

*Quantum Monte Carlo (GFMC) Studies of
Superfluid Fermi Gas*

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Introduction

Pairing is a central problem of many-body physics.

Theories for weak coupling regime: BCS, Gorkov, etc.

Strong coupling limit still to be seen.

Fermi systems with attractive interaction through 1S_0 channel:

→ neutron matter at low density in the outer crust of neutron star.

→ proton fraction at low density at the inner core of neutron star.

→ dilute Fermi gas at low T, ^6Li , ^{40}K , etc.

interaction is ‘tunable’ through Feshbach resonance

temperature as low as $0.05T_F$ achieved

evidence of superfluidity ?

Superfluidity expected at low temperature → nonzero energy gap Δ .

Importance for the evolution of neutron star.

Hamiltonian

Many-body Hamiltonian;

$$\mathcal{H} = -\frac{\hbar^2}{2m} \sum_{n=1}^A \nabla_n^2 + \sum_{i,j'} v(r_{ij'})$$

Denote spin \uparrow particles by i, j, k, \dots

Denote spin \downarrow particles by i', j', k', \dots

Spin \uparrow and spin \downarrow particles interact via potential of the form,

$$v(r_{ij'}) = -v_0 \frac{2\hbar^2}{m} \frac{\mu^2}{\cosh^2(\mu r_{ij'})}$$

Interaction is characterized by dimensionless quantity; ak_F
and effective range,

$$R_{eff} = 2 \int_0^\infty (u_{asympt}^2(r) - u^2(r)) dr$$

For example, $v_0 = 1$ corresponds to $ak_F = -\infty$ and $R_{eff} = \frac{2}{\mu}$.

Work with $\mu r_0 = 12$, where $(\frac{4\pi}{3} r_0^3 \rho = 1)$.

We checked with $\mu r_0 = 24$, and we want to approximate $\mu r_0 \rightarrow \infty$.

then we have the short range limit; $R_{eff} \ll r_0$.

The unit of energy is the free Fermi gas energy per particle,

$$E_{FG} = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m}$$

Green's Function Monte Carlo: Principle

First developed by M. Kalos, *et al* in the 1970s.

Let Ψ_i be the eigenstates of \mathcal{H} ,

$$\Psi_i \mathcal{H} = E_i \Psi_i$$

The trial wave function can be expanded,

$$\Psi_V = \sum_i \alpha_i \Psi_i$$

We can project out the ground state Ψ_0 by evolution in imaginary time,

$$e^{-i\mathcal{H}t} \longrightarrow e^{-\mathcal{H}\tau} \quad , \quad \tau = it$$

We shift the energy by $E_T \approx E_0$ to control the norm, then,

$$\lim_{\tau \rightarrow \infty} e^{-(\mathcal{H}-E_T)\tau} \Psi_V = \lim_{\tau \rightarrow \infty} \sum_i \alpha_i e^{-(E_i-E_T)\tau} \Psi_i \longrightarrow \alpha_0 e^{-(E_0-E_T)\tau} \Psi_0$$

Estimate of the ground state energy is obtained from *mixed estimate*,

$$\Psi(\tau) = e^{-(\mathcal{H}-E_T)\tau} \Psi_V(\tau=0)$$
$$\langle \mathcal{H} \rangle_{mix} = \frac{\langle \Psi_V | \mathcal{H} | \Psi(\tau) \rangle}{\langle \Psi_V | \Psi(\tau) \rangle} = E_0 \quad , \quad \lim \tau \rightarrow \infty$$

E_T is updated to keep $\langle \Psi(\tau) | \Psi(\tau) \rangle$ constant \longrightarrow *growth estimate*.

Green's Function

In general, for any value of τ the time evolution operator is not known.

Exception: system of free particles.

