Structure and reactions of light nuclei studied in fermionic molecular dynamics

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"Astrophysics and Nuclear Structure"

International Workshop XLI on Gross Properties of Nuclei and Nuclear Excitations

Hirschegg, Austria

January 26 - February 1, 2013





Overview

Realistic Effective Nucleon-Nucleon interaction: Unitary Correlation Operator Method

R. Roth, T. Neff, H. Feldmeier, Prog. Part. Nucl. Phys. 65 (2010) 50

• Short-range Correlations and Effective Interaction

Many-Body Approach:

Fermionic Molecular Dynamics

- Model
- ³He(α , γ)⁷Be Radiative Capture Reaction

T. Neff, Phys. Rev. Lett. 106, 042502 (2011)

Beryllium Isotopes

A. Krieger et al., Phys. Rev. Lett. 108, 142501 (2012)



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

Universality of short-range correlations **Two-body densities in** A = 2, 3, 4 **Nuclei — AV8'**



- normalize two-body density in coordinate space at r=1.0 fm
- normalized two-body densities in coordinate space are identical at short distances for all nuclei
- use the same normalization factor in momentum space high momentum tails agree for all nuclei

Feldmeier, Horiuchi, Neff, Suzuki, Phys. Rev. C 84, 054003 (2011)

3

4

Unitary Correlation Operator Method

Correlation Operator

• induce short-range (two-body) central and tensor correlations into the many-body state

$$\mathcal{L} = \mathcal{L}_{\Omega} \mathcal{L}_{r} = \exp\left[-i\sum_{i < j} \mathcal{L}_{\Omega, ij}\right] \exp\left[-i\sum_{i < j} \mathcal{L}_{r, ij}\right] \quad , \quad \mathcal{L}^{\dagger} \mathcal{L} = 1$$

 correlation operator should conserve the symmetries of the Hamiltonian and should be of finite-range, correlated interaction phase shift equivalent to bare interaction by construction

Correlated Operators

• correlated operators will have contributions in higher cluster orders

$$\hat{C}^{\dagger} \hat{O} \hat{C} = \hat{Q}^{[1]} + \hat{Q}^{[2]} + \hat{Q}^{[3]} + \dots$$

 two-body approximation: correlation range should be small compared to mean particle distance

Correlated Interaction

$$\underline{C}^{\dagger} (\underline{T} + \underline{V}) \underline{C} = \underline{T} + \underline{V}_{UCOM} + \underline{V}_{UCOM}^{[3]} + \dots$$

• UCOM

Central and Tensor Correlations

$$\mathbf{p} = \mathbf{p}_r + \mathbf{p}_\Omega$$
$$\mathbf{p}_r = \frac{1}{2} \left\{ \frac{\mathbf{r}}{r} \left(\frac{\mathbf{r}}{r} \mathbf{p} \right) + \left(\mathbf{p} \frac{\mathbf{r}}{r} \right) \frac{\mathbf{r}}{r} \right\}, \qquad \mathbf{p}_\Omega = \frac{1}{2r} \left\{ \mathbf{I} \times \frac{\mathbf{r}}{r} - \frac{\mathbf{r}}{r} \times \mathbf{I} \right\}$$

• UCOM

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Central Correlations

$$c_r = \exp\left\{-\frac{i}{2}\left\{p_r s(r) + s(r)p_r\right\}\right\}$$

probability density shifted out of the repulsive core



• UCOM

Central and Tensor Correlations

 $C = C_{\Omega}C_{r}$

$\mathbf{p} = \mathbf{p}_r + \mathbf{p}_\Omega$ $\mathbf{p}_r = \frac{1}{2} \left\{ \frac{\mathbf{r}}{r} \left(\frac{\mathbf{r}}{r} \mathbf{p} \right) + \left(\mathbf{p} \frac{\mathbf{r}}{r} \right) \frac{\mathbf{r}}{r} \right\}, \qquad \mathbf{p}_\Omega = \frac{1}{2r} \left\{ \mathbf{I} \times \frac{\mathbf{r}}{r} - \frac{\mathbf{r}}{r} \times \mathbf{I} \right\}$

