/2⁻ and 1/2⁻ states too small, but centroid energy and charge radius well reproduced
- with frozen configurations only the 1/2⁻ is and the 3/2⁻ state is almost unbound – polarization effects are essential

³He(*α*, γ)⁷Be **S-Factor**



³He(α, γ)⁷Be **S-Factor**



• dipole transitions from $1/2^+$, $3/2^+$, $5/2^+$ scattering states into $3/2^-$, $1/2^-$ bound states

- energy dependence and normalization of new high quality data well described
- cross section depends significantly on internal part of wave function, description as an "external" capture is too simplified
- numerics becomes difficult at very low energies, extrapolation to E = 0 therefore hard

Summary

Unitary Correlation Operator Method

- Explicit description of short-range central and tensor correlations
- Decouples low- and high-momentum modes

Fermionic Molecular Dynamics

- Microscopic many-body approach using Gaussian wave-packets
- Projection and multiconfiguration mixing
- Consistent description of well bound states with shell structure and loosely bound states of cluster or halo nature

³He(α, γ)⁷Be **Radiative Capture**

- Fully microscopic calculation with realisitic two-body interaction
- Bound states, resonance and scattering wave functions
- S-Factor: energy dependence and normalization reproduced
- analyze internal part of wave function, extrapolation to E = 0
- role of three-body forces ?

Thanks

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