However, we can obtain small time propagator with controllable errors,

$$\Delta\tau = \tau/n \quad , \quad n = \text{total number of time steps}$$

$$e^{-(\mathcal{H}-E_T)\tau} = \prod e^{-(\mathcal{H}-E_T)\Delta\tau}$$

$$\Psi(\tau) = \left[\prod e^{-(\mathcal{H}-E_T)\Delta\tau} \right] \Psi_V(\tau = 0)$$

Let \mathbf{R} be a vector in the configuration space of A particles,

$$\mathbf{R} = \{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A\}$$

Green's function for short time $\Delta\tau$,

$$G(\mathbf{R}, \mathbf{R}') = \langle \mathbf{R} | e^{-(\mathcal{H}-E_T)\Delta\tau} | \mathbf{R}' \rangle$$

Green's function is used in order to advance one step in time,

$$\Psi^j(\mathbf{R}^j) = \int G(\mathbf{R}^j, \mathbf{R}^{j-1}) \Psi^{j-1}(\mathbf{R}^{j-1}) d\mathbf{R}^{j-1}$$

After n time steps we have,

$$\Psi^n(\mathbf{R}^n) = \int d\mathbf{R}^{n-1} \dots d\mathbf{R}^0 G(\mathbf{R}^n, \mathbf{R}^{n-1}) \dots G(\mathbf{R}^2, \mathbf{R}^1) G(\mathbf{R}^1, \mathbf{R}^0) \Psi_V(\mathbf{R}^0)$$

Short Time Green's Function

We need analytical expression for,

$$G(\mathbf{R}, \mathbf{R}') = \langle \mathbf{R} | e^{-(\mathcal{H}-E_T)\Delta\tau} | \mathbf{R}' \rangle$$

where,

$$\mathcal{H} = \mathcal{T} + \mathcal{V} \quad \text{with} \quad \mathcal{T} = -\frac{\hbar^2}{2m} \sum_{i=1}^A \nabla_i^2 \quad , \quad \mathcal{V} = \sum_{i,j'} v(r_{ij'})$$

and $[\mathcal{T}, \mathcal{V}] \neq 0$

Short time Green's function is approximated as (Trotter & Feynman),

$$G(\mathbf{R}, \mathbf{R}') \approx \langle \mathbf{R} | e^{-\frac{\mathcal{V}}{2}\Delta\tau} e^{-\mathcal{T}\Delta\tau} e^{-\frac{\mathcal{V}}{2}\Delta\tau} | \mathbf{R}' \rangle e^{E_T\Delta\tau}$$

with an error of $\mathcal{O}(\Delta\tau^3)$

Total error after n time steps is of the order,

$$\text{Total error} \sim n\Delta\tau^3 = \frac{\tau^3}{n^2}$$

Total error $\rightarrow 0$ for large n (check by doubling n).

As $\mathcal{V}|\mathbf{R}\rangle = V(\mathbf{R})|\mathbf{R}\rangle$ where $V(\mathbf{R}) = \sum_{i,j'} v(r_{ij'})$,

$$\begin{aligned} G(\mathbf{R}, \mathbf{R}') &\approx e^{-V(\mathbf{R})\Delta\tau/2} \langle \mathbf{R} | e^{-\mathcal{T}\Delta\tau} | \mathbf{R}' \rangle e^{-V(\mathbf{R}')\Delta\tau/2} e^{E_T\Delta\tau} \\ &\approx e^{-(V(\mathbf{R})+V(\mathbf{R}')-2E_T)\frac{\Delta\tau}{2}} G_0(\mathbf{R}, \mathbf{R}') \end{aligned}$$

where $G_0(\mathbf{R}, \mathbf{R}')$ is the Green's function for A free particles,

$$G_0(\mathbf{R}, \mathbf{R}') = \left[\frac{m}{2\pi\hbar^2\Delta\tau} \right]^{\frac{3}{2}A} \exp \left[\frac{-m(\mathbf{R} - \mathbf{R}')^2}{2\hbar^2\Delta\tau} \right]$$

Expectation Value

Exact expectation value for ground state is given by,

$$\langle \mathcal{H} \rangle_{exact} = \frac{\langle \Psi(\tau) | \mathcal{H} | \Psi(\tau) \rangle}{\langle \Psi(\tau) | \Psi(\tau) \rangle}$$

Instead, we use so-called mixed estimate,

$$\langle \mathcal{H} \rangle_{mix} = \frac{\langle \Psi_V | \mathcal{H} | \Psi(\tau) \rangle}{\langle \Psi_V | \Psi(\tau) \rangle}$$

