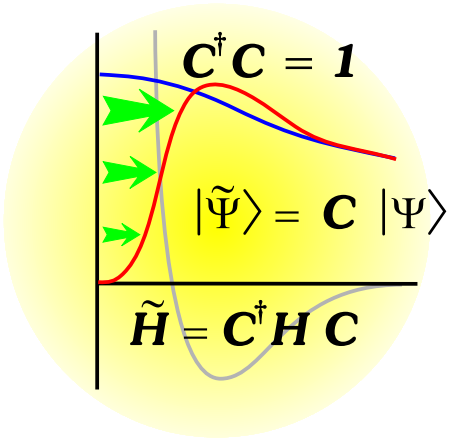

The

Unitary Correlation Operator Method

or

"The Taming of the Core"

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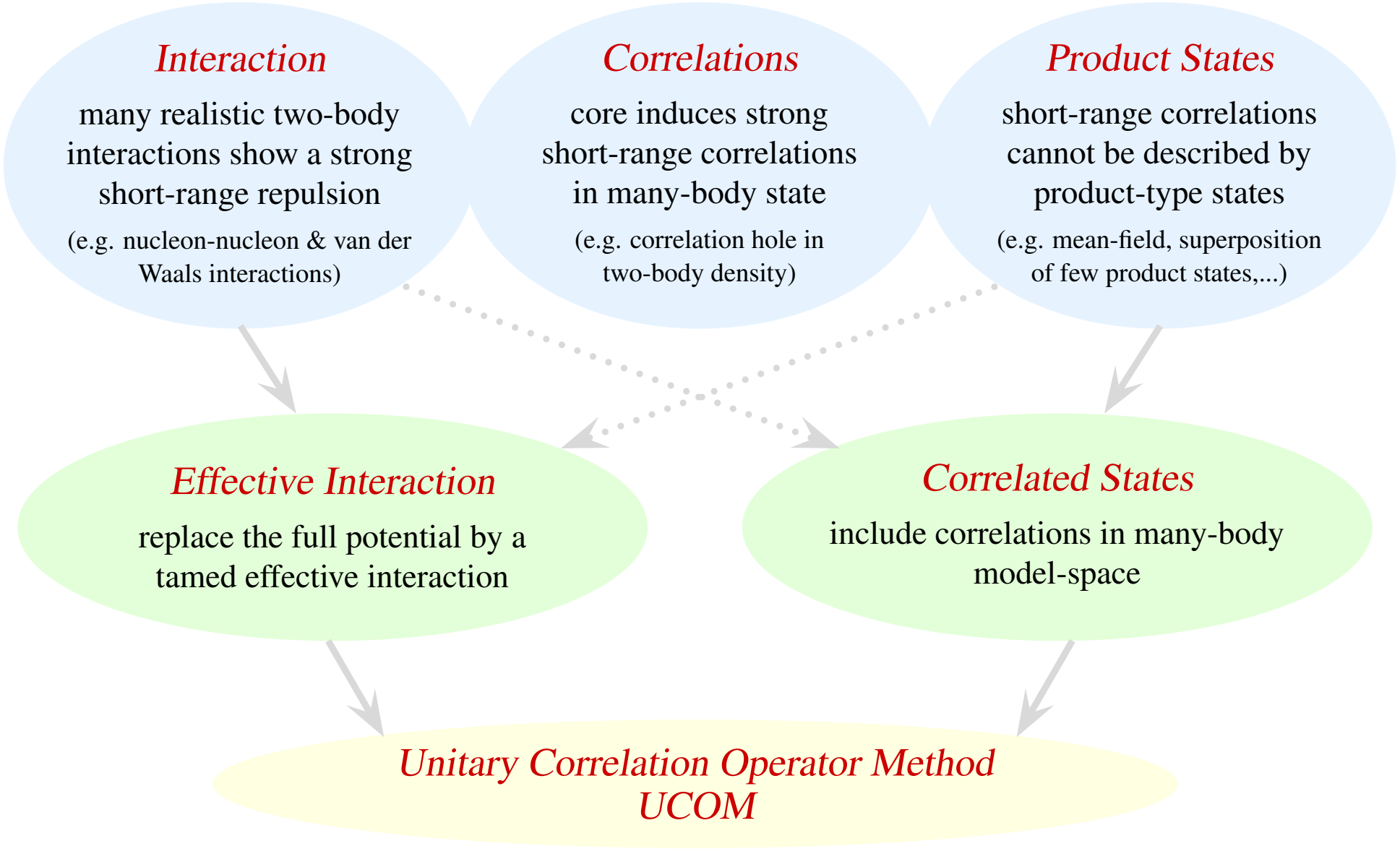
Gesellschaft für Schwerionenforschung — Darmstadt/Germany

"Nuclear Structure for the 21st Century" — INT Seattle
11/2000

Why Effective Interactions?

