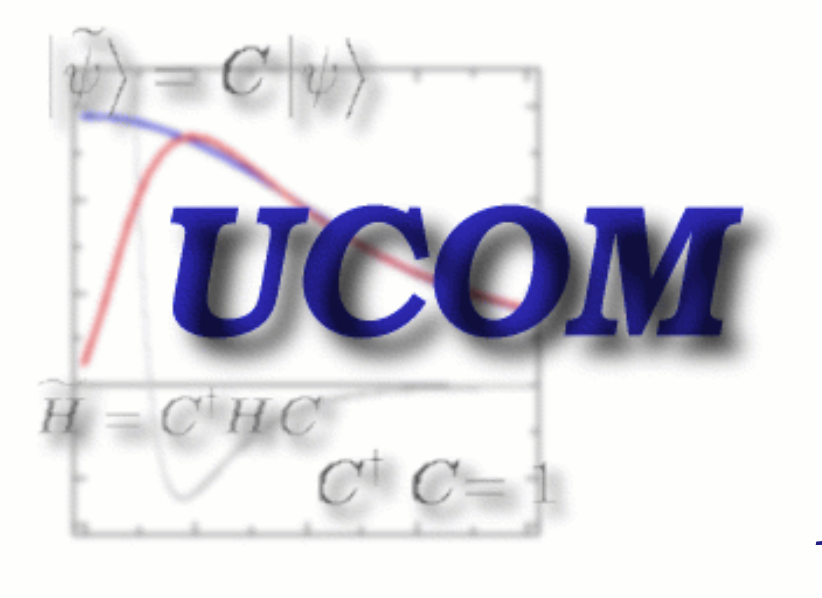


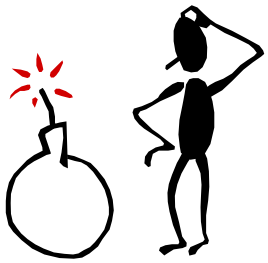
The *Unitary Correlation Operator Method*

for Interacting Fermi Gases

Robert Roth (GSI)

Rauischholzhausen XI @ Rostock, July 1-4, 1999

Problem & Overview



Q: How to treat *short-range correlations* induced by the strong repulsive core of the 2body interaction within a many-body system?

A: **Unitary Correlation Operator Method!**

...some keywords

- ★ *elements*: correlation operator/function, correlated states, correlated operators/Hamiltonian, equation of state, correlated density matrix
- ★ *approximations*: 2body approximation, 3body contributions, effective higher order contributions
- ★ *application I*: homework problem for neutron matter, equation of state, 2body density & occupation numbers
- ★ *application II*: phenomenological GCT-potential for nuclear matter, equation of state

The Concept of the

Unitary Correlation Operator Method

unitary correlation operator

$$\mathbf{C} \equiv \exp\Big\{ -\mathrm{i} \sum_{i<j} \mathbf{g}(ij) \Big\}$$

$$\mathbf{g} = \frac{1}{2}\big[s(\mathbf{r})\, \vec{\mathbf{n}}_r \vec{\mathbf{q}} + \vec{\mathbf{q}}\, \vec{\mathbf{n}}_r\, s(\mathbf{r}) \big] = \mathbf{g}^\dagger$$

- $\mathbf{C}^\dagger\, \mathbf{C} = \mathbf{1}$
- correlation function $R_\pm(r)$

$$\int_r^{R_\pm(r)} \frac{\mathrm{d}x}{s(x)} = \pm 1 \quad \rightarrow \quad R_\pm(r) \approx r \pm s(r)$$

correlated states

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

- correlated relative wave function of a 2body system

$$\langle r|\widetilde{\phi}\rangle = \frac{R_-(r)}{r} \sqrt{R_-{}'(r)}\, \langle R_-(r)|\phi\rangle$$

correlated operators

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

- correlated central potential in 2body space

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

Correlated Hamiltonian

in 2body Approximation

Hamiltonian in 2body approximation

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

$$\overset{C2}{\approx} \quad \mathbf{t}_0 \;+\; \widetilde{\mathbf{t}}_\nabla + \widetilde{\mathbf{t}}_r \;+\; \widetilde{u}(\mathbf{r}) + \widetilde{v}(\mathbf{r})$$

effective mass corrections

$$\widetilde{\mathbf{t}}_\nabla = \vec{\mathbf{q}}\; \underbrace{\frac{1}{2\mu}\left(\frac{r^2}{{R_+}^2(r)} - 1\right)}_{= 1/2\widetilde{\mu}_\nabla(r)}\; \vec{\mathbf{q}}$$

$$\widetilde{\mathbf{t}}_r = \vec{\mathbf{q}}\,\vec{\mathbf{n}}_r\; \underbrace{\frac{1}{2\mu}\left(\frac{1}{{R'_+}^2(r)} - \frac{r^2}{{R_+}^2(r)}\right)}_{= 1/2\widetilde{\mu}_r(r)}\; \vec{\mathbf{n}}_r\vec{\mathbf{q}}$$

local potentials

$$\widetilde{u}(r) = \frac{1}{2\mu\; {R'_+}^2(r)} \;\times$$

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

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

Interacting Fermi Gas

Assumptions and Trial State

many-body trial state

- free fermi gas & unitary correlation operator provides trial state for the interacting fermi gas
- free one-body states are momentum eigenstates with momentum $\vec{k}_i$ and λ-fold spin-isospin degeneracy

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

$$\left\langle \vec{x}\middle|\vec{k}_i\right\rangle = \frac{1}{\sqrt{V}} \exp(\mathrm{i}\,\vec{k}_i\,\vec{x})$$

- many-body trial state $\left|\widetilde{\Psi}\right\rangle$ is a correlated Slater determinant of all one-body states with $\left|\vec{k}_i\right| \leq k_F$

$$\left|\widetilde{\Psi}\right\rangle = \mathbf{C}\left|\Psi\right\rangle = \mathbf{C}\ \mathbf{A}\left(\left|i_1\right\rangle \otimes \cdots \otimes \left|i_A\right\rangle\right)$$

next steps...