\mathcal{H} and time evolution operator commute

→ mixed estimate and exact estimate become equal for large τ ,

$$\begin{aligned} \langle \mathcal{H} \rangle_{mix} &= \frac{\langle \Psi_V | \mathcal{H} e^{-(\mathcal{H}-E_T)\tau} | \Psi_V \rangle}{\langle \Psi_V | e^{-(\mathcal{H}-E_T)\tau} | \Psi_V \rangle} \\ &= \frac{\langle \Psi_V | e^{-(\mathcal{H}-E_T)\tau/2} \mathcal{H} e^{-(\mathcal{H}-E_T)\tau/2} | \Psi_V \rangle}{\langle \Psi_V | e^{-(\mathcal{H}-E_T)\tau/2} e^{-(\mathcal{H}-E_T)\tau/2} | \Psi_V \rangle} \\ &= \frac{\langle \Psi(\tau/2) | \mathcal{H} | \Psi(\tau/2) \rangle}{\langle \Psi(\tau/2) | \Psi(\tau/2) \rangle} \rightarrow \langle \mathcal{H} \rangle_{exact} \quad \text{for large } \tau \end{aligned}$$

In terms of the Green's functions,

$$\langle \mathcal{H} \rangle_{mix} = \frac{\int d\mathbf{R}^n \dots d\mathbf{R}^0 E_L(\mathbf{R}^n) \Psi_V^\dagger(\mathbf{R}^n) G(\mathbf{R}^n, \mathbf{R}^{n-1}) \dots G(\mathbf{R}^1, \mathbf{R}^0) \Psi_V(\mathbf{R}^0)}{\int d\mathbf{R}^n \dots d\mathbf{R}^0 \Psi_V^\dagger(\mathbf{R}^n) G(\mathbf{R}^n, \mathbf{R}^{n-1}) \dots G(\mathbf{R}^1, \mathbf{R}^0) \Psi_V(\mathbf{R}^0)}$$

where,

$$E_L(\mathbf{R}^n) = \frac{\langle \Psi_V | \mathcal{H} | \mathbf{R}^n \rangle}{\langle \Psi_V | \mathbf{R}^n \rangle}$$

And,

$$\langle \mathcal{H} \rangle_{mix} \longrightarrow E_0 \quad \text{for large enough } n$$

Fermion Green's Function Monte Carlo

First introduced by J. B. Anderson in 1975.

Integrals evaluated stochastically (Monte Carlo),

$$path_i = \{\mathbf{R}_i^n, \dots, \mathbf{R}_i^0\}$$

subscript (i) = path index

superscript (n) = time step

$P(\mathbf{R}_i^n, \dots, \mathbf{R}_i^0)$ = probability used to sample the paths

N_t = total number of sampled paths

then,

$$\langle \mathcal{H} \rangle = \frac{\sum_{i=1}^{N_t} N p_i}{\sum_{i=1}^{N_t} D p_i}$$

where we have defined,

$$N p_i = \frac{E_L(\mathbf{R}_i^n) \Psi_V(\mathbf{R}_i^n) G(\mathbf{R}_i^n, \mathbf{R}_i^{n-1}) \dots G(\mathbf{R}_i^1, \mathbf{R}_i^0) \Psi_V(\mathbf{R}_i^0)}{P(\mathbf{R}_i^n, \dots, \mathbf{R}_i^0)}$$

$$D p_i = \frac{\Psi_V(\mathbf{R}_i^n) G(\mathbf{R}_i^n, \mathbf{R}_i^{n-1}) \dots G(\mathbf{R}_i^1, \mathbf{R}_i^0) \Psi_V(\mathbf{R}_i^0)}{P(\mathbf{R}_i^n, \dots, \mathbf{R}_i^0)}$$

The path probability (by Kalos) is,

$$P(path_i) = \left[\prod_{j=1, n} I(\mathbf{R}_i^j) G(\mathbf{R}_i^j, \mathbf{R}_i^{j-1}) \frac{1}{I(\mathbf{R}_i^{j-1})} \right] I(\mathbf{R}_i^0) |\Psi_V(\mathbf{R}_i^0)|$$

We take 'Importance Function' $I(\mathbf{R}_i^j) = |\Psi_V(\mathbf{R}_i^j)|$,

then path probability becomes,

$$P(path_i) = |\Psi_V(\mathbf{R}_i^n)| G(\mathbf{R}_i^n, \mathbf{R}_i^{n-1}) \dots G(\mathbf{R}_i^1, \mathbf{R}_i^0) |\Psi_V(\mathbf{R}_i^0)|$$