The Problem: Short-Range Correlations



Concept of the

Unitary Correlation Operator Method

Correlation Operator

Short-range correlations are represented by a state-independent *unitary correlation operator* $\mathbf{C}$ that describes a *radial distance-dependent shift* in the relative coordinate of the two-body system.

$$\mathbf{C} = \exp[-\mathrm{i}\,\mathbf{G}] = \exp\Big[-\mathrm{i}\sum_{i<j}\mathbf{g}_{ij}\Big]$$

$$\mathbf{g} = \tfrac{1}{2}[\, s(\mathbf{r})\ \tfrac{\vec{\mathbf{r}}}{\mathbf{r}} \cdot \vec{\mathbf{q}}\ +\ \text{h.c.}\,]$$

$\mathbf{G}^\dagger = \mathbf{G}$
$\mathbf{C}^\dagger\mathbf{C} = 1$

$s(r) \sim$ shift distance

Correlated States

$$|\widetilde{\psi}\rangle = \mathbf{C}\ |\psi\rangle$$

Correlated Operators

$$\widetilde{\mathbf{O}} = \mathbf{C}^\dagger\ \mathbf{O}\ \mathbf{C}$$

$$\langle\widetilde{\psi}|\,\mathbf{O}\,|\widetilde{\psi}'\rangle = \langle\psi|\,\mathbf{C}^\dagger\ \mathbf{O}\ \mathbf{C}\,|\psi'\rangle = \langle\psi|\,\widetilde{\mathbf{O}}\,|\psi'\rangle$$

Correlated Wave Function

Correlated Wave Function

- correlator acts on the relative part of the two-body wave function

$$\langle \vec{r}, \vec{X} | \, \mathbf{C} \, | \psi \rangle = \mathcal{R}_-(r) \, \langle R_-(\vec{r}) \tfrac{\vec{r}}{r}, \vec{X} | \psi \rangle$$

$$\langle \vec{r}, \vec{X} | \, \mathbf{C}^\dagger \, | \psi \rangle = \mathcal{R}_+(r) \, \langle R_+(\vec{r}) \tfrac{\vec{r}}{r}, \vec{X} | \psi \rangle$$

- norm-conserving coordinate transformation

$$\vec{r} \;\mapsto\; R_\pm(r) \, \tfrac{\vec{r}}{r}$$

Correlation Function $R_\pm(r)$

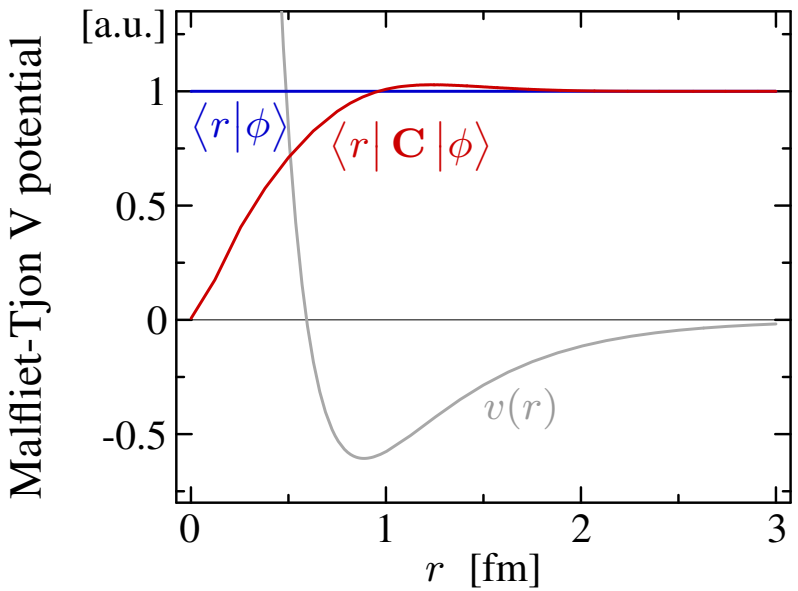
- metric factor and inverse transformation

