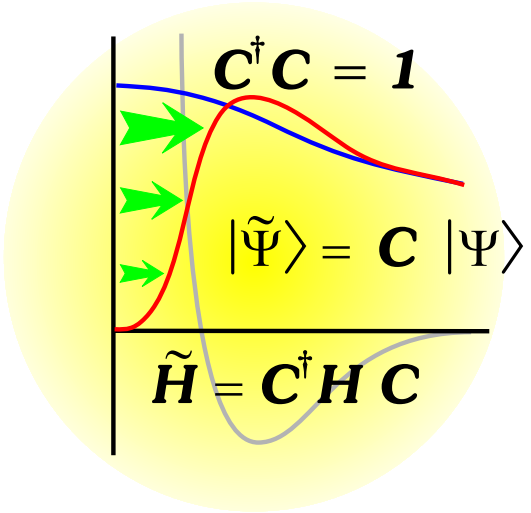

The *Unitary Correlation Operator Method*

for Dense Quantum Liquids

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Short-Range Correlations

Unitary Correlation Operator

^{4}He-Liquid & Droplets

Homework: Neutron Matter

Why Effective Interactions?

The Problem: Short-Range Correlations

Interaction

many realistic two-body interactions show a strong short-range repulsion

(e.g. nucleon-nucleon & van der Waals interactions)

Correlations

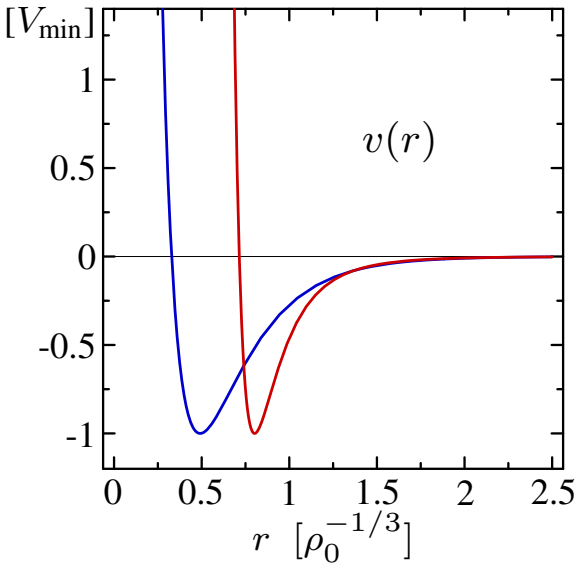
core induces strong short-range correlations in many-body state

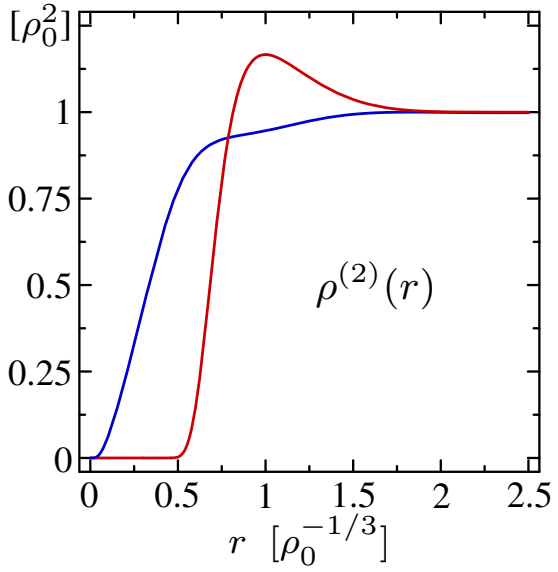
(e.g. correlation hole in two-body density)

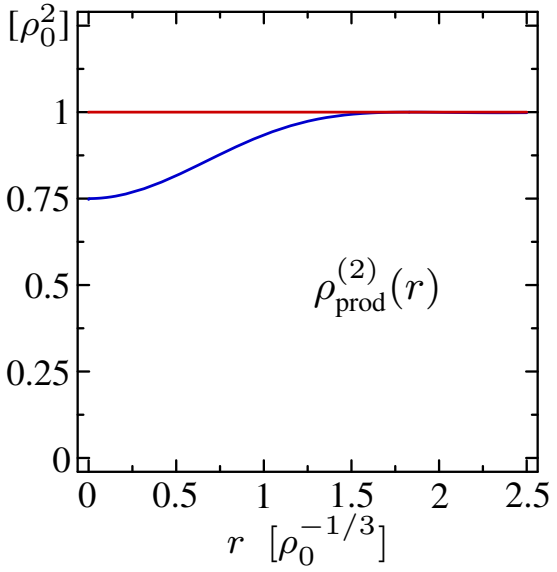
Product States

short-range correlations cannot be described by product-type states

(e.g. mean-field, superposition of few product states,...)





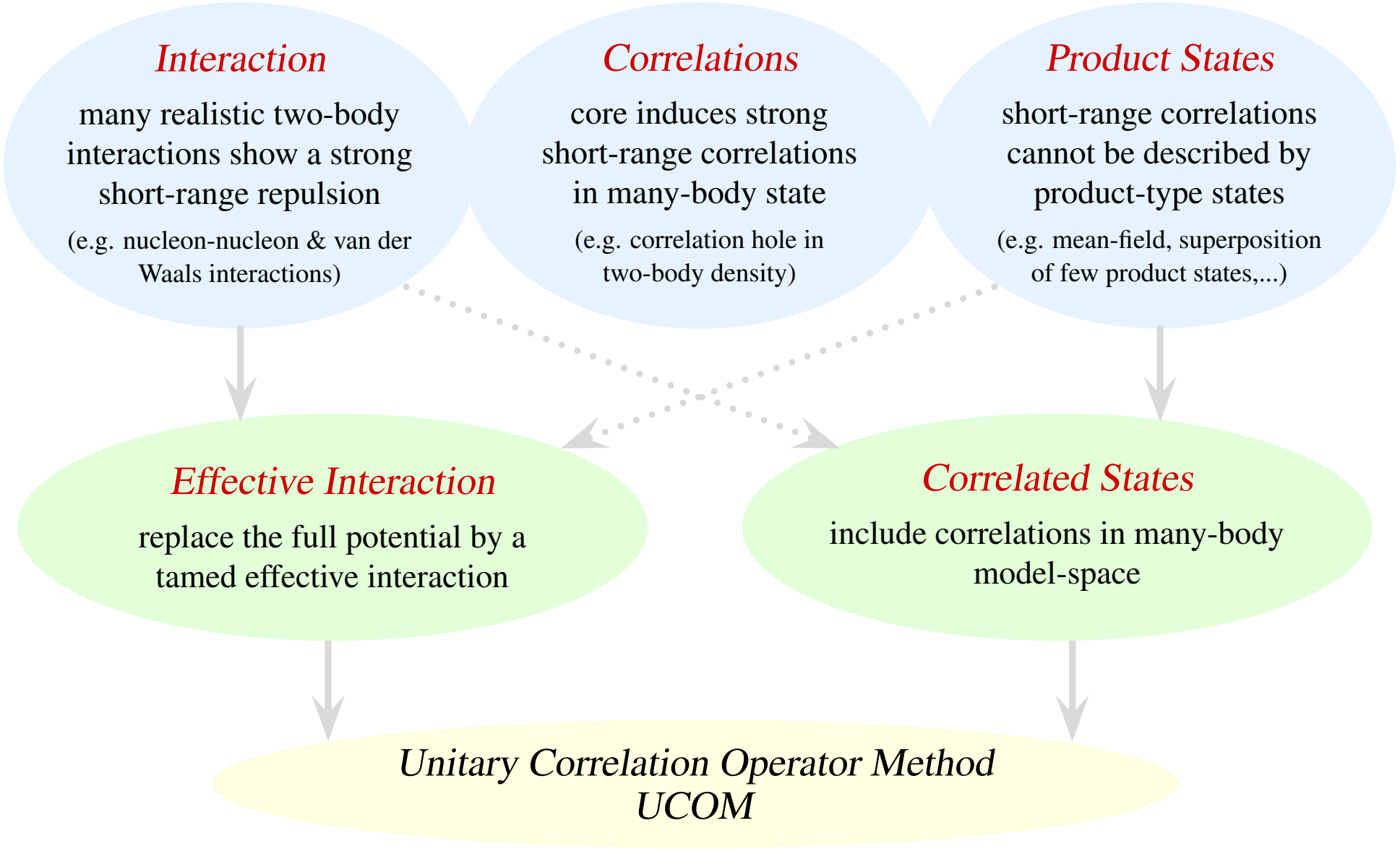


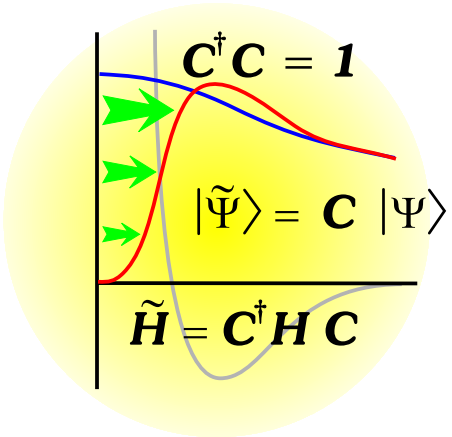
nuclear matter $\rho_0 = 0.17\,\mathrm{fm}^{-3}$

liquid ^{4}He (bosonic) $\rho_0 = 0.022\,\mathrm{Å}^{-3}$

Why Effective Interactions?

The Problem: Short-Range Correlations





Basic Elements of the

Unitary Correlation Operator Method

- Correlation Operator
- Correlated States & Effective Interaction
- Two-Body Approximation
- Many-Body 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.