Denominator of the mixed estimate becomes,

$$\begin{aligned}\sum_{i=1}^{N_t} N p_i &= \sum_{i=1}^{N_t} \frac{\Psi_V(\mathbf{R}_i^n) \Psi_V(\mathbf{R}_i^0)}{|\Psi_V(\mathbf{R}_i^n)| |\Psi_V(\mathbf{R}_i^0)|} \\ &= \sum_{i=1}^{N_t} \{ +1 \text{ or } -1 \}\end{aligned}$$

Positive domain : $\{\mathbf{R}^+\}$ such that $\Psi_V(\mathbf{R}^+) > 0$

Negative domain : $\{\mathbf{R}^-\}$ such that $\Psi_V(\mathbf{R}^-) < 0$

Nodal surface : $\{\mathbf{R}^{ns}\}$ such that $\Psi_V(\mathbf{R}^{ns}) = 0$

Neither positive domain nor negative domain is preferred by path probability.

This means,

$$\sum_{i=1}^{N_t} \frac{\Psi_V(\mathbf{R}_i^n) \Psi(\mathbf{R}_i^0)}{|\Psi_V(\mathbf{R}_i^n) \Psi(\mathbf{R}_i^0)|} \longrightarrow 0 \text{ for large } N_t$$

Similarly for the numerator, assuming that $E_L(\mathbf{R}_i^n) \approx E_0$,

$$\begin{aligned}\sum_{i=1}^{N_t} D p_i &= \sum_{i=1}^{N_t} \frac{E_L(\mathbf{R}_i^n) \Psi_V(\mathbf{R}_i^n) \Psi(\mathbf{R}_i^0)}{|\Psi_V(\mathbf{R}_i^n) \Psi(\mathbf{R}_i^0)|} \\ &\approx E_0 \sum_{i=1}^{N_t} \frac{\Psi_V(\mathbf{R}_i^n) \Psi(\mathbf{R}_i^0)}{|\Psi_V(\mathbf{R}_i^n) \Psi(\mathbf{R}_i^0)|} \\ &\longrightarrow 0 \text{ for large } N_t\end{aligned}$$

In the end, the so-called ‘Fermion Sign Problem’ of GFMC,

$$\langle \mathcal{H} \rangle \longrightarrow \frac{0}{0} \text{ for large } N_t$$

NOTE: Bose ground state wave function $\Psi_{Bose}(\mathbf{R}) \geq 0$, hence no sign problem.

Fixed Node GFMC

Fermion Sign Problem appears because $\Psi_V(\mathbf{R}_i^j)$ can change sign as the time step j increases.

A remedy; 'Fixed Node' GFMC.

Let $\Psi_V(\mathbf{R}_i^0) > 0$ for the initial time step.

Then constrain the path to the positive domain; $\Psi_V(\mathbf{R}_i^j) > 0$ for all j .

$$|e^{-(\mathcal{H}-E_T)\tau}|_{FN} \Psi_V(\mathbf{R}^+, 0) \longrightarrow \Psi(\mathbf{R}^+, \tau)$$

or

Let $\Psi_V(\mathbf{R}_i^0) < 0$ for the initial time step.

Then constrain the path to the negative domain; $\Psi_V(\mathbf{R}_i^j) < 0$ for all j .

$$|e^{-(\mathcal{H}-E_T)\tau}|_{FN} \Psi_V(\mathbf{R}^-, 0) \longrightarrow \Psi(\mathbf{R}^-, \tau)$$

When the constraint is imposed with the nodal surface of the exact $\Psi_0(\mathbf{R})$,

we get the exact E_0 ,

$$\longrightarrow \lim_{\tau \rightarrow \infty} \Psi(\mathbf{R}^\pm, \tau) = \Psi_0(\mathbf{R}^\pm)$$

$$\longrightarrow \langle \mathcal{H} \rangle_{mix} = E_0$$

Instead, when the nodal surface of $\Psi_V(\mathbf{R})$ is used to constrain,

$$\longrightarrow \lim_{\tau \rightarrow \infty} \Psi(\mathbf{R}^\pm, \tau) \text{ is only } \approx \Psi_0(\mathbf{R}^\pm)$$

$$\longrightarrow \langle \mathcal{H} \rangle_{mix} \geq E_0$$

We minimize variationally Fixed Node $\langle \mathcal{H} \rangle_{mix}$.