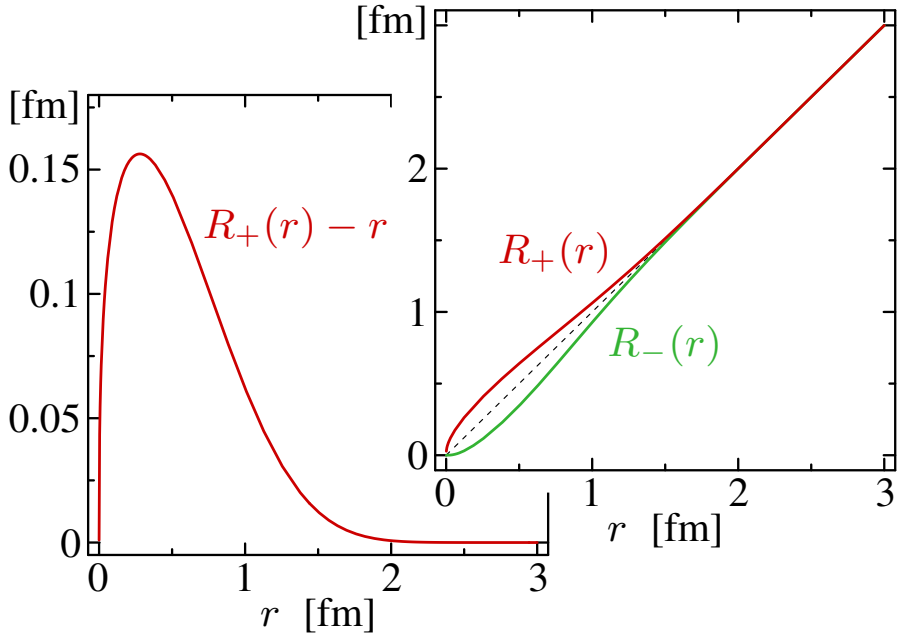
$$\mathcal{R}_\pm(r) = \frac{R_\pm(r)}{r} \sqrt{R'_\pm(r)}$$

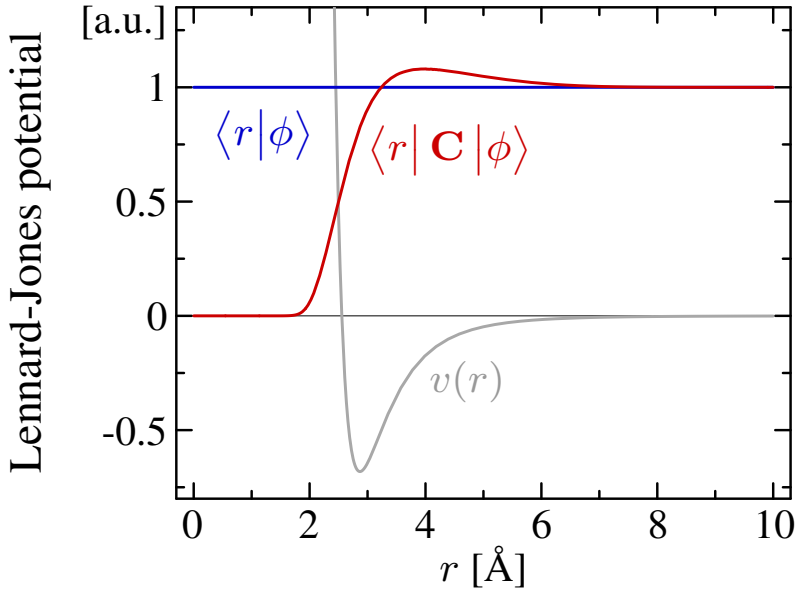
$$R_\pm[R_\mp(r)] = r$$

- connection with $s(r)$

$$\pm 1 = \int_r^{R_\pm(r)} \frac{\mathrm{d}\xi}{s(\xi)} \qquad R_\pm(r) \approx r \pm s(r)$$






Lennard-Jones potential
[a.u.]
1
0.5
0
-0.5
0
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r [Å]
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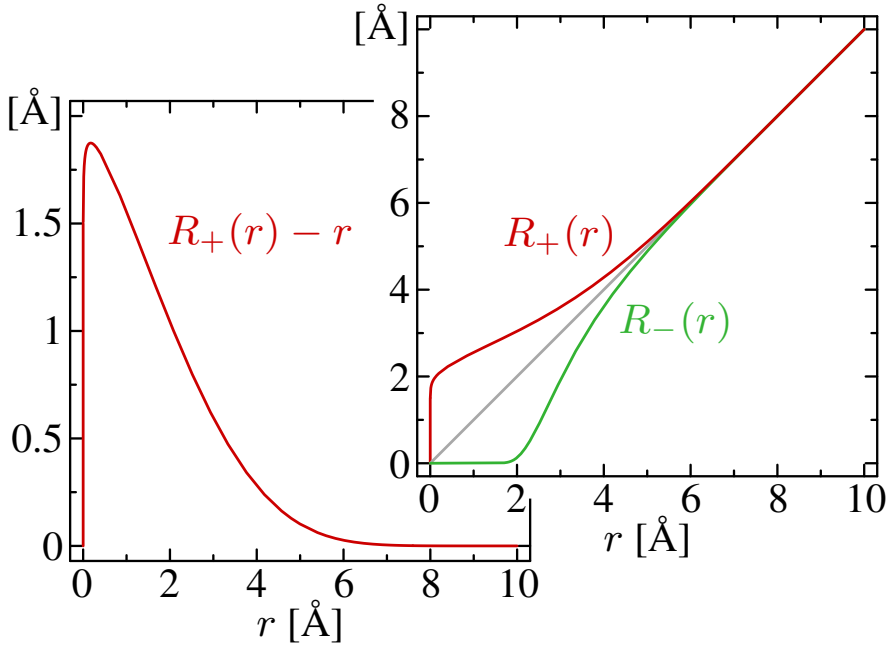
v(r)