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

$$\mathbf{g} = \tfrac{1}{2}[s(\mathbf{r})\;\tfrac{\vec{\mathbf{r}}}{\mathbf{r}}\,\vec{\mathbf{q}} + \vec{\mathbf{q}}\,\tfrac{\vec{\mathbf{r}}}{\mathbf{r}}\;s(\mathbf{r})]$$

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

$s(r) \sim$ shift distance

Correlated States

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

Correlated Operators

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

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

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Correlated Wave Function

Correlated Wave Function

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

$$\langle \vec{X}, \vec{r}\,| \mathbf{C} \,|\psi\rangle = \langle \vec{X}|\Phi_{\rm cm}\rangle \langle \vec{r}\,| \mathbf{C} \,|\phi\rangle$$

- norm-conserving coordinate transformation

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

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

Correlation Function $R_\pm(r)$

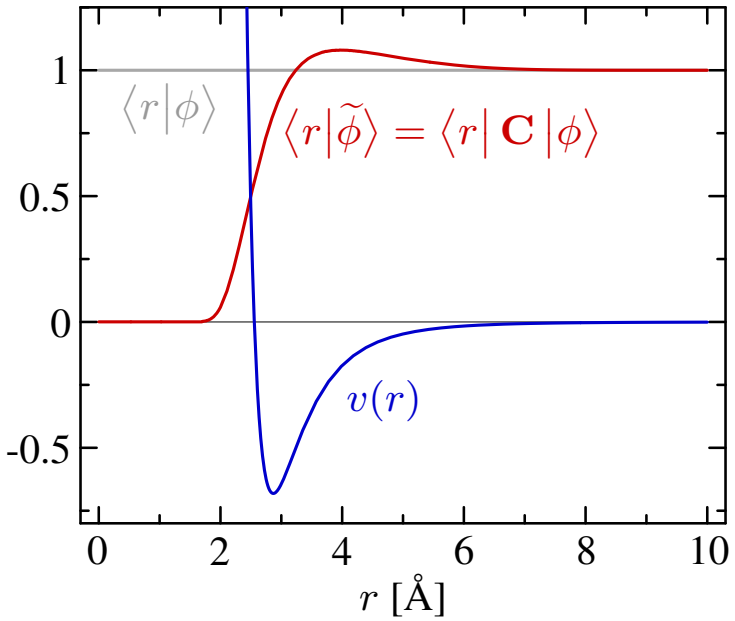
- metric factor and inverse transformation

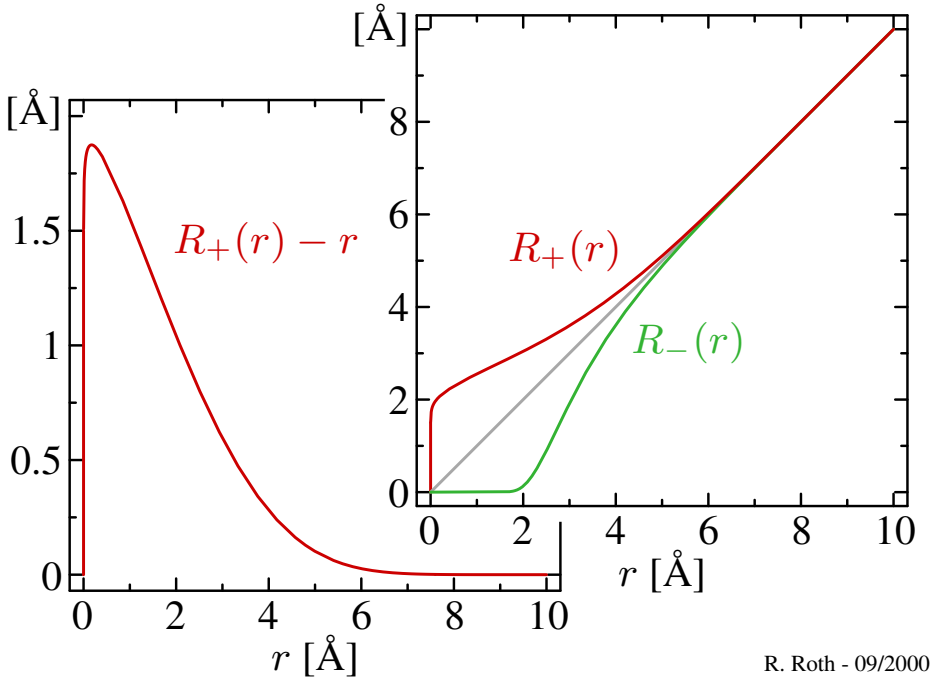
$$\mathcal{R}_\pm(r) = \frac{R_\pm(r)}{r}\sqrt{R'_\pm(r)}$$

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

- connection with $s(r)$

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

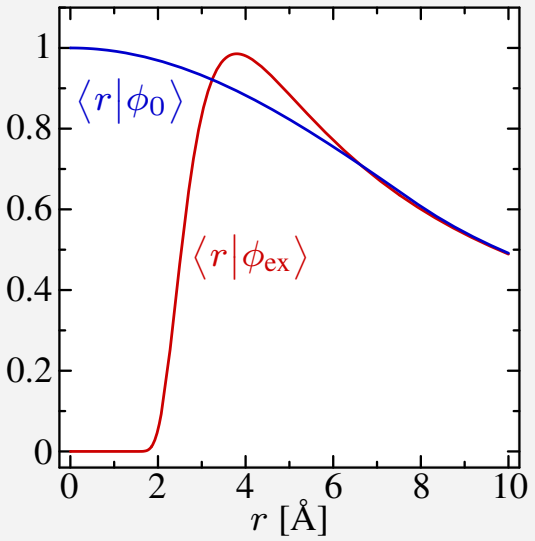




Optimal Correlation Function — One Way

Exact Two-Body Solution

- take full two-body interaction, e.g. Lennard-Jones potential
- calculate exact $E = 0$ solution for rel. wave function $\langle r|\phi_{\rm ex}\rangle$
- construct a suitable trial state $\langle r|\phi_0\rangle$ with correct long-range behavior but without correlations



the optimal correlator should map the short range part of a given trial state onto the exact two-body solution

$$\langle r|\,\mathbf{C}\,|\phi_0\rangle \stackrel{!}{=} \langle r|\phi_{\rm ex}\rangle \quad \text{for } r < \lambda$$

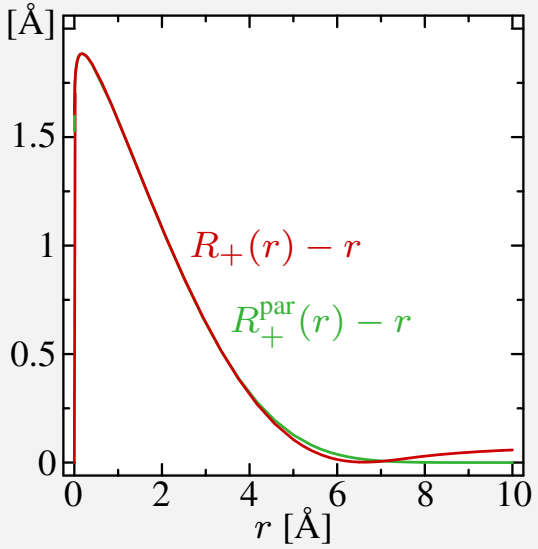
Optimal Correlator

- solve implicit integral equation by iteration

$$R_+^3(r) = 3\int_0^r \mathrm{d}\xi\ \xi^2 \frac{\langle \xi|\phi_0\rangle^2}{\langle R_+(\xi)|\phi_{\rm ex}\rangle^2}$$

- parameterize short range part

$$R_+^{\rm par}(r) = r + \alpha(r/\beta)^\eta \exp(-e^{r/\beta})$$



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

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

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

$\kappa \ll 1$

Two-Body Approximation

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

$\kappa \not\ll 1$

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 $\widetilde{\mathbf{H}}^{C2}$

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Two-Body Approximation

Correlated Hamiltonian & Effective Interaction

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

$$\overset{C2}{=} \mathbf{T}_0 + \sum_{i<j} \left[\widetilde{v}(\mathbf{r}_{ij}) + \widetilde{u}(\mathbf{r}_{ij}) + \vec{\mathbf{q}}_{ij} \frac{1}{2\widetilde{\mu}_\nabla(\mathbf{r}_{ij})} \vec{\mathbf{q}}_{ij} + \vec{\mathbf{q}}_{ij} \frac{\vec{\mathbf{r}}_{ij}}{\mathbf{r}_{ij}} \frac{1}{2\widetilde{\mu}_r(\mathbf{r}_{ij})} \frac{\vec{\mathbf{r}}_{ij}}{\mathbf{r}_{ij}} \vec{\mathbf{q}}_{ij} \right]$$

Local Potentials

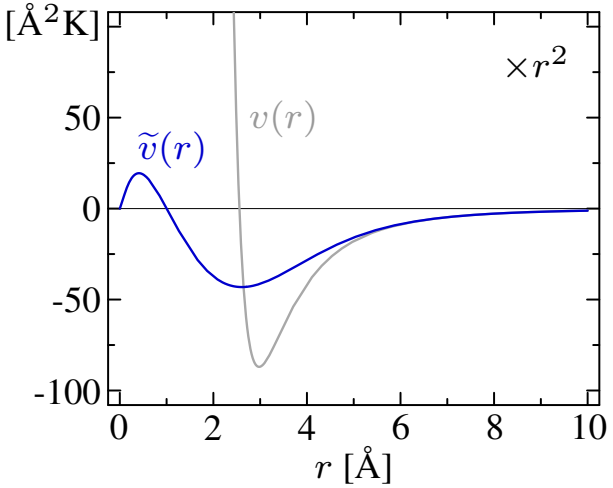
$$\widetilde{v}(r) = v[R_+(r)]$$

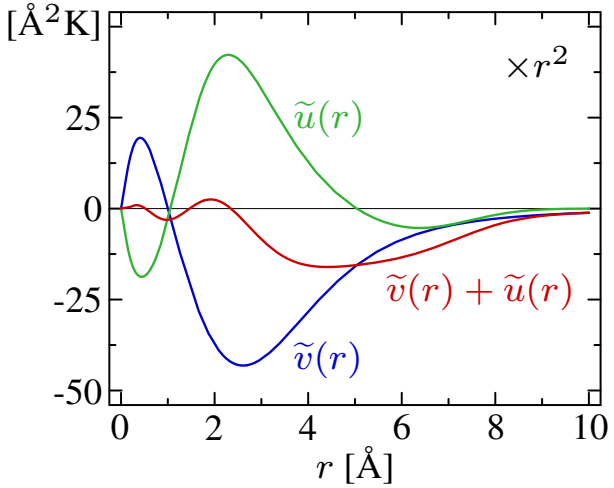
$$\widetilde{u}(r) = \frac{1}{2\mu {R'_+}^2(r)} \left(2\frac{R''_+(r)}{r R'_+(r)} - \frac{5}{4}\frac{{R''_+}^2(r)}{{R'_+}^2(r)} + \frac{1}{2}\frac{R'''_+(r)}{R'_+(r)} \right)$$

