## **Clusters and Halos studied in Fermionic Molecular Dynamics**

10 <sup>17</sup>Ne - p <sup>17</sup>Ne - n 0.001-0.01 5 0.00, z [fm] 0 -5 -10 -5 1-01 0 10 -10 0 5 -5 0 5 x [fm] x [fm]

**Thomas Neff** 

EENEN 09 First EMMI-EFES Workshop on Neutron-Rich Nuclei

> GSI Darmstadt February 10, 2009



## **Overview**

## Introduction

## **Unitary Correlation Operator Method**

- Short-range Correlations
- Correlated Interaction

## **Fermionic Molecular Dynamics**

- Cluster States in <sup>12</sup>C
- Neon Isotopes di-proton halo in <sup>17</sup>Ne

## Central and Tensor Correlations

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

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### **Central Correlations**

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

 probability density shifted out of the repulsive core



## **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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## **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



 $\mathbf{p}_r$ 

p

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Thomas Neff — EENEN09, 02/10/09

 $\mathbf{p}_r$ 

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## ucoм Correlated Two-Body Densities and Energies





central correlator  $C_r$ shifts density out of the repulsive core tensor correlator  $C_{\Omega}$ aligns density with spin

orientation

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

## ucoм Correlated Two-Body Densities and Energies





## central correlator C<sub>r</sub> shifts density out of the repulsive core

tensor correlator  $C_{\Omega}$ aligns density with spin orientation

both central and tensor correlations are essential for binding



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

## ucoм Correlated Interaction in Momentum Space





# **Correlated Interaction in Momentum Space**



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

off-diagonal matrix elements

connecting low- and high- momentum states are **strongly** reduced





## **Fermionic Molecular Dynamics**

## **Motivation**

**FMD Wave Functions** 

**Nucleon-Nucleon Interaction** 

**Mean-Field Calculations** 

**Projection After Variation, Variation After Projection and Multiconfiguration** 

# **Exotica: Special Challenges**



Al-Khalili, Nunes, J. Phys. G 29, R89 (2003)



### **Fermionic**

Slater determinant

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

• antisymmetrized A-body state

## FMD Fermionic Molecular Dynamics

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• antisymmetrized A-body state

#### **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<sub>i</sub> encodes mean position and mean momentum), spin is free, isospin is fixed
- width  $a_i$  is an independent variational parameter for each wave packet
- superposition of two wave packets for each single particle state

Rev. Mod. Phys. **72** (2000) 655 Nucl. Phys. **A745** (2004) 3

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Rev. Mod. Phys. **72** (2000) 655 Nucl. Phys. **A745** (2004) 3 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

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

- analytical formulas for matrix elements

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

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

tensor correlations also change the spin-orbit part of the interaction

Nucl. Phys. **A745** (2004) 3

### **Effective two-body interaction**

- FMD model space can't describe correlations induced by residual medium-long ranged tensor forces
- use **longer ranged tensor correlator** to partly account for that
- no three-body forces, saturation with UCOM force not correct
- add phenomenological two-body correction term with a momentumdependend central and (isospin-dependend) spin-orbit part (about 15% contribution to potential)
- fit correction term to binding energies and radii of "closed-shell" nuclei (<sup>4</sup>He, <sup>16</sup>O, <sup>40</sup>Cα), (<sup>24</sup>O, <sup>34</sup>Si, <sup>48</sup>Cα)

#### **–** Todo:

use **three-body** or **density dependent two-body force** instead of two-body correction term

## FMD Perform Variation

## **Minimization**

• minimize Hamiltonian expectation value with respect to all single-particle parameters  $q_k$ 

$$\min_{\{q_k\}} \frac{\langle Q | H - T_{cm} | Q \rangle}{\langle Q | Q \rangle}$$

- this is a Hartree-Fock calculation in our particular single-particle basis
- the mean-field may break the symmetries of the Hamiltonian



## 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

## **PAV, VAP and Multiconfiguration**

## **Projection After Variation (PAV)**

- mean-field may break symmetries of Hamiltonian
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## Variation After Projection (VAP)

- effect of projection can be large
- perform Variation after Parity Projection PAV  $^{\pi}$
- full Variation after Angular Momentum Projection (VAP)
- 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

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

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

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## **Multiconfiguration Calculations**

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

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

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

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

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

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

## **Cluster States in** <sup>12</sup>C

## **Astrophysical Motivation**

## Structure

• Is the Hoyle state a pure  $\alpha$ -cluster state ?

- Other excited 0<sup>+</sup> and 2<sup>+</sup> states
- Compare FMD results to  $\alpha$ -cluster model
- Analyze wave functions in harmonic oscillator basis
- No-Core Shell Model Calculations ?