- calculate correlated energy expectation value

$$\widetilde{\varepsilon} = \left\langle\widetilde{\Psi}\middle|\,\mathbf{H}\,\middle|\widetilde{\Psi}\right\rangle/A = \left\langle\Psi\middle|\,\widetilde{\mathbf{H}}\,\middle|\Psi\right\rangle/A$$

- minimize the energy as a function(al) of the correlation function ➨ optimal correlator
- calculate any observable you like, e.g. equation of state, densities...

Equation of State

for an Interacting Fermi Gas in 2body Approximation

corr. Hamiltonian

$$\widetilde{\mathbf{H}}^{C2} = \mathbf{t}_0 + \widetilde{v}(\mathbf{r}) + \widetilde{u}(\mathbf{r}) + \widetilde{\mathbf{t}}_\nabla + \widetilde{\mathbf{t}}_r$$

energy per particle as function of k_F

$$\widetilde{\varepsilon}^{C2} = \frac{3}{10m} k_F^2 + \frac{\lambda}{12\pi^2} k_F^3 \int \mathrm{d}^3 r \left[\widetilde{v}(r) + \widetilde{u}(r)\right] + \text{xch.} + \frac{\lambda}{80\pi^2} k_F^5 \int \mathrm{d}^3 r \left[\widetilde{\mu}_\nabla^{-1}(r) + \tfrac{1}{3}\widetilde{\mu}_r^{-1}(r)\right] + \text{xch.}$$

- direct terms of orders k_F^2, k_F^3 and k_F^5, resp. $\rho^{2/3}$, ρ and $\rho^{5/3}$ ($\rho = \frac{\lambda}{6\pi^2} k_F^3$)
- exchange terms grow with smaller powers of k_F than the direct terms
- high density behavior is determined by the effective mass terms ($\propto k_F^5, \rho^{5/3}$)

Potential & Optimal Correlator

Bethe's homework problem (1973)

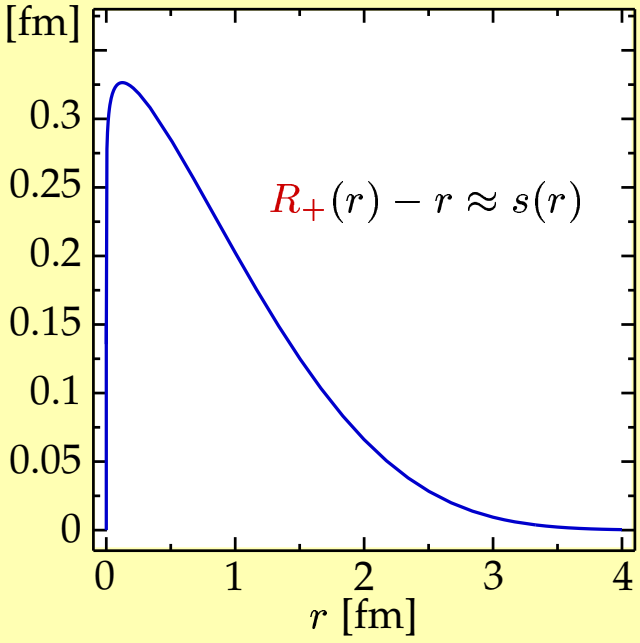
- neutron matter ($\lambda = 2$) interacting via the repulsive core of the ${}^1S_0$ component of the Reid potential

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

parametrization & matter-optimal correlator

- choose a parametrization for the correlation function R_+ and minimize the energy expectation value $\widetilde{\varepsilon}^{C2}(\rho)$ at some given density ($\rho = 1\,\text{fm}^{-3}$)

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



➨ $\alpha = 1.149\,\text{fm}$

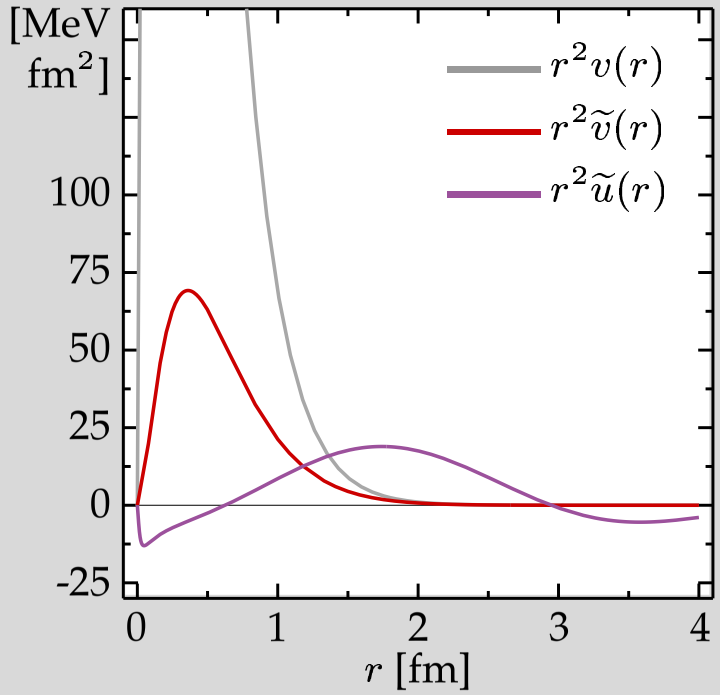
$\beta = 1.903\,\text{fm}$

$\eta = 0.07$

Homework Problem

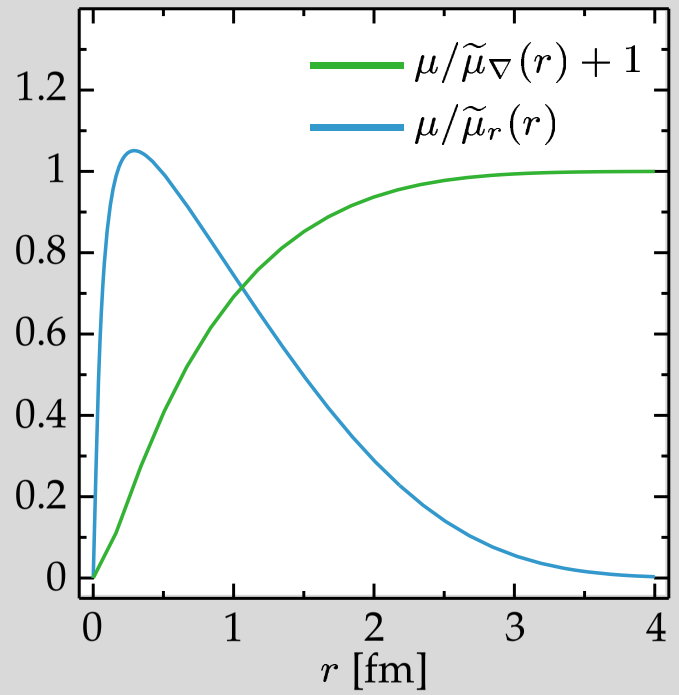
Local Potentials & Eff. Mass Corrections

local potentials



- core of the potential is dramatically reduced
- additional medium range repulsion by the kinetic potential