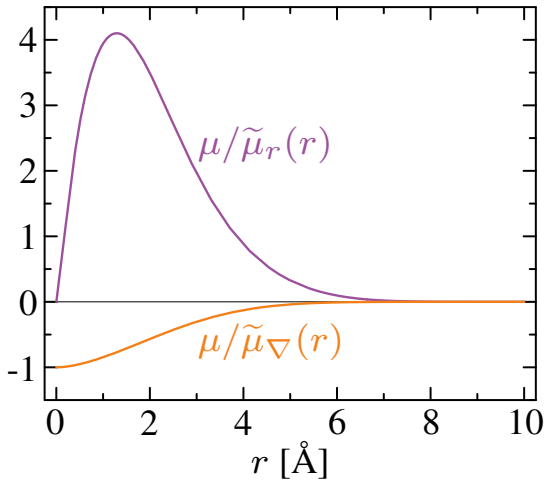
Effective Mass Corrections

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

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







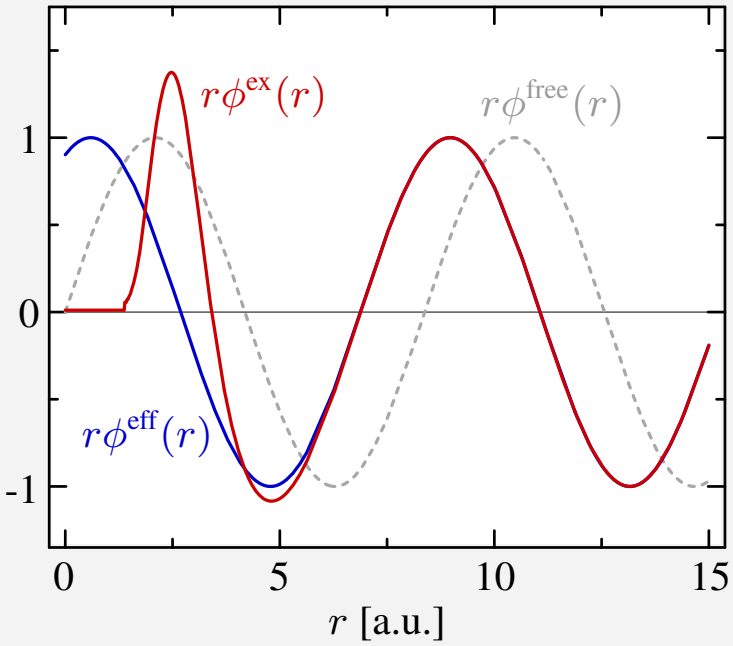
Properties of the Effective Interaction

$$\mathbf{H} \quad |\psi_n^{\text{ex}}\rangle = E_n \quad |\psi_n^{\text{ex}}\rangle$$

$$\underbrace{\mathbf{C}^\dagger \mathbf{H}\, \mathbf{C}}_{\widetilde{\mathbf{H}}} \underbrace{\mathbf{C}^\dagger |\psi_n^{\text{ex}}\rangle}_{|\psi_n^{\text{eff}}\rangle} = E_n \underbrace{\mathbf{C}^\dagger |\psi_n^{\text{ex}}\rangle}_{|\psi_n^{\text{eff}}\rangle}$$

- the eigenstates of the original Hamiltonian $\mathbf{H}$ and the correlated Hamiltonian $\widetilde{\mathbf{H}} = \mathbf{C}^\dagger \mathbf{H} \mathbf{C}$ are connected by the unitary transformation

$$|\psi_n^{\text{ex}}\rangle = \mathbf{C}\, |\psi_n^{\text{eff}}\rangle$$



- consider the two-body scattering problem for the original $\mathbf{H}$ and the correlated Hamiltonian $\widetilde{\mathbf{H}}$
- the scattering solutions for a given energy differ only within the range of the correlator, i.e. all asymptotic properties are equal

- effective interaction and original potential are phase-shift equivalent by construction!
- tool to generate systematically a class of infinitely many phase-shift equivalent interactions

Many-Body System

Generalized Coordinate Transformation

Two-Body Correlations — Revisited

- the correlator acts like a norm conserving coordinate transformation

$$\langle \vec{r}, \vec{X} | \widetilde{\psi} \rangle = \mathcal{R}_-(r) \, \langle R_-(\vec{r}) \tfrac{\vec{r}}{r} | \phi \rangle \langle \vec{X} | \Phi_{\rm cm} \rangle$$

- rewrite the transformation in terms of the one-body coordinates

$$\langle \vec{x}_1, \vec{x}_2 | \widetilde{\psi} \rangle = \mathcal{X}_-(\vec{x}_1, \vec{x}_2) \, \langle \vec{X}_1^-(\vec{x}_1, \vec{x}_2), \vec{X}_2^-(\vec{x}_1, \vec{x}_2) | \psi \rangle$$

$$\begin{aligned} \vec{X}_1^-(\vec{x}_1, \vec{x}_2) &= \vec{x}_1 + \vec{\Delta}_-(\vec{r}_{12}) \\ \vec{X}_2^-(\vec{x}_1, \vec{x}_2) &= \vec{\Delta}_-(\vec{r}_{21}) + \vec{x}_2 \end{aligned}$$

$\vec{\Delta}_-(\vec{r}) = \frac{1}{2}[R_-(r) - r]\frac{\vec{r}}{r}$ $\qquad$ $\mathcal{X}_-(\vec{x}_1, \vec{x}_2) =$ Jacobian of $\vec{X}_i^-$

Three-Body Correlations

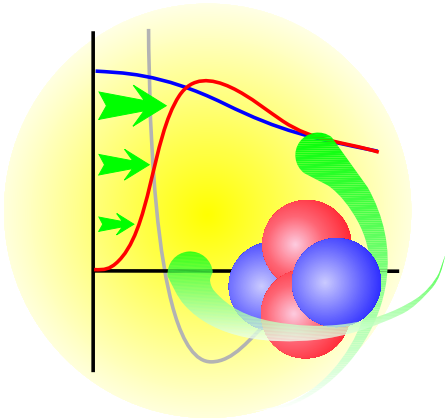
- define a correlated three-body wave function in an analogous way

$$\begin{aligned} \langle \vec{x}_1, \vec{x}_2, \vec{x}_3 | \widetilde{\psi} \rangle := \mathcal{X}_-(\vec{x}_1, \vec{x}_2, \vec{x}_3) \; \times \\ \times \langle \vec{X}_1^-(\vec{x}_1, \vec{x}_2, \vec{x}_3), \vec{X}_2^-(\vec{x}_1, \vec{x}_2, \vec{x}_3), \vec{X}_3^-(\vec{x}_1, \vec{x}_2, \vec{x}_3) | \psi \rangle \end{aligned}$$

- simplest generalization of the two-body transformation that obeys the cluster decomposition principle

$$\begin{aligned} \vec{X}_1^-(\vec{x}_1, \vec{x}_2, \vec{x}_3) &= \vec{x}_1 + \vec{\Delta}_-(\vec{r}_{12}) + \vec{\Delta}_-(\vec{r}_{13}) \\ \vec{X}_2^-(\vec{x}_1, \vec{x}_2, \vec{x}_3) &= \vec{\Delta}_-(\vec{r}_{21}) + \vec{x}_2 + \vec{\Delta}_-(\vec{r}_{23}) \\ \vec{X}_3^-(\vec{x}_1, \vec{x}_2, \vec{x}_3) &= \vec{\Delta}_-(\vec{r}_{31}) + \vec{\Delta}_-(\vec{r}_{32}) + \vec{x}_3 \end{aligned}$$

✘ question: formal link to the correlation operator in three-body system



Dense Bosonic Matter:

Helium-4 Liquid & Small Droplets

- Equation of State
- Two- & Three-Body Approximation
- Density-Dependent Correlators
- Energies & Radii of Small Droplets

Unitary Correlation Operator Method

A Simple Model For Liquid ^{4}He

looking for the equation of state $\varepsilon(\rho)$ for a homogeneous liquid of ^{4}He at $T = 0\,\mathrm{K}$

Interaction

$$v(r) = 4\epsilon\left[(\sigma/r)^{12} - (\sigma/r)^{6}\right]$$

$$\sigma = 2.556\,\text{Å}\,, \quad \epsilon = 10.22\,\mathrm{K}$$

Optimal Correlator

- parameters determined by mapping of the exact $E = 0$ two-body solution

$$R_+(r) = r + \alpha\left(\frac{r}{\beta}\right)^{\eta}\exp(-\exp[r/\beta])$$

$$\alpha = 6.267\text{Å},\ \beta = 3.520\text{Å},\ \eta = 0.052$$

Uncorrelated State

- direct product of N identical constant one-body states

$$\big|\psi, N\big\rangle = \underbrace{\big|\psi, 1\big\rangle \otimes \cdots \otimes \big|\psi, 1\big\rangle}_{N \text{ states}}$$

$$\big\langle \vec{x}\big|\psi, 1\big\rangle = 1/\sqrt{V}$$

$\widetilde{\mathbf{H}}^{C2}$, $\widetilde{\mathbf{H}}^{C3}$

correlated Hamiltonian in two- or three-body approximation

$\widetilde{\varepsilon}^{C2}(\rho)$, $\widetilde{\varepsilon}^{C3}(\rho)$

energy per particle in two- and three-body approximation

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^{4}*He Liquid*

Equation of State in Two-Body and Three-Body Approx.

$$\widetilde{\varepsilon}^{C2}(\rho) = \widetilde{v}^{[2]}(\rho) + \widetilde{u}^{[2]}(\rho) = C_2\,\rho$$

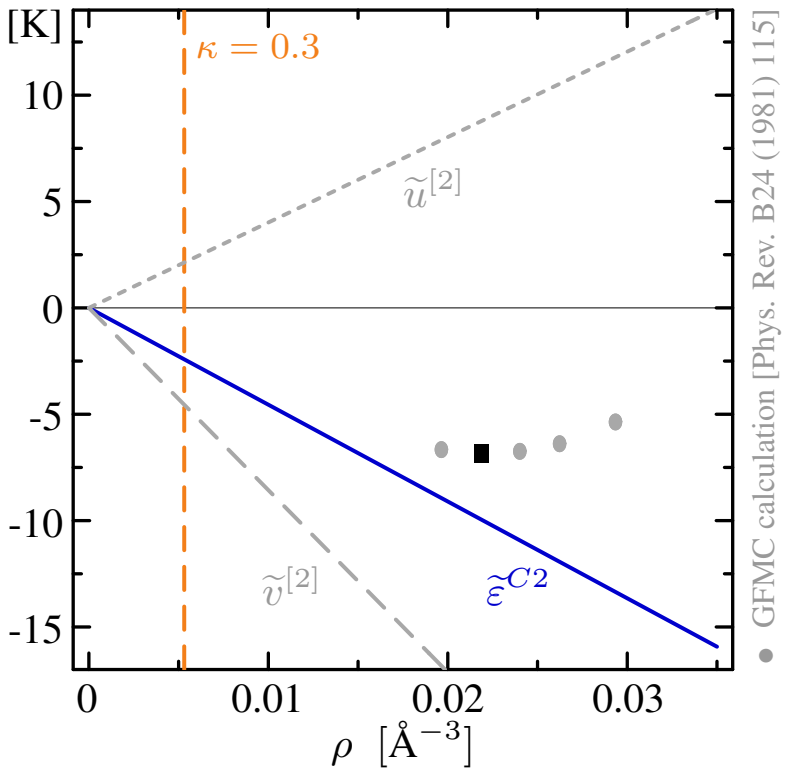
$$\widetilde{v}^{[2]}(\rho) = \frac{\rho}{2}\int \mathrm{d}^3 r\; \widetilde{v}(r)$$