[Å]
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r [Å]
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R−(r)

Many-Body System

Correlated Operators & Cluster Expansion

Cluster Decomposition Principle

Cluster Expansion

decompose the correlated operator into a sum of irreducible k-body operators

$$\widetilde{\mathbf{H}} = \mathbf{C}^\dagger \, \mathbf{H} \, \mathbf{C} = \widetilde{\mathbf{H}}^{[1]} + \widetilde{\mathbf{H}}^{[2]} + \widetilde{\mathbf{H}}^{[3]} + \cdots$$

if the range of correlations is small compared to the average distance between the particles then higher cluster orders are negligible

Smallness Parameter

$$\kappa = \rho \, V_C$$

$$V_C = \int \mathrm{d}^3 r \left[\langle r | \, \mathbf{C} \, | 1 \rangle - \langle r | 1 \rangle \right]^2 = \int \mathrm{d}^3 r \left[\mathcal{R}_+(r) - 1 \right]^2$$

$\kappa \ll 1$ | $\kappa \not\ll 1$

Two-Body Approximation

$$\widetilde{\mathbf{H}}^{C2} = \widetilde{\mathbf{H}}^{[1]} + \widetilde{\mathbf{H}}^{[2]}$$

Three-Body Approximation

$$\widetilde{\mathbf{H}}^{C3} = \widetilde{\mathbf{H}}^{[1]} + \widetilde{\mathbf{H}}^{[2]} + \widetilde{\mathbf{H}}^{[3]}$$

Effective Corrections

e.g. density-dependent correlation functions in $\widetilde{\mathbf{H}}^{C2}$

Two-Body Approximation

Correlated Hamiltonian & Effective Interaction

$$\mathbf{H} = \mathbf{T}_0 + \sum_{i<j} v(\mathbf{r}_{ij})$$

$$\widetilde{\mathbf{H}}^{C2} = \mathbf{T}_0 + \sum_{i<j} \left[\widetilde{v}(\mathbf{r}_{ij}) + \widetilde{u}(\mathbf{r}_{ij}) + \vec{\mathbf{q}}_{ij} \frac{1}{2\,\widetilde{\mathfrak{M}}(\vec{\mathbf{r}}_{ij})} \vec{\mathbf{q}}_{ij} \right]$$

Local Potentials

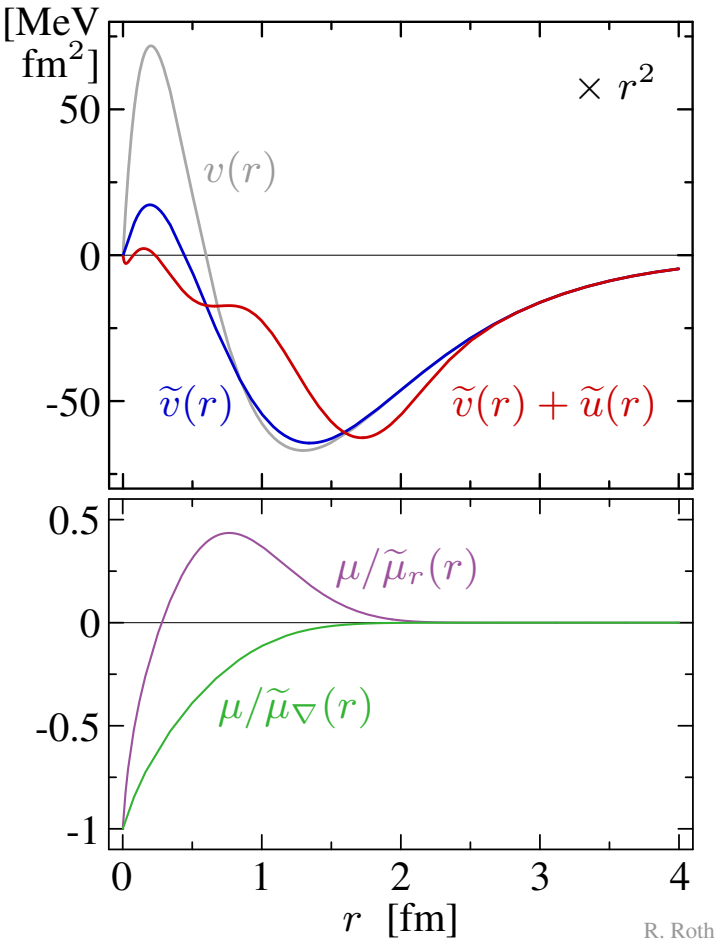
$$\widetilde{v}(r) = v[R_+(r)]$$

$$\widetilde{u}(r) = \frac{1}{2\mu R_+'^2(r)} \left(\frac{2R_+''(r)}{rR_+'(r)} - \frac{5R_+''^2(r)}{4R_+'^2(r)} + \frac{R_+'''(r)}{2R_+'(r)} \right)$$