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probability density shifted out of the repulsive core



$$c_{\Omega} = \exp\left\{-i\vartheta(r)\left\{\frac{3}{2}(\boldsymbol{\sigma}_{1}\cdot\boldsymbol{p}_{\Omega})(\boldsymbol{\sigma}_{2}\cdot\boldsymbol{r}) + \frac{3}{2}(\boldsymbol{\sigma}_{1}\cdot\boldsymbol{r})(\boldsymbol{\sigma}_{2}\cdot\boldsymbol{p}_{\Omega})\right\}\right\}$$

tensor force admixes other angular momenta





 \mathbf{p}_r

 \mathbf{p}_{Ω}

p

UCOM

Central and Tensor Correlations

 $\underset{\sim}{C} = \underset{\sim}{C}_{\Omega}\underset{\sim}{C}_{r}$

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Central Correlations

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probability density shifted out of the repulsive core



Tensor Correlations

$$c_{\Omega} = \exp\left\{-i\vartheta(r)\left\{\frac{3}{2}(\boldsymbol{\sigma}_{1}\cdot\boldsymbol{p}_{\Omega})(\boldsymbol{\sigma}_{2}\cdot\boldsymbol{r}) + \frac{3}{2}(\boldsymbol{\sigma}_{1}\cdot\boldsymbol{r})(\boldsymbol{\sigma}_{2}\cdot\boldsymbol{p}_{\Omega})\right\}\right\}$$

tensor force admixes other angular momenta



 \mathbf{p}_r

Unitary Correlation Operator Method Correlations and Energies





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 Correlations and Energies







both central and tensor correlations are essential for binding



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

Unitary Correlation Operator Method Correlated Interaction in Momentum Space

${}^{3}S_{1}$ bare



bare interaction has strong off-diagonal matrix elements connecting to high momenta



Roth, Hergert, Papakonstaninou, Neff, Feldmeier, Phys. Rev. C 72, 034002 (2005)

Unitary Correlation Operator Method Correlated Interaction in Momentum Space





bare interaction has strong off-diagonal matrix elements connecting to high momenta

correlated interaction is **more attractive** at low momenta



off-diagonal matrix elements connecting low- and

high- momentum states are **strongly** reduced



${}^{3}S_{1} - {}^{3}D_{1}$ bare





Unitary Correlation Operator Method Correlated Interaction in Momentum Space





bare interaction has strong off-diagonal matrix elements connecting to high momenta

correlated interaction is **more attractive** at low momenta



matrix elements connecting low- and high- momentum states are strongly reduced

off-diagonal







Roth, Hergert, Papakonstaninou, Neff, Feldmeier, Phys. Rev. C 72, 034002 (2005)

UCOM(SRG) No-Core Shell Model Calculations



- convergence much improved compared to bare interaction
- effective interaction in two-body approximation converges to different energy then bare interaction
- transformed interaction can be tuned to obtain simultaneously (almost) exact ³He and ⁴He binding energies

Roth, Neff, Feldmeier, Prog. Part. Nucl. Phys. 65, 50 (2010)

UCOM(SRG) NCSM ⁶Li/⁷Li ground state energy



• effective two-body interaction also works reasonably well for (slightly) heavier nuclei





- states close to one-nucleon, two-nucleon or cluster thresholds can have well developed halo or cluster structure
- >> these are hard to tackle in the harmonic oscillator basis



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

Feldmeier, Schnack, Rev. Mod. Phys. **72** (2000) 655 Neff, Feldmeier, Nucl. Phys. **A738** (2004) 357

FMD Fermionic Molecular Dynamics

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Molecular

single-particle states

$$\langle \mathbf{x} | q \rangle = \sum_{i} c_{i} \exp \left\{ -\frac{(\mathbf{x} - \mathbf{b}_{i})^{2}}{2a_{i}} \right\} \otimes \left| \chi^{\dagger}_{i}, \chi^{\downarrow}_{i} \right\rangle \otimes \left| \xi \right\rangle$$

- Gaussian wave-packets in phase-space (complex parameter b_i encodes mean position and mean momentum), spin is free, isospin is fixed
- width a_i is an independent variational parameter for each wave packet
- use one or two wave packets for each single particle state

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Feldmeier, Schnack, Rev. Mod. Phys. **72** (2000) 655 Neff, Feldmeier, Nucl. Phys. **A738** (2004) 357 Antisymmetrization

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Feldmeier, Schnack, Rev. Mod. Phys. **72** (2000) 655 Neff, Feldmeier, Nucl. Phys. **A738** (2004) 357 see also Antisymmetrized Molecular Dynamics

Horiuchi, Kanada-En'yo, Kimura, . . .