- ✔ core is tamed completely; overall attraction
- ✘ two-body approx. by construction not able to describe saturation in homogeneous Bose liquid
- ✘ interesting region far beyond smallness-limit

$$\widetilde{\varepsilon}^{C3}(\rho) = \widetilde{\varepsilon}^{C2}(\rho) + \widetilde{v}^{[3]}(\rho) + \widetilde{u}^{[3]}(\rho) = C_2\,\rho + C_3\,\rho^2$$

$$\widetilde{v}^{[3]}(\rho) = \frac{\rho^2}{6}\int \mathrm{d}^3 r_{12}\; \mathrm{d}^3 r_{13}\; \widetilde{v}^{[3]}(\vec{r}_{12}, \vec{r}_{13})$$

- ✔ three-body approximation is able to describe saturation
- ✘ correlator has to be optimized in three-body approximation; genuine three-body correlations
- ✘ how about four-body, five-body...?



better look for an effective description of higher-order correlations

Beyond Two-Body Approximation

Density-Dependent Correlators

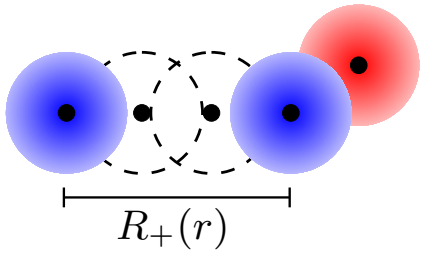
simulate the effects of

- higher orders of the cluster expansion
- genuine many-body correlations

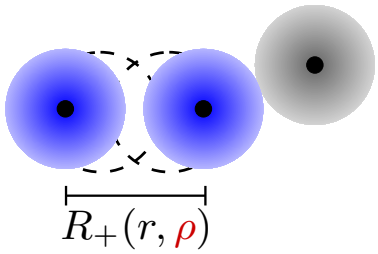
by an effective density-dependent correlator that is used in two-body approximation

density-dependent effective interaction

- two-body approximation may shift a particle pair into the core of a neighboring "third particle"



- three-body correlations will prevent from a shift into the core of a "third particle"

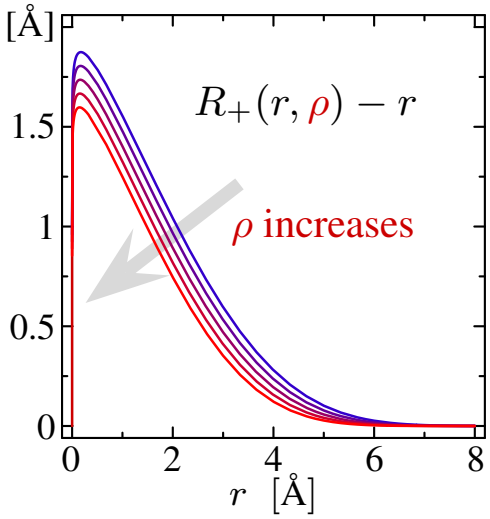


- reduce the range β and the shift-distance α of the correlator linear with density

$$\xi(\rho) = 1 - \gamma\ \rho$$

$$R_+(r,\rho) = r + \alpha\xi(\rho)\ \left(\frac{r}{\beta\xi(\rho)}\right)^{\eta}\ H\left[\frac{r}{\beta\xi(\rho)}\right]$$

- fix γ by experimental results or "exact" many-body calculations



Equation of State with Density-Dependent Correlators

$$\widetilde{\varepsilon}^{C2\rho}(\rho) = \widetilde{v}^{[2]\rho}(\rho) + \widetilde{u}^{[2]\rho}(\rho)$$

$$\widetilde{v}^{[2]\rho}(\rho) = \frac{\rho}{2}\int \mathrm{d}^3 r \;\; \widetilde{v}(r,\rho)$$

- the parameter γ of the density-dependence is chosen such that

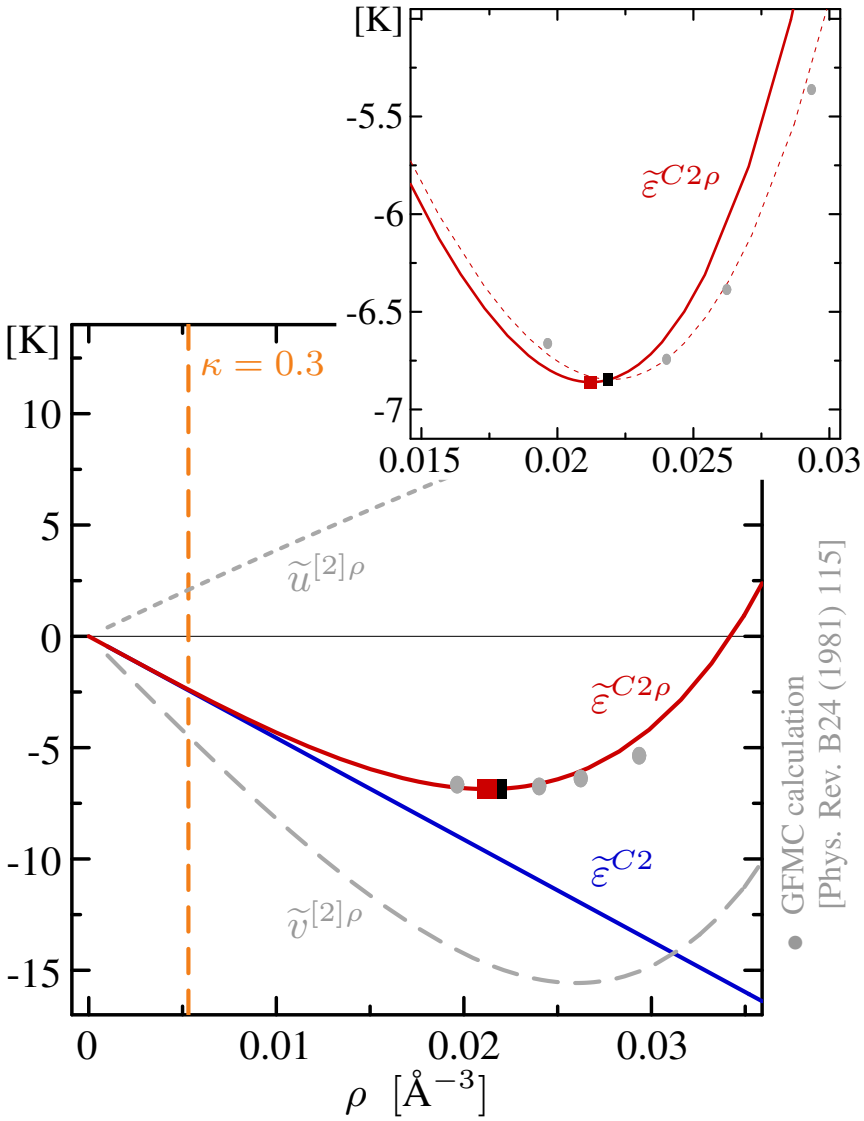
$$\widetilde{\varepsilon}^{C2\rho}(\rho^{\mathrm{ref}}_{\mathrm{sat}}) = \varepsilon^{\mathrm{ref}}_{\mathrm{sat}}$$

$$\rho^{\mathrm{ref}}_{\mathrm{sat}} = 0.0219\text{Å}^{-3} \qquad \varepsilon^{\mathrm{ref}}_{\mathrm{sat}} = -6.58\text{K}$$

- ✔ density-dependent correlator gives saturation at the right point

$$\rho_{\mathrm{sat}} = 0.0212\text{Å}^{-3} \qquad \varepsilon_{\mathrm{sat}} = -6.86\text{K}$$

- ✔ one free parameter enables to reproduce the position of the minimum and the shape of $\varepsilon(\rho)$
- ✔ contains the relevant physics of many-body correlations in a very efficient way



Unitary Correlation Operator Method

Small Droplets of ^{4}He

calculate binding energies and
radii of small droplets ($N = 3, ..., 70$) of
^{4}He at $T = 0\,\mathrm{K}$

Interaction

$$v(r) = 4\epsilon \left[(\sigma/r)^{12} - (\sigma/r)^{6}\right]$$

$$\sigma = 2.556\,\text{Å}\,, \quad \epsilon = 10.22\,\mathrm{K}$$

Correlator (Density-Dep.)

- determined by mapping of the exact $E = 0$ two-body solution

$$R_+(r) = r + \alpha \left(\frac{r}{\beta}\right)^{\eta} \exp(-\exp[r/\beta])$$

$$\alpha = 6.267\text{Å},\ \beta = 3.520\text{Å},\ \eta = 0.052$$

- density dependence fixed for the homogeneous liquid

$$\xi(\rho) = 1 - \gamma\,\rho$$

$$\gamma = 3.696\,\text{Å}^3$$

Uncorrelated State

- Gaussian one-body trial state with variable width a

$$\big|\psi, N\big\rangle = \big|\psi, 1\big\rangle \otimes \cdots \otimes \big|\psi, 1\big\rangle$$

$$\big\langle \vec{x}\big|\psi, 1\big\rangle = \frac{1}{(\pi a)^{3/4}} \exp\!\left(-\frac{\vec{x}^2}{2a}\right)$$

$\widetilde{\mathbf{H}}^{C2}$, $\widetilde{\mathbf{H}}^{C2\rho}$

correlated Hamiltonian in two-body approx. without and with dens-dep.

$\widetilde{\varepsilon}^{C2}$, $\widetilde{\varepsilon}^{C2\rho}$

energy per particle in two-body approx. without and with dens-dep.