Effective Mass Corrections

$$\frac{1}{\widetilde{\mathfrak{M}}(\vec{r})} = \frac{1}{\widetilde{\mu}_\nabla(r)} + \frac{1}{\widetilde{\mu}_r(r)} \left(\tfrac{\vec{r}}{r} \otimes \tfrac{\vec{r}}{r}\right)$$

$$\frac{\mu}{\widetilde{\mu}_\nabla(r)} = \frac{r^2}{R_+^2(r)} - 1, \qquad \frac{\mu}{\widetilde{\mu}_r(r)} = \frac{1}{R_+'^2(r)} - \frac{r^2}{R_+^2(r)}$$



The Basics of Fermionic Molecular Dynamics

One-Body States

$$\langle \vec{x} | \psi \rangle = \sum_{\nu=1}^{n} \exp\left(- \frac{(\vec{x} - \vec{\xi}_\nu)^2}{2\,\alpha_\nu} - \mathrm{i}\,\vec{\pi}_\nu \vec{x} \right) \; | m_\nu^s \rangle \otimes | m^t \rangle$$

$\vec{\xi}_\nu$: mean position
$\vec{\pi}_\nu$: mean momentum
α_ν : complex width

- $8n$ variational parameters per nucleon

Many-Body State

$$| \widetilde{\Psi} \rangle = \mathbf{C}\,\mathbf{A} \left(| \psi_1 \rangle \otimes | \psi_2 \rangle \otimes \cdots \otimes | \psi_A \rangle \right)$$

- exactly antisymmetrized product states
- short-range correlations described by UCOM

Structure

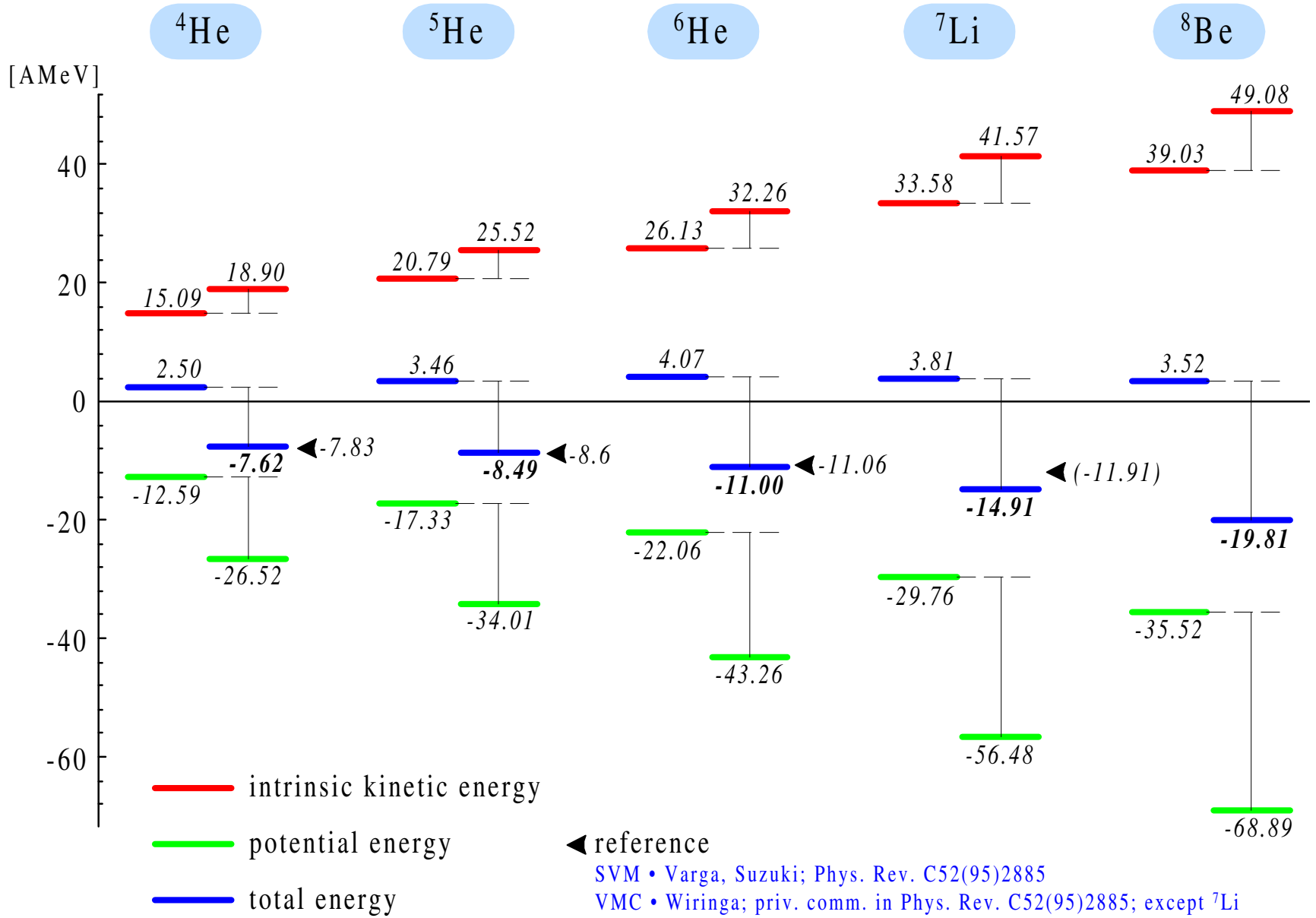
- energy minimization by variation of the parameters gives groundstate wave function
- diagonalization within a small subspace (spanned by rotation & scaling of the variational groundstate)