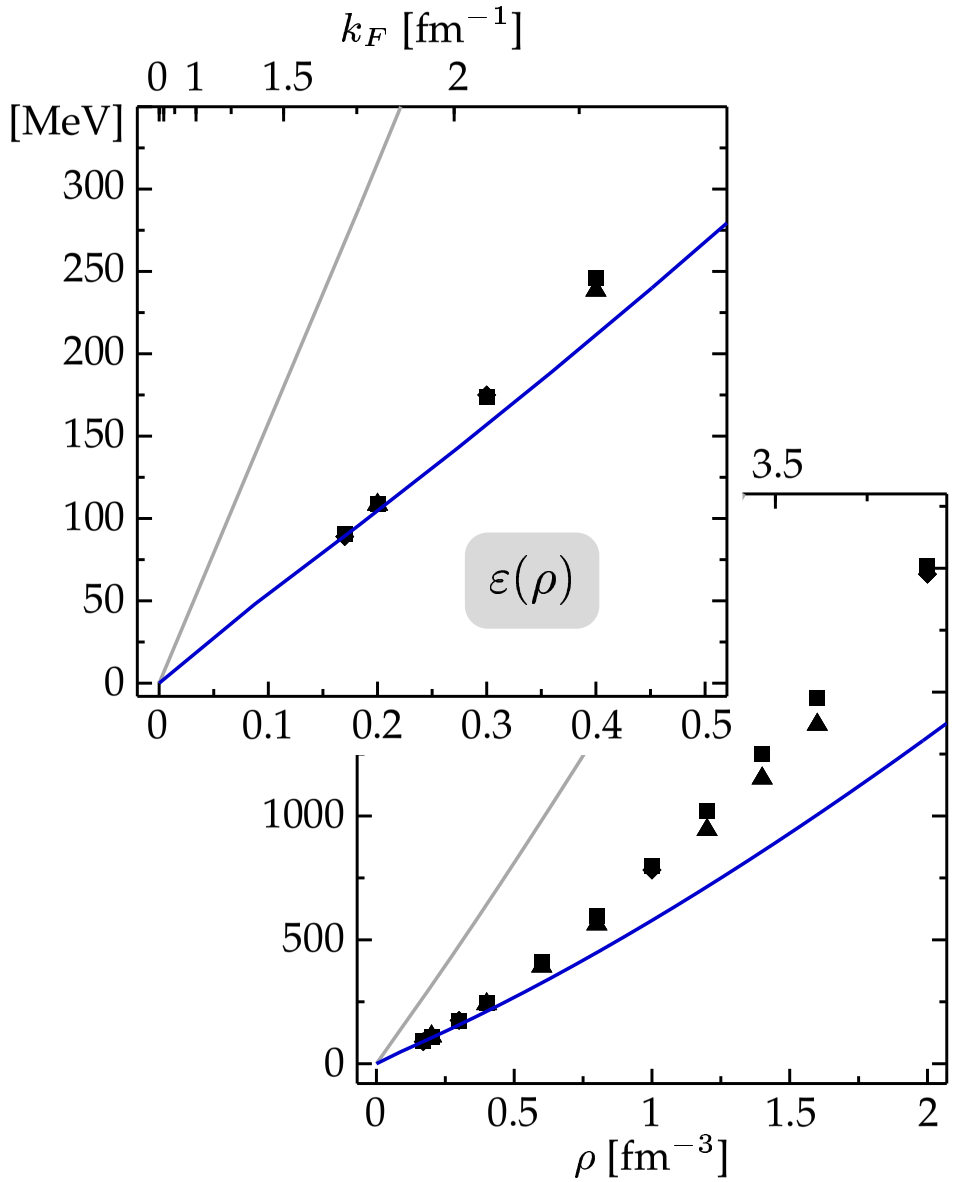
effective mass corrections



- mass reduction within the range of the interaction
- enhancement of the kinetic energy by additional radial mass

Homework Problem

Equation of State in 2body Approx.



- ✔ reduction of the energy to 1/3 of the uncorrelated value
- ✔ good agreement with reference for low densities $\leq 0.3\,\mathrm{fm}^{-3}$
- ✘ "overbinding" of up to 20% at high densities $\geq 1\,\mathrm{fm}^{-3}$
- ➨ 2body approximation gives resonable description for low densities but needs corrections for high densities
- ➨ 3body contributions relevant!!!

no correlator

$\widetilde{\varepsilon}^{C2}$ with matter-optimal correlator

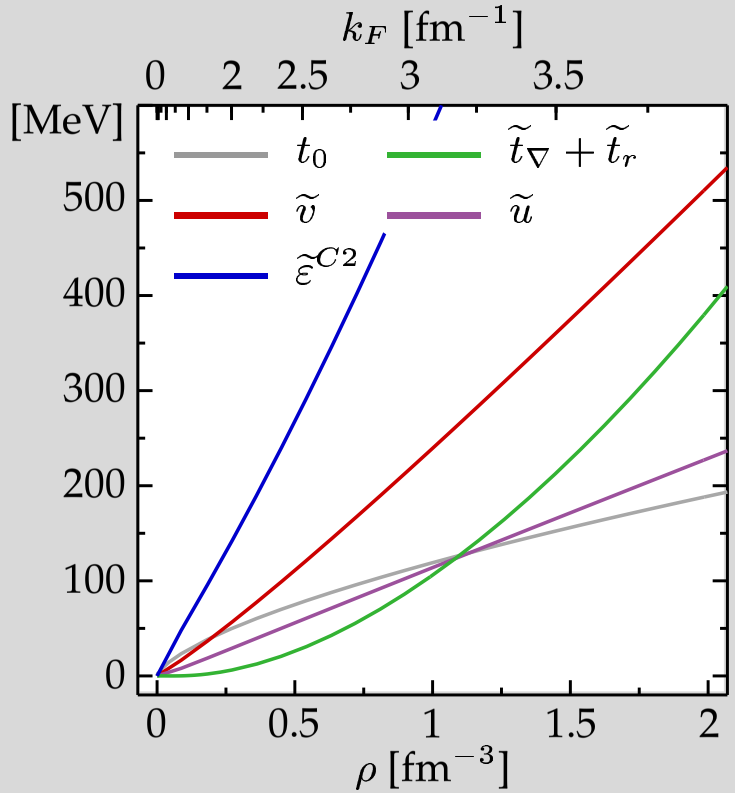
♦ MC Variation [PRD 16(77)3081]