7.2747

30



http://outreach.atnf.csiro.au/education/senior/astrophysics/stellarevolution\_postmain.html

## Cluster States in <sup>12</sup>C Microscopic *α*-Cluster Model



 $R_{12} = (2, 4, \dots, 10) \text{ fm}$  $R_{13} = (2, 4, \dots, 10) \text{ fm}$  $\cos(\vartheta) = (1.0, 0.8, \dots, -1.0)$ 

alltogether 165 configurations

## **Basis States**

• describe Hoyle State as a system of 3 <sup>4</sup>He nuclei

 $\begin{aligned} \left| \Psi_{3\alpha}(\mathbf{R}_{1}, \mathbf{R}_{2}, \mathbf{R}_{3}); JMK\pi \right\rangle = \\ P^{J}_{MK} P^{\pi} \mathcal{A} \left\{ \left| \psi_{\alpha}(\mathbf{R}_{1}) \right\rangle \otimes \left| \psi_{\alpha}(\mathbf{R}_{2}) \right\rangle \otimes \left| \psi_{\alpha}(\mathbf{R}_{3}) \right\rangle \right\} \end{aligned}$ 

## **Volkov Interaction**

- simple central interaction
- parameters adjusted to reproduce  $\alpha$  binding energy and radius,  $\alpha - \alpha$  scattering data and C12 ground state energy
- ✗ only reasonable for <sup>4</sup>He, <sup>8</sup>Be and <sup>12</sup>C nuclei

#### **'BEC'** wave functions

• same interaction and  $\alpha$ -cluster parameters used by Funaki et al.

Kamimura, Nuc. Phys. **A351** (1981) 456 Funaki et al., Phys. Rev. C **67** (2003) 051306(R)

## **Basis States**

**Cluster States in**<sup>12</sup>C

FMD

- 20 FMD states obtained in Variation after Projection on 0<sup>+</sup> and 2<sup>+</sup> with constraints on the radius
- 42 FMD states obtained in Variation after Projection on parity with constraints on radius and quadrupole deformation
- 165  $\alpha$ -cluster configurations
- projected on angular momentum and linear momentum

#### Interaction

• not tuned for  $\alpha$ - $\alpha$  scattering or <sup>12</sup>C properties





## Cluster States in <sup>12</sup>C $\alpha$ - $\alpha$ Phaseshifts



- Phaseshifts calculated with cluster configurations only (dashed lines)
- Phaseshifts calculated with additional FMD VAP configurations in the interaction region (solid lines)

 only cluster configurations included

- similar quality for description of  $\alpha$ - $\alpha$ -scattering





## **Cluster States in** <sup>12</sup>C Comparison

	Exp <sup>1</sup>	Exp <sup>2</sup>	Exp <sup>3</sup>	FMD	$\alpha$ -cluster	'BEC' <sup>4</sup>	
<i>E</i> (0 <sup>+</sup> <sub>1</sub> )	-92.16			-92.64	-89.56	-89.52	
$E^{*}(2_{1}^{+})$	4.44			5.31	2.56	2.81	experimental
Ε(3α)	-84.89			-83.59	-82.05	-82.05	situation for $0^+_3$ and $2^+_2$ states still unsettled
$E(0_{2}^{+}) - E(3\alpha)$	0.38			0.43	0.38	0.26	
$E(0_{3}^{+}) - E(3\alpha)$	(3.0)	2.7(3)	3.96(5)	2.84	2.81		
$E(2^{+}_{2}) - E(3\alpha)$	(3.89)	2.6(3)	6.63(3)	2.77	1.70		
$r_{\rm charge}(0^+_1)$	2.47(2)			2.53	2.54		
$r(0^+_1)$				2.39	2.40	2.40	$2\frac{1}{2}$ resonance at
$r(0^{+}_{2})$				3.38	3.71	3.83	treshold included in NACRE compilation
$r(0_{3}^{+})$				4.62	4.75		
$r(2_{1}^{+})$				2.50	2.37	2.38	
$r(2^{+}_{2})$				4.43	4.02		
$M(E0, 0^+_1 \rightarrow 0^+_2)$	5.4(2)			6.53	6.52	6.45	-
$B(E2,2^+_1\rightarrow 0^+_1)$	7.6(4)			8.69	9.16		
$B(E2, 2_{1}^{+} \rightarrow 0_{2}^{+})$	2.6(4)			3.83	0.84		

<sup>1</sup> Ajzenberg-Selove, Nuc. Phys. A506, 1 (1990)
<sup>2</sup> Itoh et al., Nuc. Phys. A738, 268 (2004)
<sup>3</sup> Fynbo et al., Nature 433, 137 (2005). Diget et al., Nuc. Phys. A738, 760 (2005)
<sup>4</sup> Funaki et al., Phys. Rev. C 67, 051306(R) (2003)

## Cluster States in <sup>12</sup>C Electron Scattering Data





- compare with precise electron scattering data up to high momenta in Distorted Wave Born Approximation
- use intrinsic density

$$\rho(\mathbf{x}) = \sum_{k=1}^{A} \langle \Psi \, \big| \, \delta(\mathbf{x}_{k} - \mathbf{X} - \mathbf{x}) \, \big| \Psi \, \rangle$$

- elastic form factor described very well by FMD
- transition form factor better described by cluster model

M. Chernykh, H. Feldmeier, T. Neff, P. von Neumann-Cosel, and A. Richter, Phys. Rev. Lett. 98 (2007) 032501

## Cluster States in <sup>12</sup>C Important Configurations

• Calculate the overlap with FMD basis states to find the most important contributions to the Hoyle state



loosely bound, gas-like states

FMD basis states are not orthogonal!