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Minimization in Two-Body Approximation

- minimization of the correlated energy expectation value in two-body approximation

$$\widetilde{\varepsilon}^{C2} = \frac{1}{N}\left\langle \mathbf{T}_{\text{int}} + \widetilde{\mathbf{V}}^{[2]} + \widetilde{\mathbf{U}}^{[2]} + \widetilde{\mathbf{T}}^{[2]}_{\nabla} + \widetilde{\mathbf{T}}^{[2]}_{r} \right\rangle$$

✔ unitary correlator is able to tame the core and describe the extremely weak bound ^{4}He-droplets

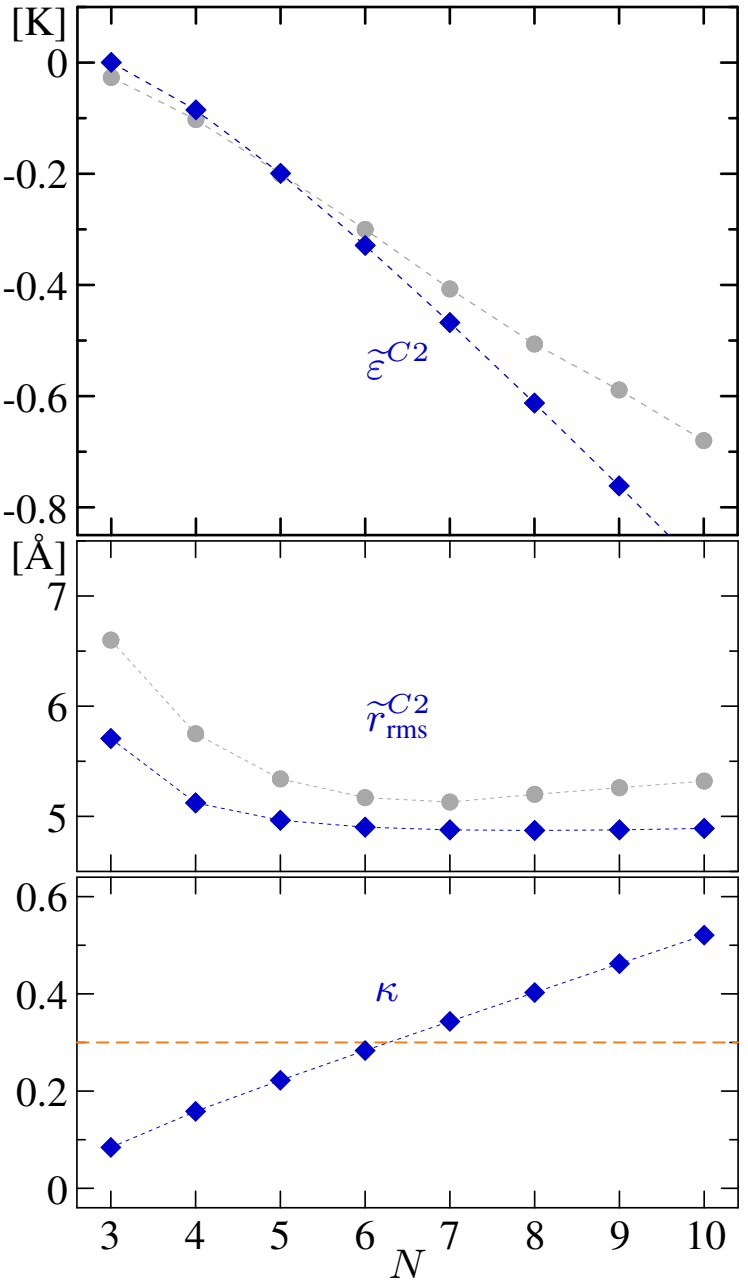
✔ binding energies for $N \leq 6$ are in very good agreement with VMC calculations

✘ for $N > 6$ overbinding occurs; simultaneously the smallness parameter exceeds the limit $\kappa = 0.3$

✘ rms-radii are systematically too low; for small particle numbers caused by Gaussian trial state; for higher particle number consequence of overbinding

▶ $\kappa < 0.3$: two-body approximation gives good results

▶ $\kappa > 0.3$: many-body correlations become important; include three-body contributions or use density-dependent correlators



• VMC calculation [Physica 31 (1965) 1143]

Minimization with Density-Dependent Correlator

- minimization of the correlated energy expectation value in two-body approximation with density-dependent correlator

$$\widetilde{\varepsilon}^{C2\rho} = \frac{1}{N}\left\langle \mathbf{T}_{\rm int} + \widetilde{\mathbf{V}}^{[2]\rho} + \widetilde{\mathbf{U}}^{[2]\rho} + \widetilde{\mathbf{T}}^{[2]\rho}_{\nabla} + \widetilde{\mathbf{T}}^{[2]\rho}_{r} \right\rangle$$

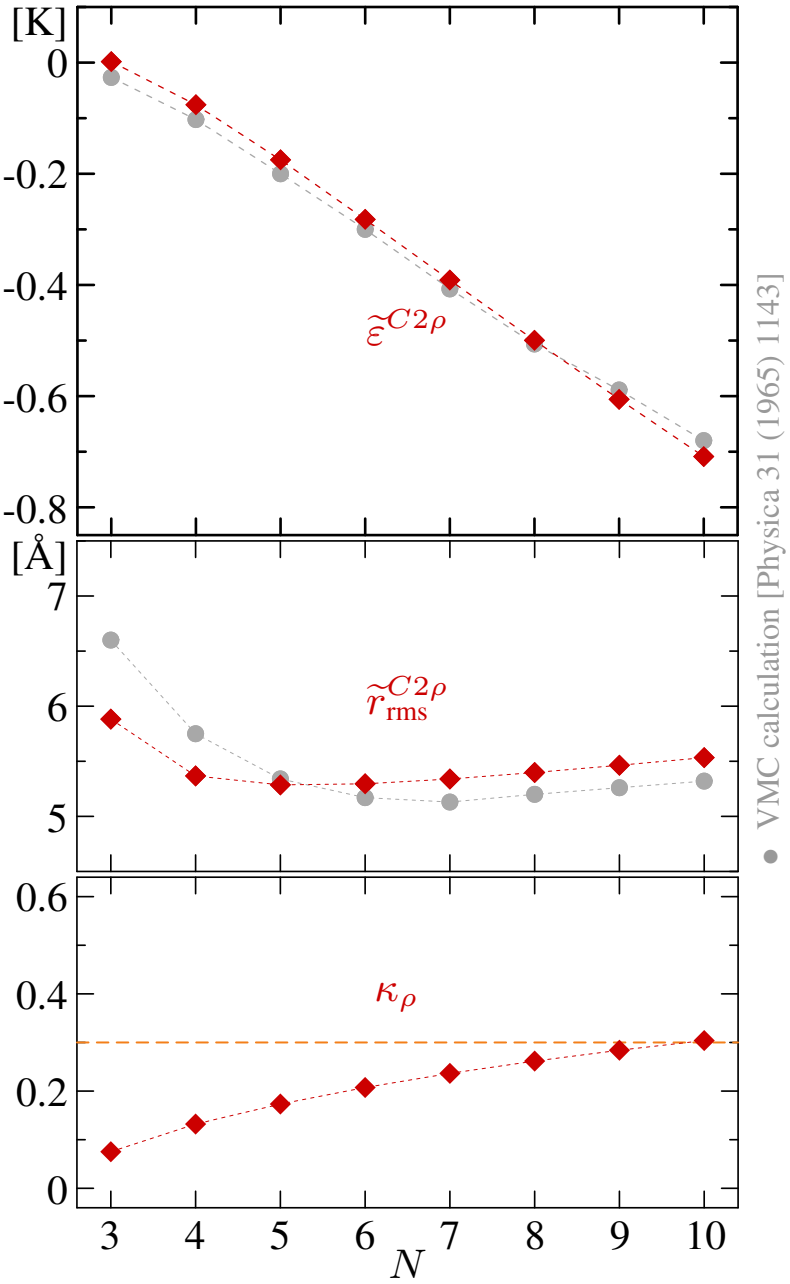
- correlator and effective interaction are completely fixed by two-body system and homogeneous liquid, i.e. there is no free parameter

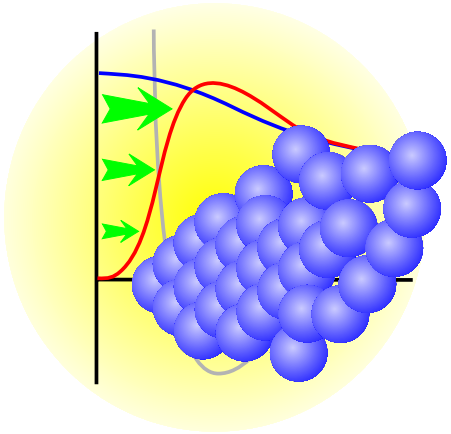
✔ density-dependent correlator reproduces the binding energy with high accuracy

✔ rms-radii are qualitatively right; underestimation for small droplets is due to the Gaussian trial state

▶ calculations have full predictive power and can be done for any droplet size

▶ even better accuracy could be achieved with improved trial states





Dense Fermionic Matter: Bethe's Homework Problem

- Equation of State for Neutron Matter
- Density-Dependent Correlators
- Correlated Densities and Occupation Numbers

Unitary Correlation Operator Method

Interacting Fermi Liquid

looking for the equation of state $\varepsilon(\rho)$
and densities/occupation numbers for a
homogeneous Fermi liquid at $T = 0\,\mathrm{K}$

Interaction — Homework Problem

- neutron matter ($\lambda = 2$) interacting via the repulsive core of the ${}^1S_0$ component of the Reid potential

$$v(r) = 9263.1\,\mathrm{MeV\,fm}\ \exp(-4.9\,\mathrm{fm}^{-1}\ r)/r$$

Correlator

- mapping onto an exact two-body solution works only if there is some attraction
- energy minimization for the two-body system with constrained range parameter β
- energy minimization in the many-body system without constraint

Uncorrelated State

- one-body states with momentum $\vec{k}_i$ and spin-isospin quantum number $m_i = 1, ..., \lambda$

$$|i\rangle = |\vec{k}_i\rangle \otimes |m_i\rangle$$

- antisymmetrized product of all N one-body states with $|\vec{k}_i| \leq k_F$

$$|\psi, N\rangle = \mathbf{A}\big(\,|i_1\rangle \otimes \cdots \otimes |i_N\rangle\big)$$

$\widetilde{\mathbf{H}}^{C2}$
$\widetilde{\mathbf{H}}^{C3}$
$\widetilde{\mathbf{H}}^{C2\rho}$

$\widetilde{\varepsilon}^{C2}(\rho)$
$\widetilde{\varepsilon}^{C3}(\rho)$
$\widetilde{\varepsilon}^{C2\rho}(\rho)$