▲/■ FHNC [PL 61B(76)393]/[PRA 16(77)1258]

Homework Problem

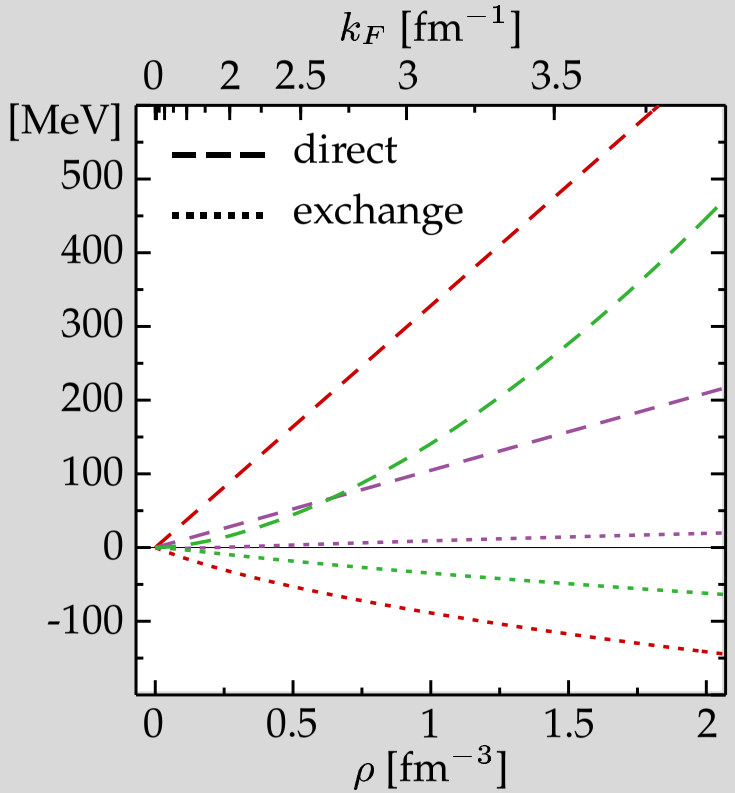
Energy Contributions in Detail

energy contributions



- local terms ($\propto k_F^3, \rho$) give main contribution, effective mass term ($\propto k_F^5, \rho^{5/3}$) wins at high densities

direct & exchange terms



- exchange contribution is in the order of 10% of the direct terms

Contributions of the 3rd Cluster Order

3body correlations

✘ no closed analytic expression for 3body correlated operators available

➨ product approximation: partial summation of the Baker-Hausdorff expansion of the correlated operator

➨ generalized coordinate transformation: correlations formulated by a norm conserving 3body coordinate transformation

3body approximation of the EoS

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

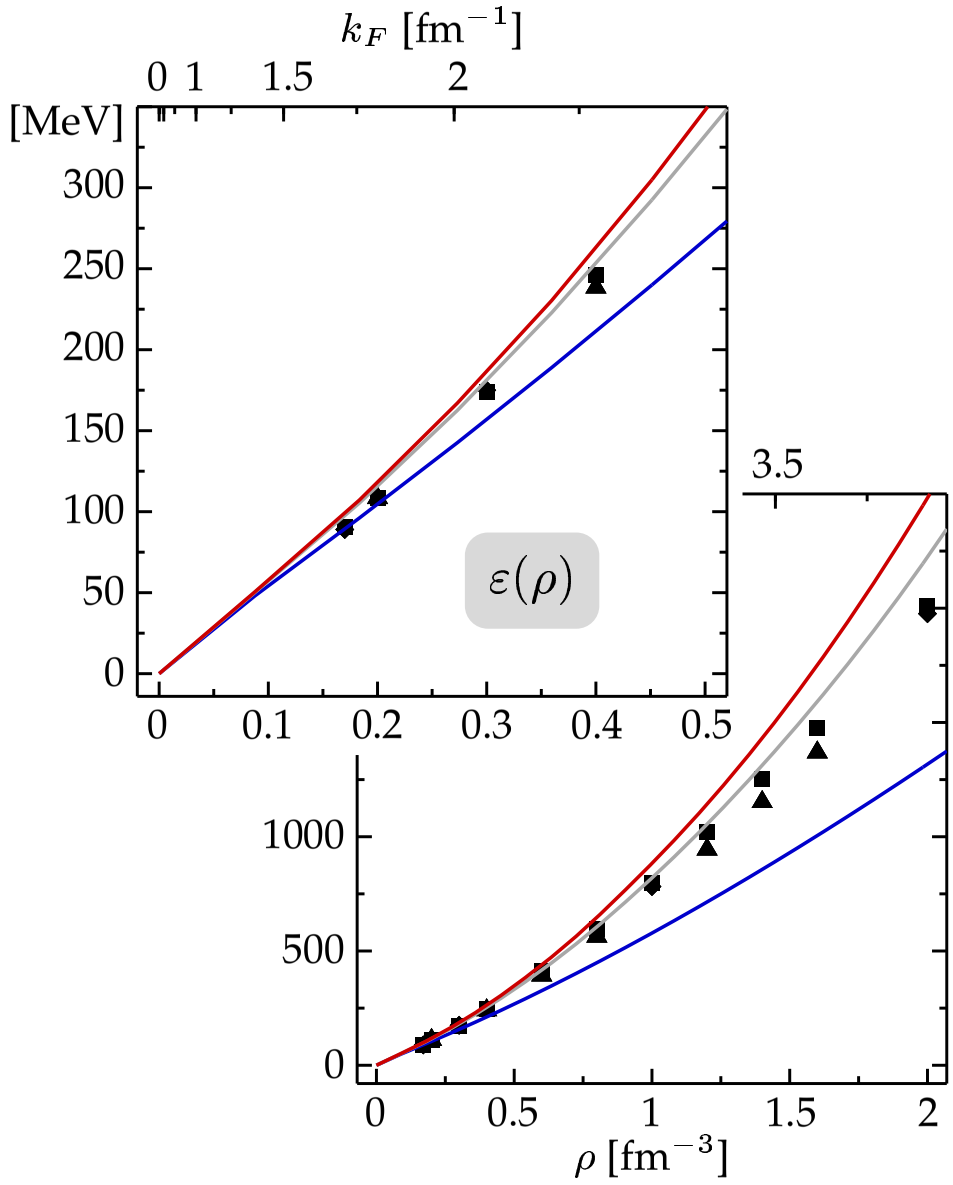
$$\widetilde{v}^{[3]} = \frac{\lambda^2}{216\pi^4}\, k_F^6 \iint \mathrm{d}^3 r_{12}\, \mathrm{d}^3 r_{13}\;\; \widetilde{v}^{[3]}(\vec{r}_{12}, \vec{r}_{13}) + \text{xch.} + \text{xxch.}$$