Antisymmetrization

(One-body) Kinetic Energy

 $\langle q_{k} | \underline{\mathcal{T}} | q_{l} \rangle = \langle a_{k} \mathbf{b}_{k} | \underline{\mathcal{T}} | a_{l} \mathbf{b}_{l} \rangle \langle \chi_{k} | \chi_{l} \rangle \langle \xi_{k} | \xi_{l} \rangle$

$$\langle a_k \mathbf{b}_k | \underline{T} | a_l \mathbf{b}_l \rangle = \frac{1}{2m} \left(\frac{3}{a_k^* + a_l} - \frac{(\mathbf{b}_k^* - \mathbf{b}_l)^2}{(a_k^* + a_l)^2} \right) R_{kl}$$

(Two-body) Potential

► fit radial dependencies by (a sum of) Gaussians $G(\mathbf{x}_1 - \mathbf{x}_2) = \exp\left\{-\frac{(\mathbf{x}_1 - \mathbf{x}_2)^2}{2\kappa}\right\}$

► Gaussian integrals

$$\langle a_k \mathbf{b}_k, a_l \mathbf{b}_l | \mathcal{Q} | a_m \mathbf{b}_m, a_n \mathbf{b}_n \rangle = R_{km} R_{ln} \left(\frac{\kappa}{\alpha_{klmn} + \kappa} \right)^{3/2} \exp \left\{ -\frac{\boldsymbol{\rho}_{klmn}^2}{2(\alpha_{klmn} + \kappa)} \right\}$$

>> analytical expressions for matrix elements

 $\alpha_{klmn} = \frac{a_k^* a_m}{a_k^* + a_m} + \frac{a_l^* a_n}{a_l^* + a_n}$

$$\boldsymbol{\rho}_{klmn} = \frac{a_m \mathbf{b}_k^* + a_k^* \mathbf{b}_m}{a_k^* + a_m} - \frac{a_n \mathbf{b}_l^* + a_l^* \mathbf{b}_m}{a_l^* + a_n}$$
$$R_{km} = \langle a_k \mathbf{b}_k | a_m \mathbf{b}_m \rangle$$

 $C^{\dagger}(T+V)C = T$ one-body kinetic energy $+\sum_{cT} \hat{V}_{c}^{ST}(r) + \frac{1}{2} (p_{r}^{2} \hat{V}_{p^{2}}^{ST}(r) + \hat{V}_{p^{2}}^{ST}(r) p_{r}^{2}) + \hat{V}_{l^{2}}^{ST}(r) \mathbf{L}^{2}$ **central** potentials $+\sum_{\tau} \hat{V}_{ls}^{T}(r) \mathbf{\underline{l}} \cdot \mathbf{\underline{s}} + \hat{V}_{l^{2}ls}^{T}(r) \mathbf{\underline{l}}^{2} \mathbf{\underline{l}} \cdot \mathbf{\underline{s}}$ **spin-orbit** potentials $+\sum_{\tau} \hat{V}_t^{\mathsf{T}}(r) \underbrace{S}_{12}(\mathbf{r}, \mathbf{r}) + \hat{V}_{trp_{\Omega}}^{\mathsf{T}}(r) \underbrace{p_r}_{\sim} \underbrace{S}_{12}(\mathbf{r}, \mathbf{p_{\Omega}}) + \hat{V}_{tll}^{\mathsf{T}}(r) \underbrace{S}_{12}(\mathbf{I}, \mathbf{I}) +$ $\hat{V}_{tn_{\Omega}n_{\Omega}}^{T}(r) \underset{\sim}{S}_{12}(\mathbf{p}_{\Omega}, \mathbf{p}_{\Omega}) + \hat{V}_{l^{2}tp_{\Omega}p_{\Omega}}^{T}(r) \underset{\sim}{\mathbf{I}}^{2} \underset{\sim}{S}_{12}(\mathbf{p}_{\Omega}, \mathbf{p}_{\Omega})$ **tensor** potentials bulk of tensor force mapped onto central part of correlated interaction tensor correlations also change the spin-orbit

part of the interaction

Nucl. Phys. A745 (2004) 3

FMD PAV, VAP and Multiconfiguration

Projection After Variation (PAV)

- mean-field 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

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Variation After Projection (VAP)

- effect of projection can be large
- Variation after Angular Momentum and Parity Projection (VAP) for light nuclei
- combine VAP with constraints on radius, dipole moment, quadrupole moment, . . . to generate additional configurations

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FMD

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Multiconfiguration Calculations

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

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

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

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

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

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



• NCSM allows good description of short-range physics, but long-range behavior suffers from harmonic oscillator asymptotics