R. Roth - 09/2000

Structure of the Equation of State

Two-Body Approximation

$$\widetilde{\varepsilon}^{C2} = \tfrac{1}{N}\langle \widetilde{\mathbf{H}}^{C2} \rangle = t_0 + \widetilde{v}^{[2]} + \widetilde{u}^{[2]} + \widetilde{t}^{[2]}_{\nabla+r}$$

- direct terms of orders k_F^2, k_F^3 and k_F^5
- possible to describe saturation for attractive potentials because of the effective mass contributions ($\sim k_F^5$)

$$t_0 = \frac{3}{10m}\, k_F^2$$

$$\widetilde{v}^{[2]} + \widetilde{u}^{[2]} = \frac{\lambda}{12\pi^2}\, k_F^3 \int \mathrm{d}^3 r\, \left[\widetilde{v}(r) + \widetilde{u}(r)\right] + \text{xch.}$$

$$\widetilde{t}^{[2]}_{\nabla+r} = \frac{\lambda}{80\pi^2}\, k_F^5 \int \mathrm{d}^3 r\, \left[\frac{1}{\widetilde{\mu}_\nabla(r)} + \frac{1}{3\widetilde{\mu}_r(r)}\right] + \text{xch.}$$

Three-Body Approximation

$$\widetilde{\varepsilon}^{C3\star} = \tfrac{1}{N}\langle \widetilde{\mathbf{H}}^{C2} + \widetilde{\mathbf{V}}^{[3]} + \widetilde{\mathbf{U}}^{[3]} \rangle = \widetilde{\varepsilon}^{C2} + \widetilde{v}^{[3]} + \widetilde{u}^{[3]}$$

- additional direct term of order k_F^6 from local three-body potentials
- non-local three-body terms neglected ($\sim k_F^8$)

$$\widetilde{v}^{[3]} + \widetilde{u}^{[3]} = \frac{\lambda^2}{216\pi^4}\, k_F^6 \int \mathrm{d}^3 r_{12}\, \mathrm{d}^3 r_{13}\ \times \left[\widetilde{v}^{[3]}(\vec{r}_{12}, \vec{r}_{13}) + \widetilde{u}^{[3]}(\vec{r}_{12}, \vec{r}_{13})\right] + \text{xch.}$$

$$\rho = \frac{\lambda}{6\pi^2}\, k_F^3$$

Homework-Problem

Energy in Two-Body Approximation

$$\widetilde{\varepsilon}^{C2} = t_0 + \widetilde{v}^{[2]} + \widetilde{u}^{[2]} + \widetilde{t}^{[2]}_{\nabla} + \widetilde{t}^{[2]}_{r}$$

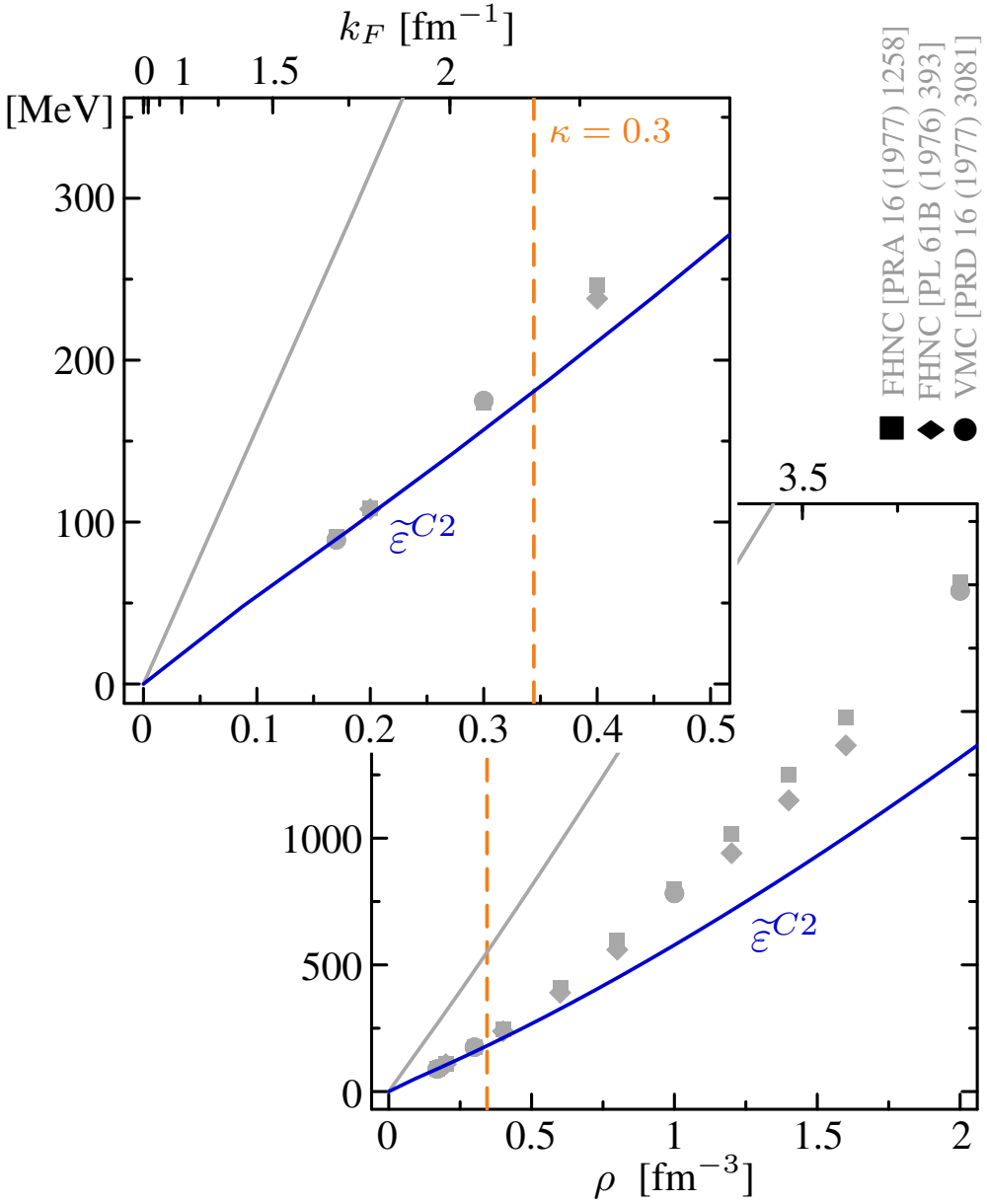
- parameters of the optimal correlator determined by minimization of $\widetilde{\varepsilon}^{C2}(\rho)$ for $\rho = 1\text{fm}^{-3}$

✔ energy is reduced by 1/3 compared to the uncorrelated expectation value

✔ good agreement with sophisticated many-body methods for low densities ($\kappa < 0.3$)

✘ underestimates energies systematically for high densities

▶ higher orders of the cluster expansion necessary to describe behavior for high densities



Homework-Problem

Energy in Three-Body Approximation

$$\widetilde{\varepsilon}^{C3\star} = \widetilde{\varepsilon}^{C2} + \widetilde{v}^{[3]} + \widetilde{u}^{[3]}$$

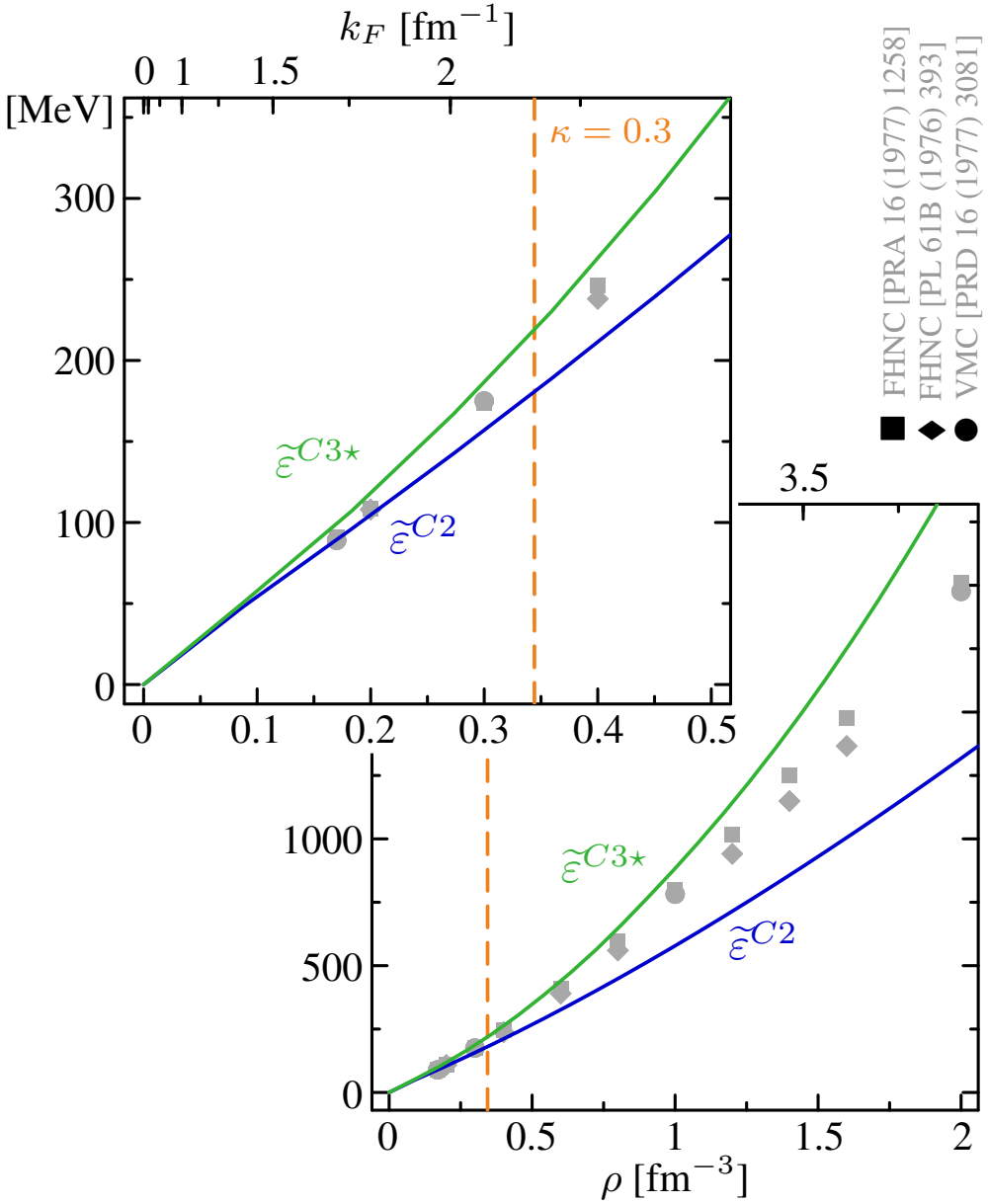
- non-local three-body terms neglected
- "optimal" correlator determined by minimization of $\widetilde{\varepsilon}^{C2}(\rho)$ for $\rho = 1\text{fm}^{-3}$