- contains all terms up to order k_F^6, especially all local 3body contributions
- 3body effective mass contributions of order k_F^8 are neglected

✘ high-dimensional numerical integrations over “rough” functions necessary (Monte Carlo methods)

Homework Problem

3body Contributions to the EoS



- ✔ local contributions of the 3body order raise the energy
- ✔ variational upper-bound property restored
- ✔ very good description of the low density regime
- ✔ potential contribution produces dominant effect
- ➨ 3body order seems to be sufficient for a reasonable approximation

$\widetilde{\varepsilon}^{C2}$ with matter-optimal corr.

$\widetilde{\varepsilon}^{C2} + \widetilde{v}^{[3]}$

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

♦ MC Variation [PRD 16(77)3081]

▲/■ FHNC [PL 61B(76)393]/[PRA 16(77)1258]

Formulation of

Effective Higher Order Contributions

density-dependent correlators

- correlator parameters with dimension of a length (i.e. α and β) are scaled as a function of density

$$\left.\begin{aligned}\alpha &\to \alpha\,\xi(\rho)\\ \beta &\to \beta\,\xi(\rho)\end{aligned}\right\} \to R_+(r,\rho)$$

$$\xi(\rho) = 1 - \gamma\,\rho^{1/3}$$

✔ effective potentials and masses become density-dependent

✔ consistent simulation of higher order effects for all correlated observables (energies, densities...)

3body contact interaction

- local 3body contributions approximated by a single 3body contact interaction

$$v_\delta^{[3]} = \Gamma\;\delta(r_{12})\delta(r_{13})$$

✔ expectation value gives an additional term proportional to k_F^6 for the EoS

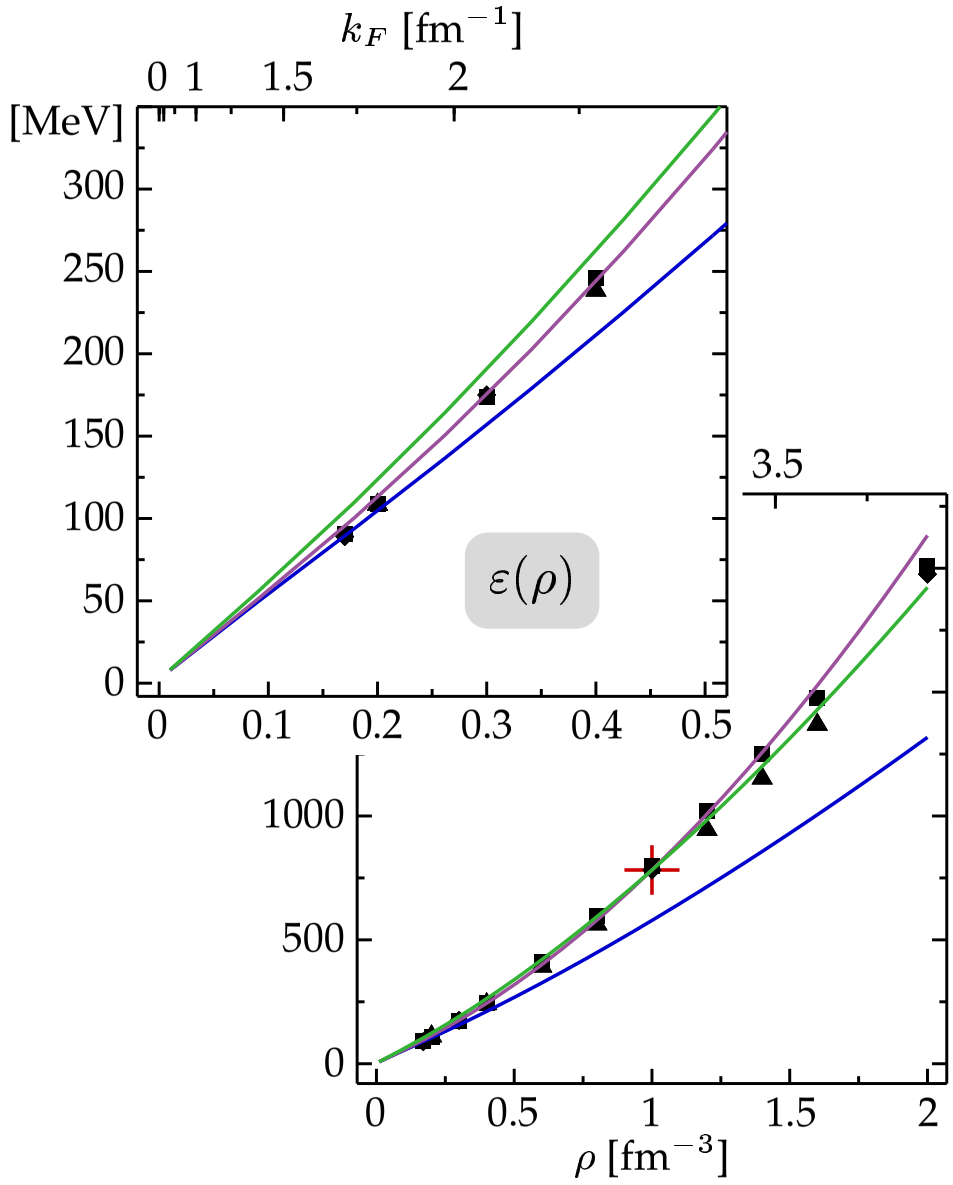
$$\widetilde{\varepsilon}^{C2+\delta} = \widetilde{\varepsilon}^{C2} + c\;\Gamma\;k_F^6$$