Dynamics

- time-dependent variational principle yields equations of motion for the parameters

Malfliet-Tjon-V Potential

Groundstate Energies



SVM • Varga, Suzuki; Phys. Rev. C52(95)2885

VMC • Wiringa; priv. comm. in Phys. Rev. C52(95)2885; except ^{7}Li

Spin-Isospin Dependent NN-Potentials

Spin-Isospin Dependent Central Interaction

- central two-body potential expressed by projection operators $\mathbf{\Pi}_{ST}$ on spin S and isospin T

$$\mathbf{v} = \sum_{S,T} v_{ST}(\mathbf{r})\ \mathbf{\Pi}_{ST}$$

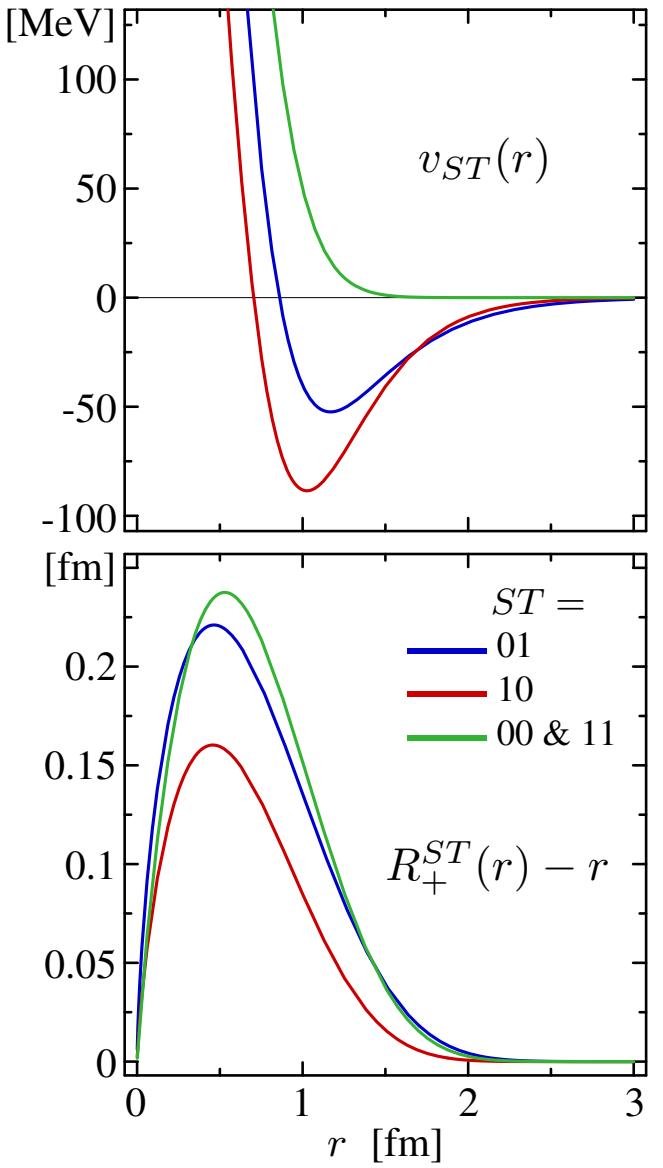
- e.g. Afnan-Tang S3M potential

Spin-Isospin Dependent Correlator

- unitary transformation depending on the (S,T) quantum numbers of the particle pair (two-body space)

$$\mathbf{c} = \exp\Big(-\mathrm{i}\sum_{S,T} \mathbf{g}_{ST}\ \mathbf{\Pi}_{ST}\Big)$$
$$= \sum_{S,T} \exp(-\mathrm{i}\,\mathbf{g}_{ST})\ \mathbf{\Pi}_{ST} = \sum_{S,T} \mathbf{c}_{ST}\ \mathbf{\Pi}_{ST}$$