FMD FMD vs NCSM model spaces



- NCSM allows good description of short-range physics, but long-range behavior suffers from harmonic oscillator asymptotics
- FMD allows to describe long-range physics by superposition of localized cluster configurations, but limited in description of short-range physics

Cluster States in ¹²C Harmonic Oscillator NħΩ Excitations



• Hoyle state very difficult to converge in no-core shell model

Chernykh, Feldmeier, Neff, von Neumann-Cosel, Richter, PRL **98**, 032501 (2007) Neff, Feldmeier, Few-Body Syst. **45**, 145 (2009)



Many-Body Approach:

Fermionic Molecular Dynamics

- Internal region: VAP configurations with radius constraint
- External region: Brink-type cluster configurations
- Matching to Coulomb solutions: Microscopic *R*-matrix method

Results:

- ⁷Be bound and scattering states
- Astrophysical S-factor

T. Neff, Phys. Rev. Lett. 106, 042502 (2011)

³He(α, γ)⁷Be **FMD model space**

Frozen configurations

• 15 antisymmetrized wave function built with ⁴He and ³He FMD clusters up to channel radius α =12 fm

Polarized configurations

 30 FMD wave functions obtained by VAP on 1/2⁻, 3/2⁻, 5/2⁻, 7/2⁻ and 1/2⁺, 3/2⁺ and 5/2⁺ combined with radius constraint in the interaction region

Boundary conditions

 Match relative motion of clusters at channel radius to Whittaker/Coulomb functions with the microscopic *R*matrix method of the Brussels group D. Baye, P.-H. Heenen, P. Descouvemont



Bound states

		Experiment	FMD
⁷ Be	E _{3/2-}	-1.59 MeV	-1.49 MeV
	E _{1/2-}	-1.15 MeV	-1.31 MeV
	r _{ch}	2.647(17) fm	2.67 fm
	Q	-	-6.83 <i>e</i> fm²
⁷ Li	E _{3/2-}	-2.467 MeV	-2.39 MeV
	E _{1/2-}	-1.989 MeV	-2.17 MeV
	<i>r</i> _{ch}	2.444(43) fm	2.46 fm
	Q	-4.00(3) <i>e</i> fm ²	-3.91 <i>e</i> fm²

- centroid of bound state energies well described if polarized configurations included
- tail of wave functions tested by charge radii and quadrupole moments

Phase shift analysis:

Spiger and Tombrello, PR **163**, 964 (1967)



dashed lines – frozen configurations only solid lines – polarized configurations in interaction region included

 Scattering phase shifts well described, polarization effects important

³He(α, γ)⁷Be S-, d- and f-wave Scattering States



dashed lines – frozen configurations only – solid lines – FMD configurations in interaction region included

- polarization effects important
- s- and d-wave scattering phase shifts well described
- 7/2⁻ resonance too high, 5/2⁻ resonance roughly right, consistent with no-core shell model calculations





S-factor: $S(E) = \sigma(E)E \exp\{2\pi\eta\}$ $\eta = \frac{\mu Z_1 Z_2 e^2}{k}$

Nara Singh *et al.*, PRL **93**, 262503 (2004) Bemmerer *et al.*, PRL **97**, 122502 (2006) Confortola *et al.*, PRC **75**, 065803 (2007) Brown *et al.*, PRC **76**, 055801 (2007) Di Leva *et al.*, PRL **102**, 232502 (2009) Carmona-Gallardo *et al.*, PRC **86**, 032801(R) (2012)

- dipole transitions from $1/2^+$, $3/2^+$, $5/2^+$ scattering states into $3/2^-$, $1/2^-$ bound states
- FMD is the only model that describes well the energy dependence and normalization of new high quality data
- ► fully microscopic calculation, bound and scattering states are described consistently

T. Neff, Phys. Rev. Lett. 106 (2011) 042502

³He(α, γ)⁷Be **Overlap Functions and Dipole Matrixelements**



- Overlap functions from projection on RGM-cluster states
- Coulomb and Whittaker functions matched at channel radius a=12 fm
- Dipole matrix elements calculated from overlap functions reproduce full calculation within 2%
- cross section depends significantly on internal part of wave function, description as an "external" capture is too simplified

³H(α, γ)⁷Li **S-Factor**



- isospin mirror reaction of ${}^{3}\text{He}(\alpha, \gamma){}^{7}\text{Be}$
- ⁷Li bound state properties and phase shifts well described
- FMD calculation describes energy dependence of Brune et al. data but cross section is larger by about 15%

³He(α, γ)⁷Be S-Factor Contributions



- main difference between FMD and Kajino results is originating in s-wave capture both in normalization and energy dependence
- difference in normalization related to ground state properties as seen in charge radius/quadrupole moment
- difference in energy dependence not understood yet
 - long-range of realistic interaction due to explicit description of pion-exchange ?
 - polarization of clusters in the interaction region ?