✘ applicable only for the energy expectation value, no prediction for other observables

- the free parameter γ or Γ has to be fixed by fitting the energy to higher order results or to some independent calculations

Homework Problem

Effective Higher Order Contributions to the EoS



- parameter γ or Γ is choosen to fit the MCV result at $\rho = 1\,\mathrm{fm}^{-3}$
- ✔ very good agreement with reference over the whole range for the density-dep. correlator
- ✔ perfect results for low and intermediate densities with 3body contact interaction
- ➨ easy and successful way to simulate the effects beyond 2body approximation

$\widetilde{\varepsilon}^{C2}$ with matter-optimal corr.
$\widetilde{\varepsilon}^{C2}$ + density-dep. correlator
$\widetilde{\varepsilon}^{C2}$ + 3body contact interaction
♦ MC Variation [PRD 16(77)3081]
▲/■ FHNC [PL 61B(76)393]/[PRA 16(77)1258]

Densities & Occupation Numbers

correlated 2body density matrix

$$\rho^{(2)}(\vec{x}_1,\vec{x}_2;\vec{x}_3,\vec{x}_4) := \left\langle \mathbf{\Psi}^\dagger_{\vec{x}_3}\mathbf{\Psi}^\dagger_{\vec{x}_4}\mathbf{\Psi}_{\vec{x}_2}\mathbf{\Psi}_{\vec{x}_1}\right\rangle$$
$$\widetilde{\rho}^{(2)}(\vec{x}_1,\vec{x}_2;\vec{x}_3,\vec{x}_4) := \left\langle \mathbf{C}^\dagger\mathbf{\Psi}^\dagger_{\vec{x}_3}\mathbf{\Psi}^\dagger_{\vec{x}_4}\mathbf{\Psi}_{\vec{x}_2}\mathbf{\Psi}_{\vec{x}_1}\mathbf{C}\right\rangle$$

➨ diagonal elements of the correlated 2body density in 2body approximation

$$\widetilde{\rho}^{(2)C2}(r_{12}) = \frac{R_-{}^2(r)}{r^2}R'_-(r)\left(\rho^2 - \frac{1}{\lambda}\left[\rho^{(1)}(R_-(r_{12}))\right]^2\right)$$

correlated occupation numbers

$$\rho^{(1)}(\vec{x}_1;\vec{x}_2) := \left\langle \mathbf{\Psi}^\dagger_{\vec{x}_2}\mathbf{\Psi}_{\vec{x}_1}\right\rangle$$
$$\widetilde{\rho}^{(1)}(\vec{x}_1;\vec{x}_2) := \left\langle \mathbf{C}^\dagger\mathbf{\Psi}^\dagger_{\vec{x}_2}\mathbf{\Psi}_{\vec{x}_1}\mathbf{C}\right\rangle$$

- off-diagonal elements of the correlated 1body density in 2body approximation

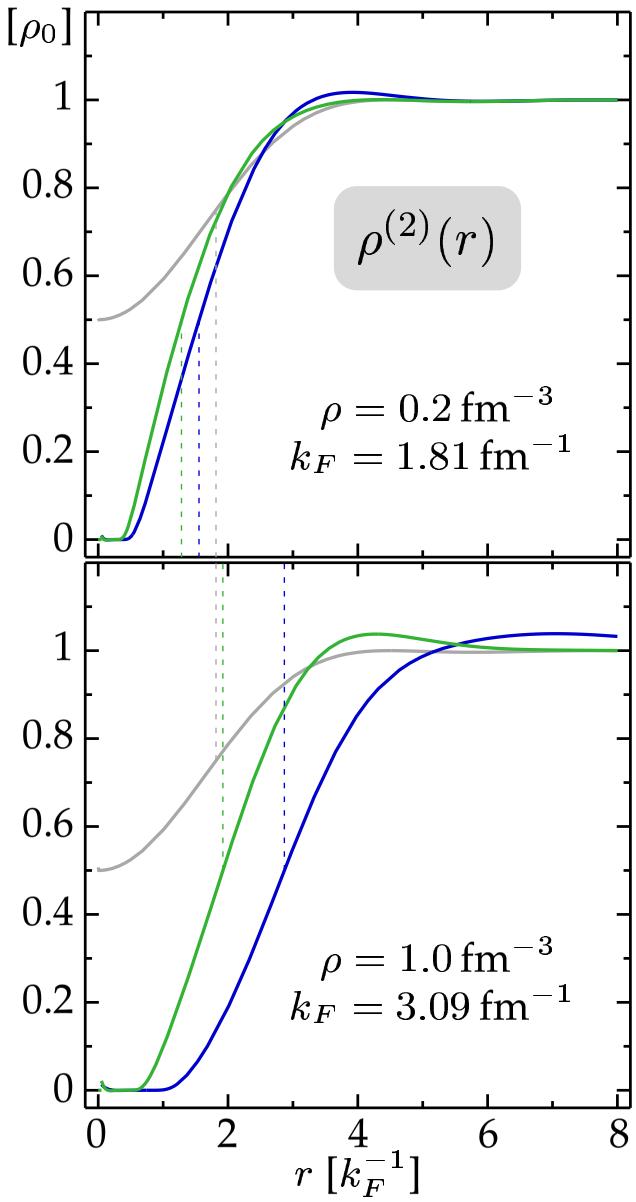
$$\widetilde{\rho}^{(1)C2}(r_{12}) = \rho^{(1)}(r_{12}) + \widetilde{\rho}^{(1)[2]}(r_{12})$$