Trial Wave Function Ψ_V

Ψ_V is used as:

- Initial guess of $\Psi_0(\mathbf{R})$.
- Importance function $I(\mathbf{R}) = |\Psi_V(\mathbf{R})|$.
- Nodal surface of $\Psi_V(\mathbf{R})$ provides the fixed node constraint.

Assume that infinite matter is approximated as a cubic box ($L \times L \times L$) with periodic boundary conditions.

The simplest nodal surface; free fermions,

$$\Psi_{JS}(\mathbf{R}) = \prod_{i,j'} f_{ij'}(r_{ij'}) |\Phi\rangle$$

$|\Phi\rangle = \text{ground state of free fermions}$

Jastrow correlation $f_{ij'}(r_{ij'})$ has no effects on the nodal structure.

More general nodal surface is given by the BCS variational wave function,

$$\Psi_{BCS} = \prod_i (u_i + v_i a_{\mathbf{k}_i \uparrow}^\dagger a_{-\mathbf{k}_i \downarrow}^\dagger) |0\rangle$$
$$|u_i|^2 + |v_i|^2 = 1$$

$|0\rangle = \text{vacuum}$

This common form of Ψ_{BCS} does not correspond to a definite number of particles N .

For N spin \uparrow and N' ($= N$) spin \downarrow particles in the paired state the number conserving Ψ_{BCS} is given by,

$$\Psi_{BCS} = \mathcal{A}[\phi(r_{11'})\phi(r_{22'})\dots\phi(r_{NN'})]$$

$$\phi(r) = \sum_i \frac{v_i}{u_i} e^{i\mathbf{k}_i \cdot \mathbf{r}} = \sum_i \alpha_i e^{i\mathbf{k}_i \cdot \mathbf{r}} \quad , \quad \alpha_i \text{ can be taken as real}$$

NOTE: $\Psi_{BCS} = \Psi_{JS}$ when $\alpha_i = \{1, 1, \dots, 1, 1, 0, 0, 0, \dots\}$.

Pair wave function $\phi(\mathbf{r})$ can be generalized,

$$\phi(\mathbf{r}) = \tilde{\beta}_{b,c}(r) + \sum_{i \leq i_c} \alpha_i e^{i\mathbf{k}_i \cdot \mathbf{r}}$$

With u and d' unpaired \uparrow and \downarrow spin particles (Bouchaud, *et al*),

$$\Psi_{BCS}(\mathbf{R}) = \mathcal{A} \left\{ [\phi(r_{11'})\dots\phi(r_{NN'})] [\psi_{1\uparrow}(\mathbf{r}_{N+1})\dots\psi_{u\uparrow}(\mathbf{r}_{N+u})] [\psi_{1\downarrow}(\mathbf{r}_{(N+1)'})\dots\psi_{d\downarrow}(\mathbf{r}_{(N+d)'})] \right\}$$

$\psi_{i\uparrow}$ and $\psi_{j\downarrow} =$ single particle states.

$\longrightarrow \Psi_{BCS} =$ Determinant of

$$\begin{pmatrix} \phi(r_{11'}) & \phi(r_{12'}) & \dots & \phi(r_{1(N+d)'}) & \psi_{1\uparrow}(\mathbf{r}_1) & \psi_{2\uparrow}(\mathbf{r}_1) \\ \phi(r_{21'}) & \phi(r_{22'}) & \dots & \phi(r_{2(N+d)'}) & \psi_{1\uparrow}(\mathbf{r}_2) & \psi_{2\uparrow}(\mathbf{r}_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \phi(r_{(N+u)1'}) & \phi(r_{(N+u)2'}) & \dots & \phi(r_{(N+u)(N+d)'}) & \psi_{1\uparrow}(\mathbf{r}_{N+u}) & \psi_{2\uparrow}(\mathbf{r}_{N+u}) \\ \psi_{1\downarrow}(\mathbf{r}_{1'}) & \psi_{1\downarrow}(\mathbf{r}_{2'}) & \dots & \psi_{1\downarrow}(\mathbf{r}_{(N+d)'}) & 0 & 0 \\ \psi_{2\downarrow}(\mathbf{r}_{1'}) & \psi_{2\downarrow}(\mathbf{r}_{2'}) & \dots & \psi_{2\downarrow}(\mathbf{r}_{(N+d)'}) & 0 & 0 \\ \psi_{3\downarrow}(\mathbf{r}_{1'}) & \psi_{3\downarrow}(\mathbf{r}_{2'}) & \dots & \psi_{3\downarrow}(\mathbf{r}_{(N+d)'}) & 0 & 0 \end{pmatrix}$$