✔ only small three-body contribution for low densities ($\kappa < 0.3$)

✔ very good agreement with the reference for low and intermediate densities

✘ energies systematically too high for high densities

▶ optimization of the correlator parameters by minimization of the energy in three-body approximation



Homework-Problem

Energy with Density-Dependent Correlator

$$\widetilde{\varepsilon}^{C2\rho} = t_0 + \widetilde{v}^{[2]\rho} + \widetilde{u}^{[2]\rho} + \widetilde{t}^{[2]\rho}_{\nabla+r}$$

- density-dependent scaling of the correlator parameters α and β

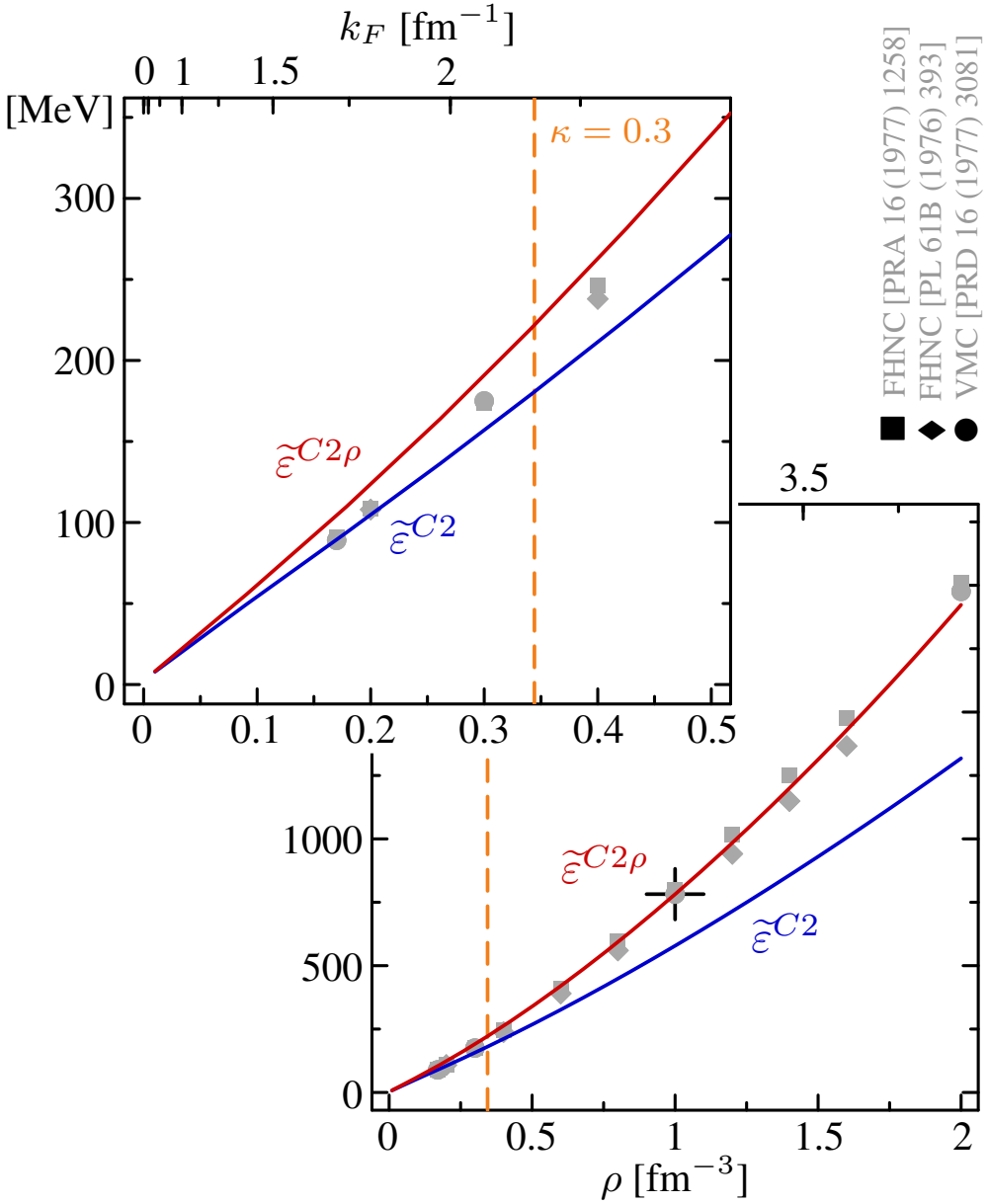
$$\alpha \to \alpha\xi(\rho) \quad ; \quad \xi(\rho) = 1 - \gamma\rho^{1/3}$$
$$\beta \to \beta\xi(\rho)$$

- parameter γ chosen such that the energy for $\rho = 1.0\text{fm}^{-3}$ matches the VMC result

✔ energies are in very good agreement with the reference for all densities

▶ one tunable parameter fixed at one selected density allows to describe the energies over a large density range

▶ again: density-dependent correlators contain the relevant physics of many-body correlations



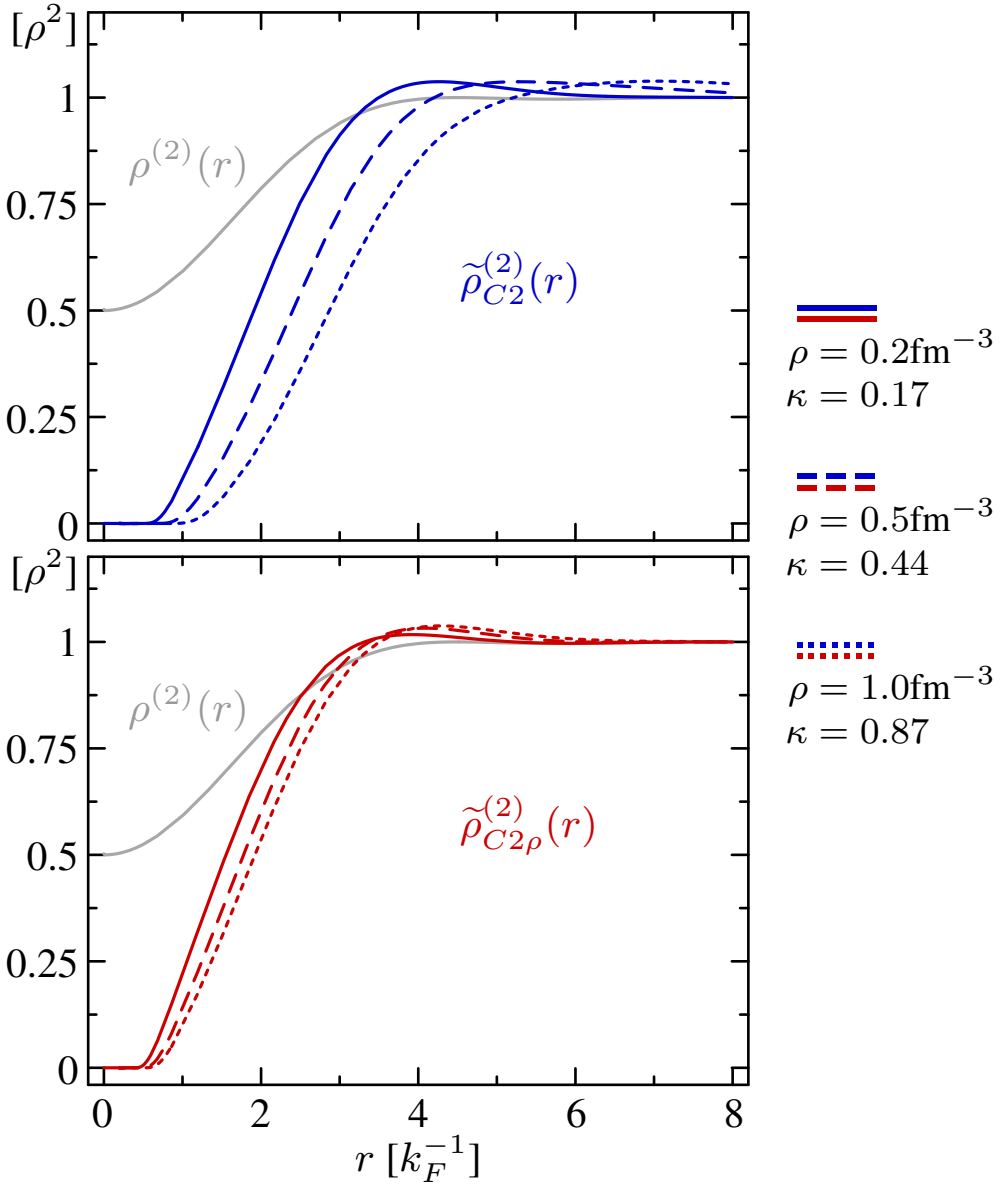
Homework-Problem

Correlated Two-Body Density

$$\rho^{(2)}(r) = \rho^2 \left[1 - \frac{9}{\lambda} \left(\frac{j_1(k_F r)}{k_F r} \right)^2 \right]$$

$$\widetilde{\rho}^{(2)}_{C2}(r) = \mathcal{R}^2_-(r) \;\; \rho^{(2)}[R_-(r)]$$

- ✔ correlator generates a large correlation hole in the two-body density
- ✔ strength is shifted out of the core-region and leads to enhanced densities at intermediate radii
- ✘ static correlator: size of the correlation hole grows with density compared to the average particle distance
- ▶ density-dependence reduces the growth and leads to a nearly constant ratio of hole size to particle distance