➨ correlated momentum space occupation numbers by Fourier transform of correlated 1body density

$$\widetilde{n}^{C2}(k) = \frac{4\pi}{k}\int \mathrm{d}r\; r\sin(kr)\;\widetilde{\rho}^{(1)C2}(r)$$

Homework Problem

Correlated 2body Density Matrix



- ✔ density is reduced to almost zero within the core region ($r \leq 0.5\,\mathrm{fm}$)
- ✔ enhancement of the density outside the core such that the integral is preserved (unitarity)
- ➨ correlation hole

- ✘ size of the correlation hole grows compared to the exchange hole with increasing density
- ✔ density-dependent correlator reduces this effect

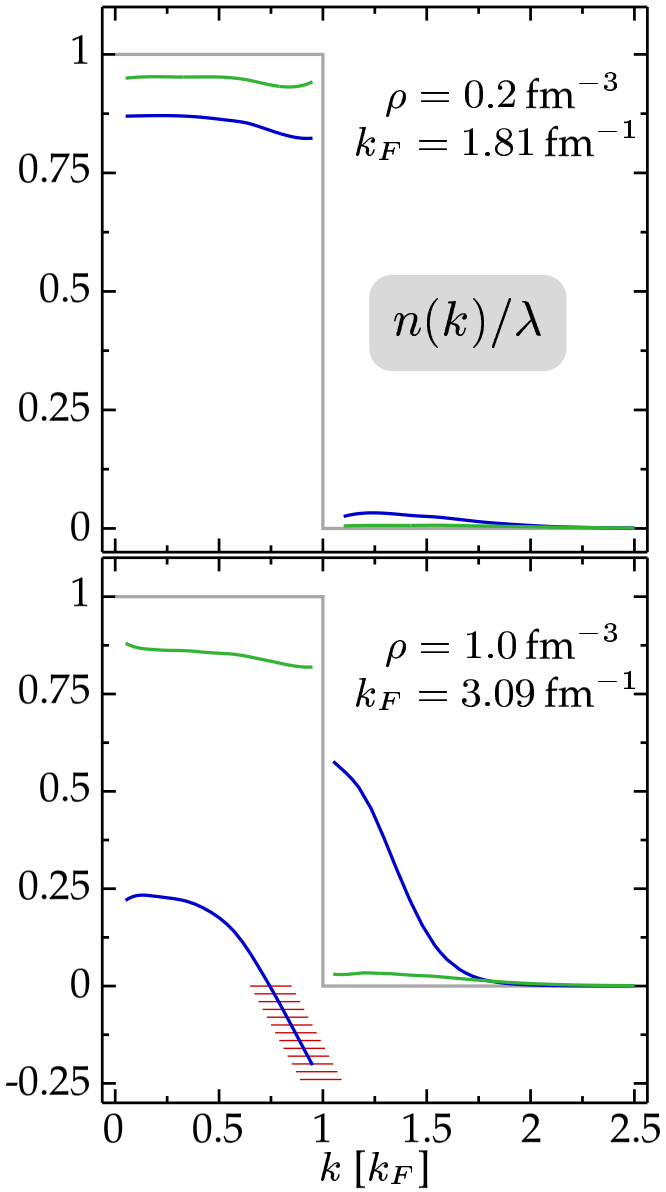
$\rho^{(2)}(r)$

$\widetilde{\rho}^{(2)C2}(r)$

$\widetilde{\rho}^{(2)C2}(r)$ + density-dependent corr.
(density-dependence fixed by energy fit)

Homework Problem

Correlated Occupation Numbers



- ✔ correlations lead to population of states above the Fermi edge
- ✔ states within the Fermi sphere are depopulated accordingly

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- ✘ negativ – unphysical – occupation numbers for high densities with density-independent correlator
- ✘ 2body approximation breaks down!
- ✔ effective higher order inclusion via the density-dependent correlator cures the problem

$n(k)/\lambda$

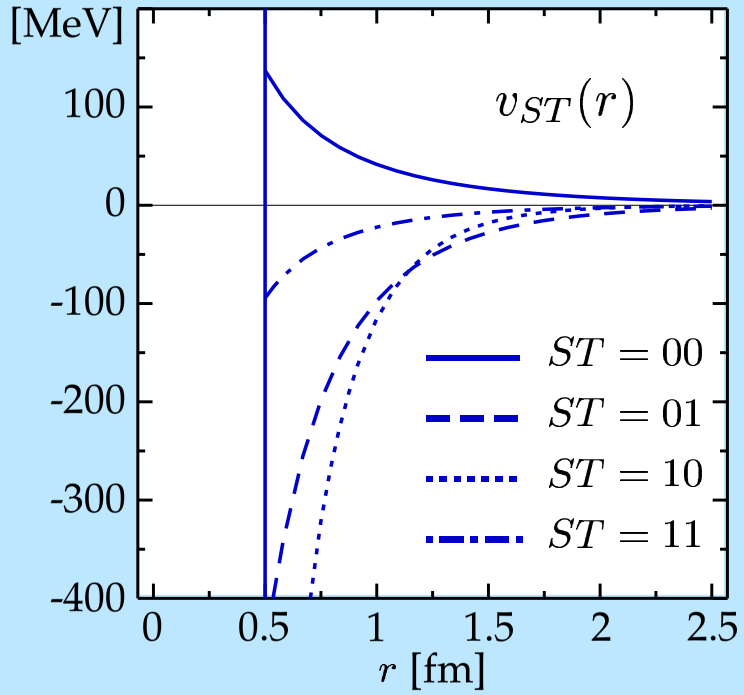
$\widetilde{n}^{C2}(k)/\lambda$

$\widetilde{n}^{C2}(k)/\lambda$ + density-dependent corr.