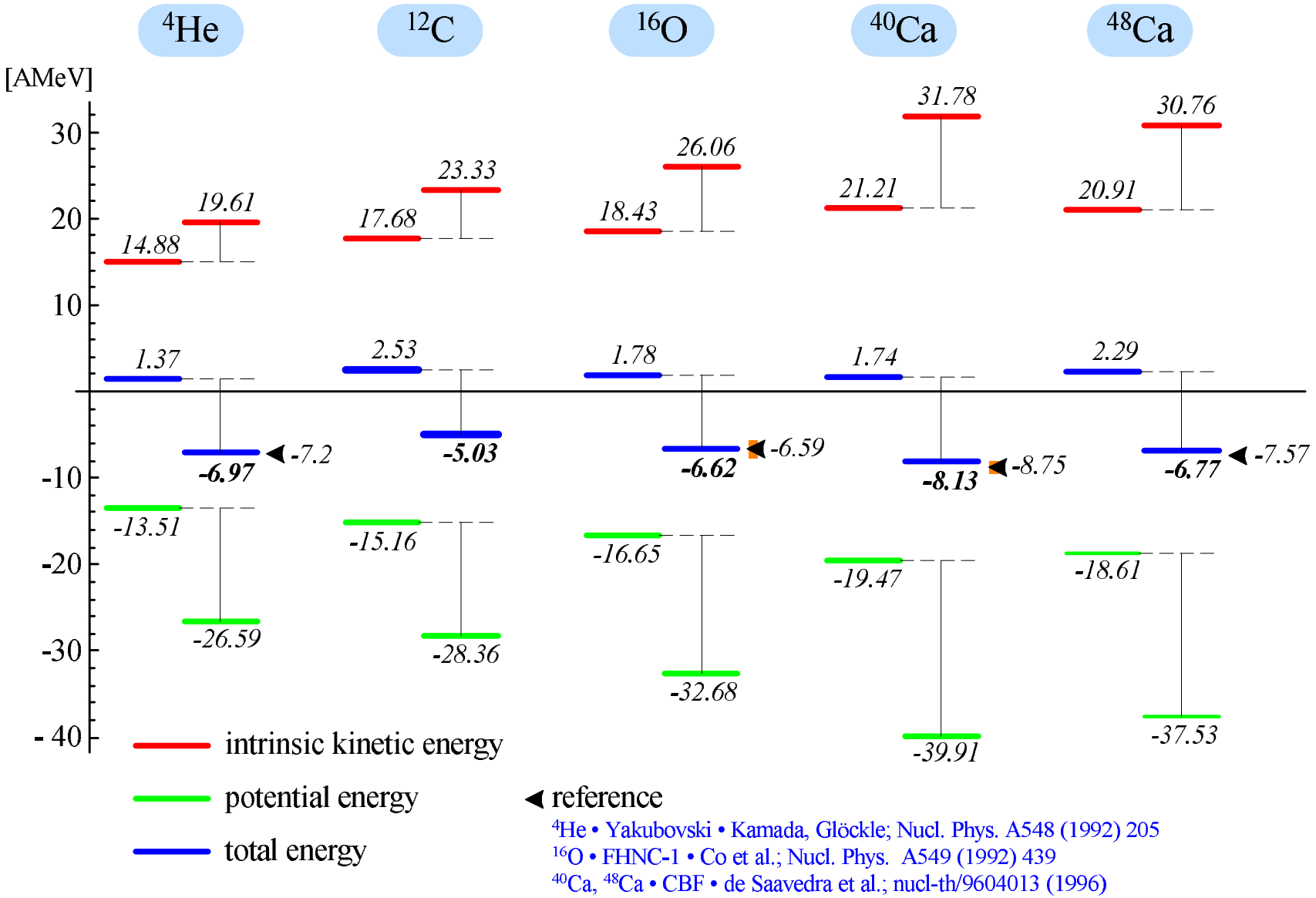
- different correlation function $R_+^{ST}(r)$ for each (S,T)-component of the potential



[Phys. Rev. 175 (1968) 1337], [Nucl. Phys. A371 (1981) 79]