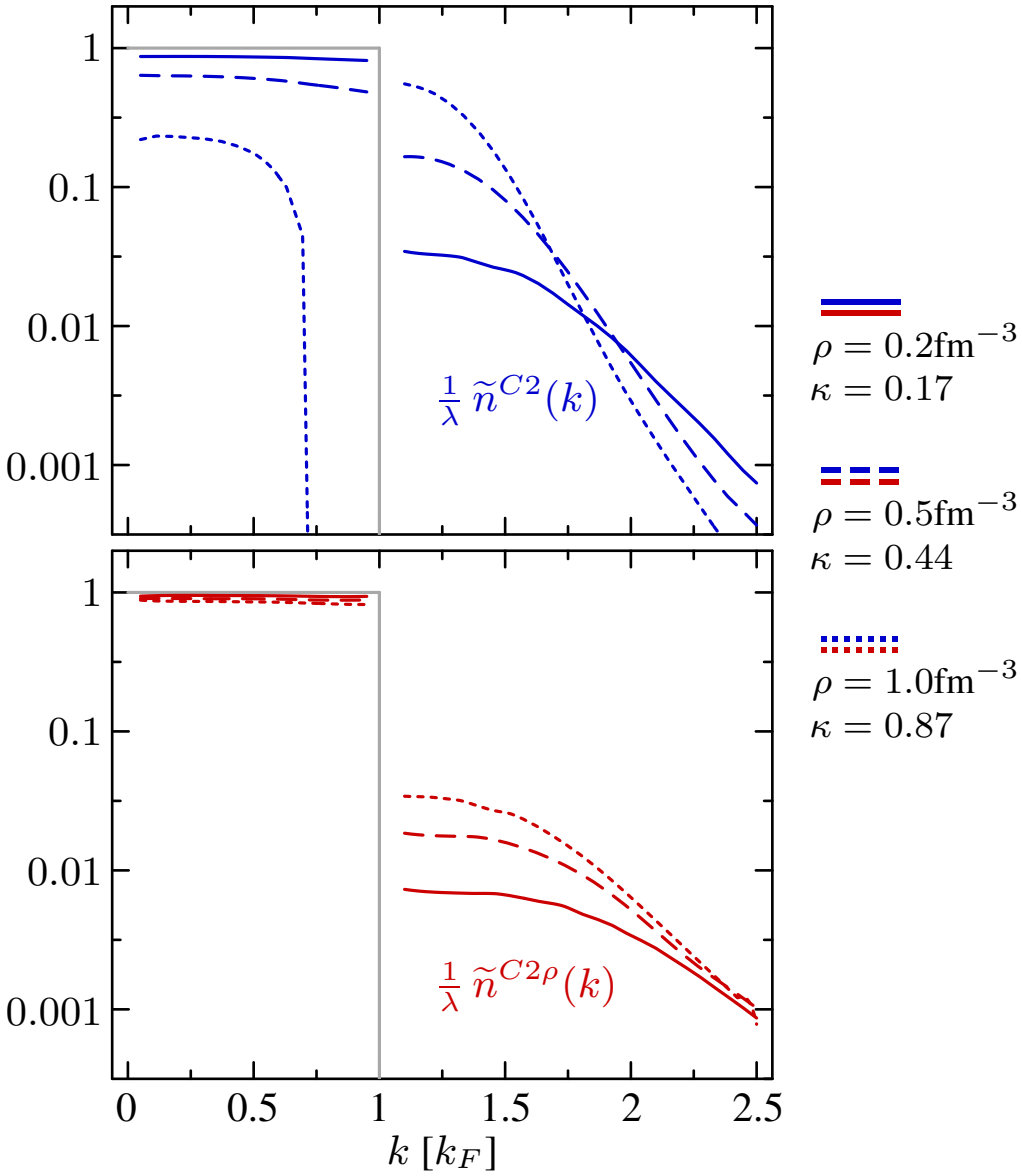
Homework-Problem

Correlated Momentum-Space Occupation Numbers

$$n(k) = \lambda\,\Theta(k_F - k)$$

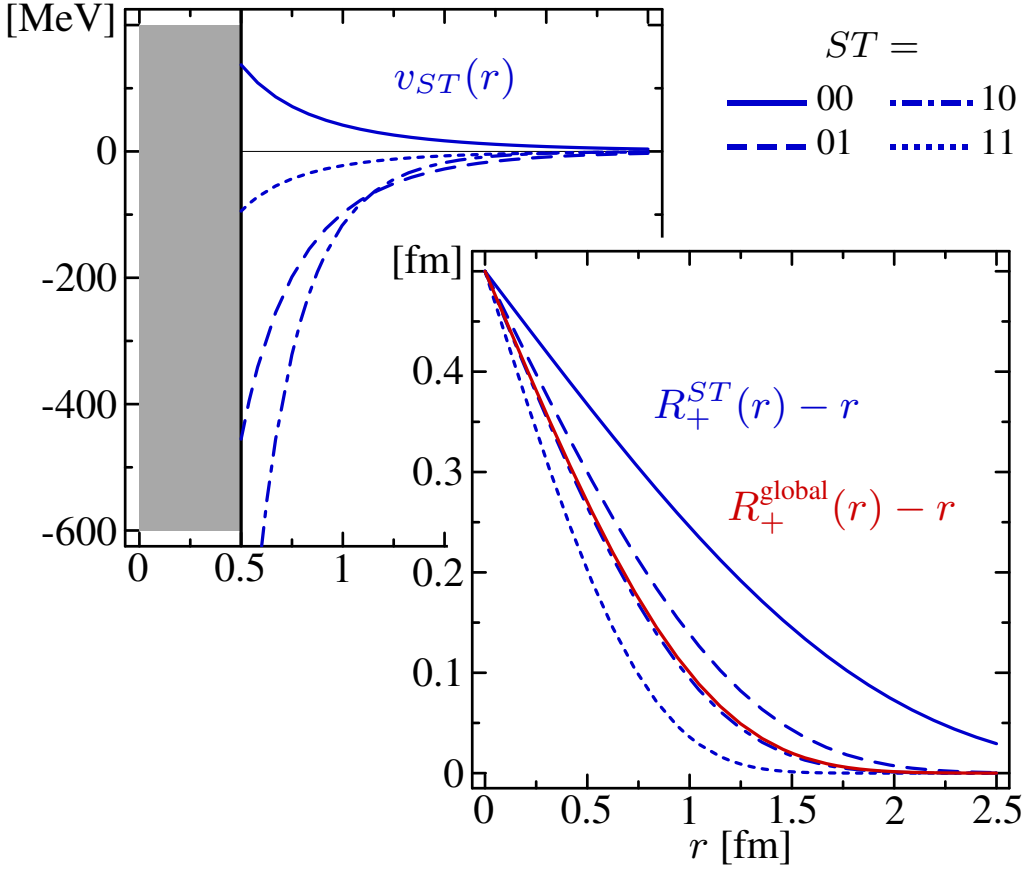
$$\widetilde{n}^{C2}(k) = n(k) + \widetilde{n}^{[2]}(k)$$

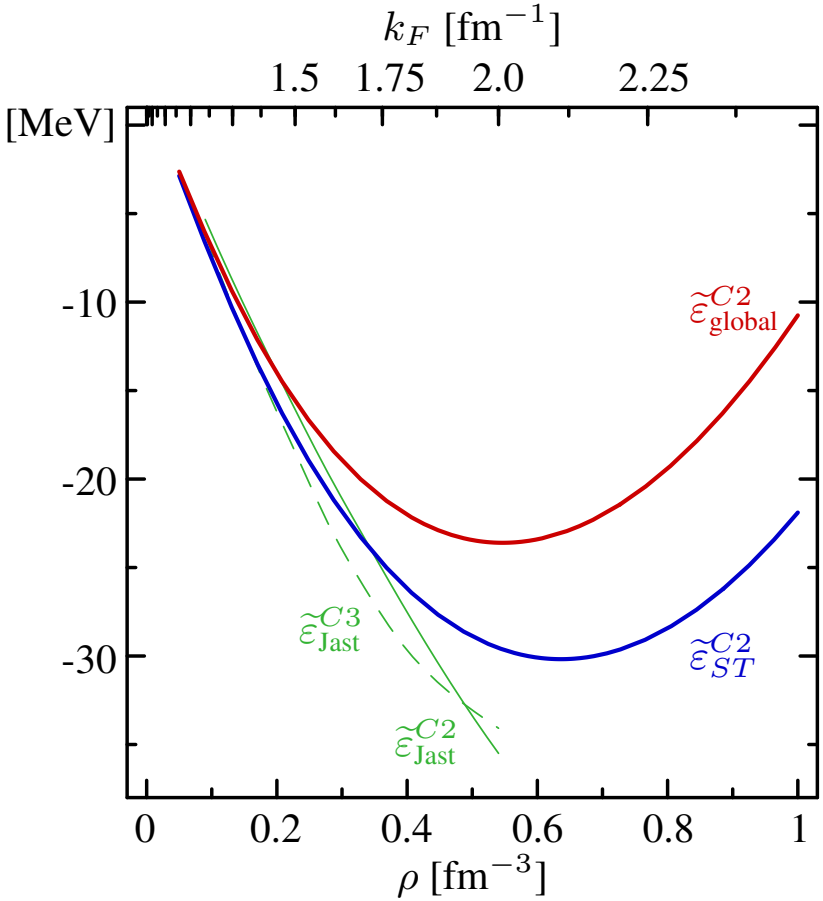
- ✔ due to short-range correlations states outside the Fermi sphere are populated
- ✔ states inside the Fermi sphere are de-populated; total particle number is conserved
- ✘ two-body approximation with static correlator leads to pathological momentum tails and negative occupation numbers for intermediate and high densities
- ▶ density-dep. correlator cures this problem and gives reasonable momentum tails
- ▶ density distributions are much more sensitive to failures of the two-body approximation than energies



Gammel-Christian-Thaler Potential

UCOM versus Jastrow-Correlators





- spin-isospin-dependent hard-core potential
- optimal global/spin-isospin-dependent correlators fixed by minimization of the nuclear-matter energy for $\rho = 0.6\,\text{fm}^{-3}$

✔ unitary correlator gives saturation in two-body approximation

✘ Jastrow correlation functions need three-body contributions to get saturation

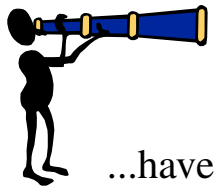
Summary

Strategy

- developed the Unitary Correlation Operator that describes short-range correlations by a two-body coordinate transformation
- evaluated the correlated Hamiltonian in two- and three-body approximation and correlated energies for the groundstate of Bose and Fermi liquids
- introduced density-dependent correlation functions

Results

- two-body approximation gives a good (ab initio) description for low densities, i.e. $\kappa = \rho V_C < 0.3$
- three-body contributions compensate the over-binding of the two-body approximation at higher densities... but expensive
- density-dependent correlators are an efficient way to describe the effects of many-body correlations
- reproduce the energy of the ^{4}He liquid with one adjustable parameter and predict the groundstate structure of droplets
- similar results for energy, densities and occupation numbers for neutron (Homework) and nuclear (GCT-potential) matter



...have a look at
http://theory.gsi.de/~rroth/phd