Beryllium Isotopes

Questions

• α -clustering, halos in ¹¹Be and ¹⁴Be, N = 8 shell closure ?

Calculation

- VAP and multiconfiguration-VAP calculations with mean proton distance as generator coordinate
- UCOM(SRG) effective spin-orbit strength is too small modify interaction by multiplying spin-orbit interaction in S = 1, T = 1 channel with factor $\eta \approx 2$

Observables

- energies
- charge and matter radii, electromagnetic transitions

Beryllium Isotopes Mean proton distance as generator coordinate



Mean proton distance

$$R_{pp}^{2} = \frac{1}{Z^{2}} \langle \sum_{i < j}^{\text{protons}} (\mathbf{r}_{i} - \mathbf{r}_{j})^{2} \rangle$$

 R_{pp} as a measure of α -cluster distance



Beryllium Isotopes

Mean proton distance as generator coordinate



¹¹Be – "*p*", "*s*" and "*d*"-configurations

- "s"- and "d"-configurations will mix in 1/2⁺ state
- energy surfaces for "p" and "s" similar to those in ¹⁰Be
- "d" surface has minimum at larger cluster distance → d-configuration has a polarized ¹⁰Be core



Beryllium Isotopes N = 8 shell closure ?



- in ¹²Be normal and intruder configurations almost degenerate in energy
- contribution of spin-orbit force larger in intruder configuration
- eigenstate composition can be tuned from dominant p^2 to dominant $(sd)^2$ by changing spin-orbit factor from 2.0 to 2.2

Beryllium Isotopes

Charge Radii



A. Krieger et al., Phys. Rev. Lett. 108, 142501 (2012)

Beryllium Isotopes

Electromagnetic transitions

¹⁰Be

	FMD(Multiconfig)	Experiment
$B(E2; 2^+_1 \to 0^+_1)$	8.07 e ² fm ⁴	9.2 ± 0.3 e ² fm ⁴
$B(E2; 2^{+}_{2} \rightarrow 0^{+}_{1})$	0.08 e ² fm ⁴	$0.11 \pm 0.02 \ e^2 \text{fm}^4$
$B(E2; 0_2^{+} \rightarrow 2_1^{+})$	0.17 <i>e</i> ² fm ⁴	3.2 ± 1.9 e ² fm ⁴

¹²Be

	FMD(Multiconfig)	Experiment
$B(E2; 2^+_1 \rightarrow 0^+_1)$	8.75 e ² fm ⁴	$8.0 \pm 3.0 \ e^{2} \text{fm}^{4}$
$B(E2; 0_2^+ \to 2_1^+)$	7.45 e ² fm ⁴	$7.0 \pm 0.6 \ e^{2} \text{fm}^{4}$
$M(E0;0^+_1\rightarrow 0^+_2)$	0.90 efm ²	$0.87 \pm 0.03 \text{ efm}^2$

- Monopole and Quadrupole transitions directly connected to mixing between normal and intruder configurations
- 2^+_1 state has dominant intruder contribution

McCutchan *et al.*, Phys. Rev. Lett. **103**, 192501 (2009). Nakamura *et al.*, Phys. Lett. **B394**, 11 (1997). Shimoura *et al.*, Phys. Lett. **B654**, 87 (2007). Iwasaki *et al.*, Phys. Lett. **B491**, 8 (2000).

Summary

Unitary Correlation Operator Method

• Realistic low-momentum interaction V_{UCOM}

Fermionic Molecular Dynamics

- Microscopic many-body approach using Gaussian wave-packets
- Projection and multiconfiguration mixing

³He(α , γ)⁷Be Radiative Capture

- Bound states, resonance and scattering wave functions
- S-Factor: energy dependence and normalization

Beryllium Isotopes

- Breakdown of N = 8 shell closure
- Charge radii

Thanks to my collaborators:

Hans Feldmeier (GSI), Wataru Horiuchi (Hokkaido), Karlheinz Langanke (GSI), Robert Roth (TUD), Yasuyuki Suzuki (Niigata), Dennis Weber (GSI)