## Cluster States in <sup>12</sup>C Overlap with Cluster Model Space

Calculate the overlap of FMD wave functions with pure  $\alpha$ -cluster model space

$$N_{\alpha} = \langle \Psi | \underbrace{P}_{\exists \alpha} | \Psi \rangle$$



## Cluster States in <sup>12</sup>C Harmonic Oscillator NħΩ Excitations

Y. Suzuki et al., Phys. Rev. C 54 (1996) 2073

$$\operatorname{Occ}(N) = \langle \Psi \left| \delta \left( \sum_{i} (\mathcal{H}_{i}^{HO} / \hbar \Omega - 3/2) - N \right) \right| \Psi \rangle$$



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Y. Suzuki et al, Phys. Rev. C 54, 2073 (1996).

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# Hoyle State $\alpha$ -cluster states in the No-Core Shell Model ?

- compare spectra in NCSM and  $\alpha\text{-cluster}$  model using the Volkov interaction
- bare interaction used in NCSM calculations
- **–** good agreement for ground state band  $(0^+_1, 2^+_1, 4^+_1)$
- very slow convergence for cluster states

#### **Binding energies**

	<sup>4</sup> He	<sup>12</sup> C
Cluster	-27.3 MeV	-89.6 MeV
NCSM	-28.3 MeV	-95.4 MeV



## Neon Isotopes <sup>17</sup>Ne-<sup>22</sup>Ne

## Structure

- $s^2/d^2$  occupation in <sup>17</sup>Ne and <sup>18</sup>Ne
- <sup>3</sup>He and <sup>4</sup>He cluster admixtures

## **Observables**

- Charge Radii
- Matter Radii
- Is <sup>17</sup>Ne a Halo nucleus ?

## Neon Isotopes Calculation



- Variation after parity projection on positive and negative parity
- Crank strength of spin-orbit force, changes properties of single-particle orbits and their occupations
- "*s*<sup>2</sup>" and "*d*<sup>2</sup>" minima in <sup>17,18</sup>Ne
- explicit cluster configurations:
  - <sup>17</sup>Ne: <sup>14</sup>O-<sup>3</sup>He <sup>18</sup>Ne: <sup>14</sup>O-<sup>4</sup>He
  - <sup>19</sup>Ne: <sup>16</sup>O-<sup>3</sup>He and <sup>15</sup>O-<sup>4</sup>He
  - <sup>20</sup>Ne: <sup>16</sup>O-<sup>4</sup>He
  - <sup>21</sup>Ne: "<sup>17</sup>O"-<sup>4</sup>He
  - <sup>22</sup>Ne: "<sup>18</sup>O"-<sup>4</sup>He

Intrinsic proton/neutron densities of dominant FMD state

#### • Neon Isotopes

## **Separation energies**



Separation Energies

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#### Neon Isotopes

## **Charge and Matter Radii**





- cluster admixtures responsible for large charge radii in <sup>19–22</sup>Ne
- measurements of charge radii by COLLAPS@ISOLDE



 matter radii from interaction cross sections

A. Ozawa *et al.*, Nuc. Phys. **A693** (2001) 32

good agreement with expection of <sup>19</sup>Ne

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

## Neon Isotopes <sup>17</sup>Ne **Halo ?**



## Summary

## **Unitary Correlation Operator Method**

- Explicit description of short-range central and tensor correlations
- Phase-shift equivalent correlated interaction  $V_{\text{UCOM}}$
- Interaction in momentum-space
- *ab initio* calculations with few- and many-body methods

## **Fermionic Molecular Dynamics**

- Microscopic many-body approach using Gaussian wave-packets
- Consistent description of well bound states with shell structure and loosely bound states of cluster or halo nature
- <sup>12</sup>C spectrum, Hoyle state and other high-lying 0<sup>+</sup> and 2<sup>+</sup> states, monopole transition form factor, analysis of FMD wave functions in harmonic oscillator basis, comparison with no-core shell model calculations
- Neon isotopes, separation energies, charge and matter radii, halo structure in <sup>17</sup>Ne, importance of cluster admixtures in <sup>19–22</sup>Ne ground states

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