Afnan-Tang S3M Potential

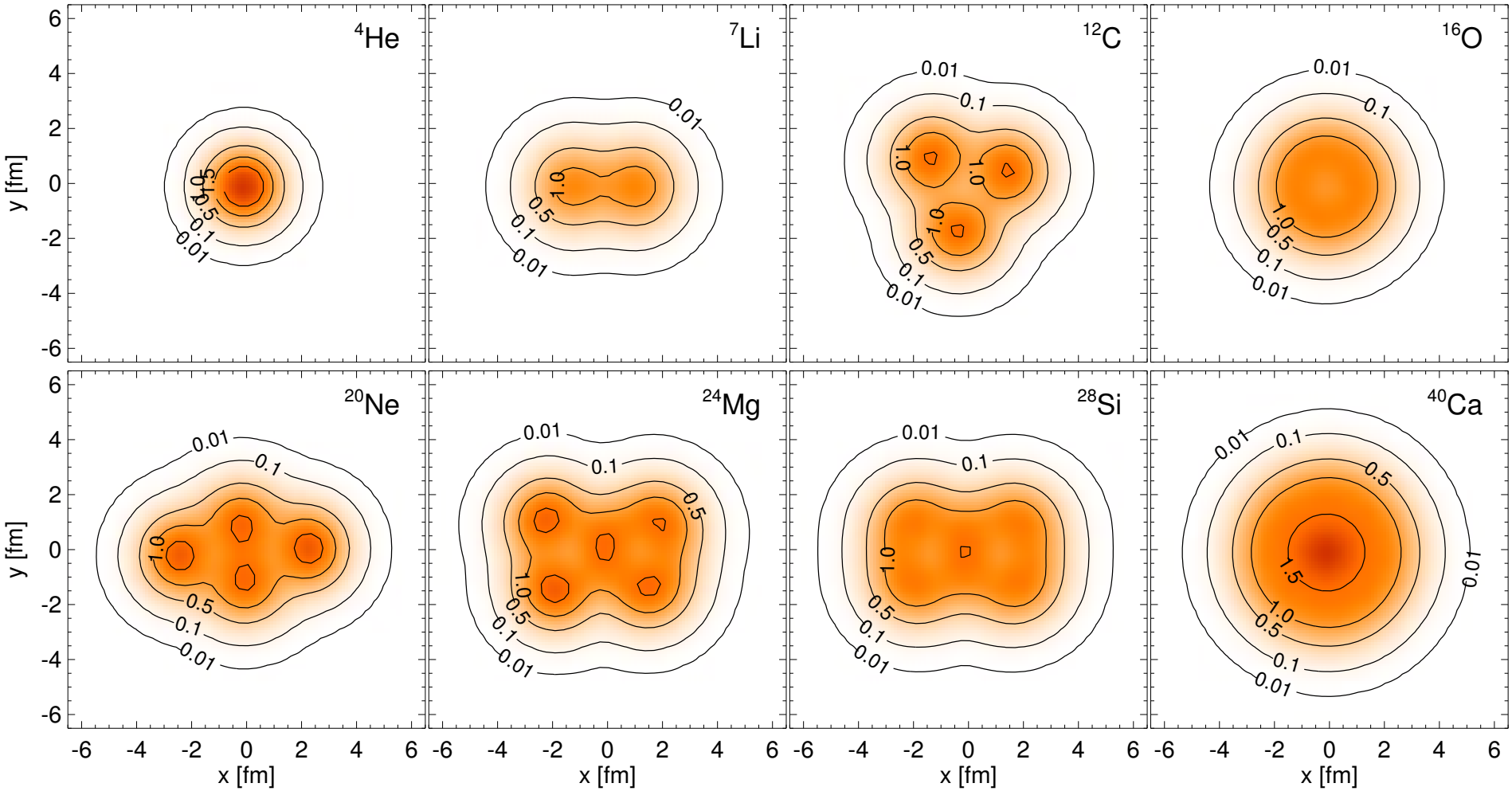
Groundstate Energies



^{4}He • Yakubovski • Kamada, Glöckle; Nucl. Phys. A548 (1992) 205
^{16}O • FHNC-1 • Co et al.; Nucl. Phys. A549 (1992) 439
^{40}Ca, ^{48}Ca • CBF • de Saavedra et al.; nucl-th/9604013 (1996)

Afnan-Tang S3M Potential

Groundstate Densities



- one gaussian per nucleon, fixed spin

Summary & Outlook

Summary

- Unitary Correlation Operator Method describes short-range correlations by a distance-dependent transformation in the relative two-body coordinate
- correlated Hamiltonian / effective interaction in two-body approximation is given in closed form; higher cluster orders are negligible in case of finite nuclei
- variational model based on a Slater determinant of Gaussian trial states (Fermionic Molecular Dynamics) to describe groundstate structure of light and intermediate mass nuclei
- for central potentials (MTV/ATS3M) the results are comparable with quasi-exact and expensive many-body techniques

Outlook

- need realistic NN-interaction, e.g. Bonn or Argonne potential, including a proper treatment of tensor correlations
- ready for systematic and nearly *ab initio* nuclear structure studies
- can be used for the description of low-energy nucleus-nucleus collisions right away