Gammel-Christian-Thaler-Potential

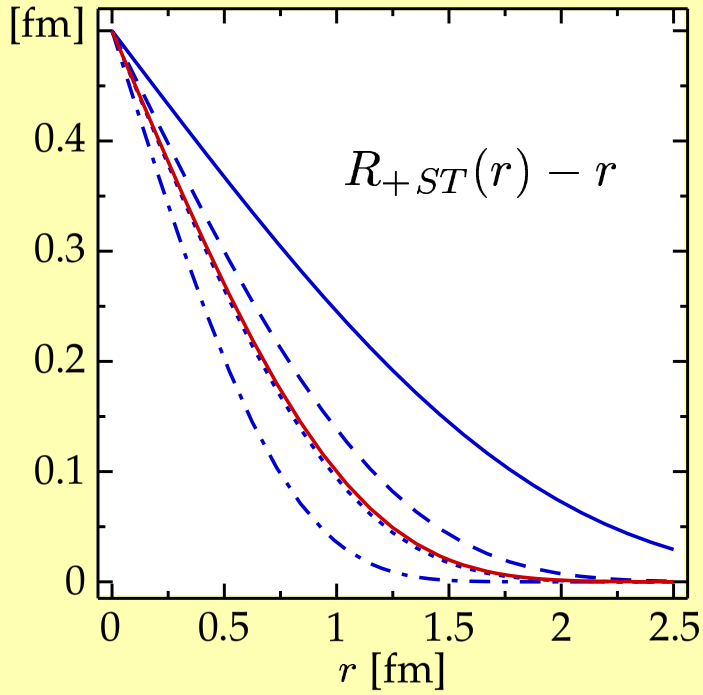
a Semi-Realistic Interaction

GCT-potential



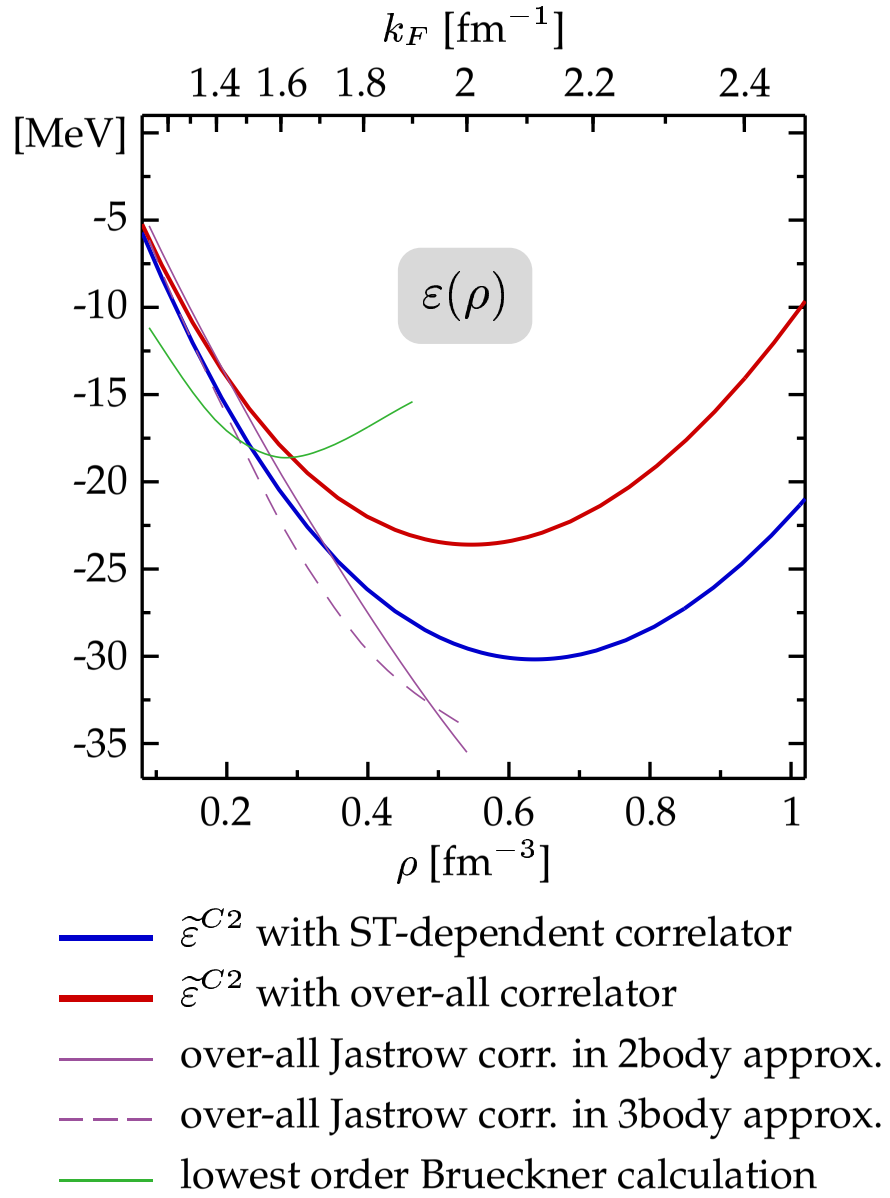
- spin-isospin-dependent hard-core potential
- tensor components not included

optimal correlators



- parameters fixed by energy minimization for nuclear matter
- full spin-isospin dependent correlator compared to over-all corr.

Equation of State in 2body Approx.



- ✔ energy minimum (saturation) at finite density already in 2body approx. due to k_F^5-term
- ✔ ST-dependent correlator gives a significant increase of binding energy (~ 6 MeV)
- ✔ good qualitative agreement with Jastrow (3body) and Brueckner calculations

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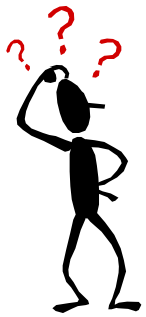
- ✘ Jastrow-method can not provide saturation in 2body approximation by construction (no k_F^5-term)
- ✘ 3body order is able to generate saturation (k_F^6-term)

Summary & Outlook

what was shown here...

- ✔ UCOM is a new and promising approach to tame short-range correlations in the context of quantum many-body problems
- ✔ unitary coordinate transformation of states or operators to introduce correlations
- ✔ in 2body approximations the correlated interaction has a *simple* analytic form
- ✔ higher order contributions can be calculated explicitly or included effectively
- ✔ convincing results for the homework problem and nuclear matter with the GCT potential



coming up next...

- ★ application to the zoo of atomic many-body system: liquid ^{3}He, liquid ^{4}He and droplets, trapped Bose-Einstein condensates...
- ★ nuclear many-body systems with realistic interactions: tensor correlations!!!
- ★ use of the correlated realistic interactions as input for simulation of dynamics: nuclear collisions (FMD) and BEC dynamics.