Variational parameters: b , c , and $\{\alpha_0, \alpha_1, \dots, \alpha_{i_c}\}$.

STRATEGY:

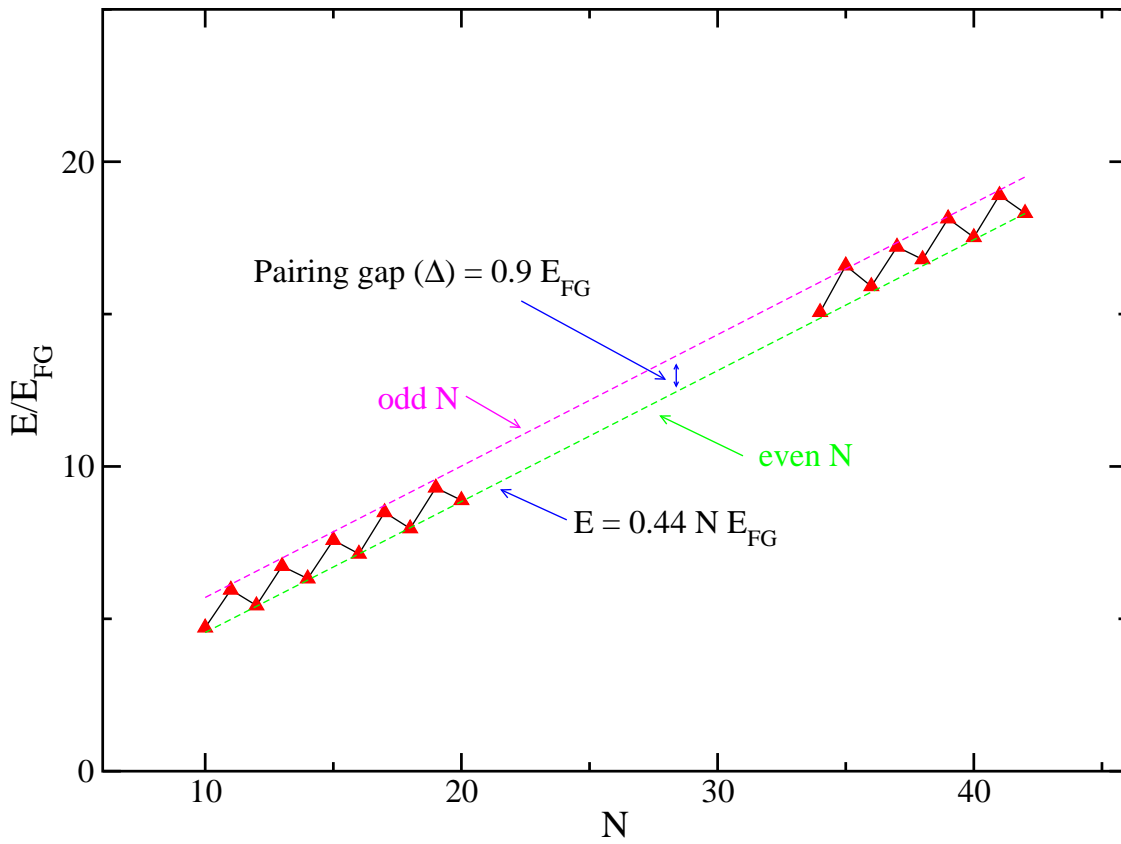
Find the optimal set of parameters by minimizing fixed node GFMC energy

\longrightarrow *best overlap with the nodal structure of the true ground state.*

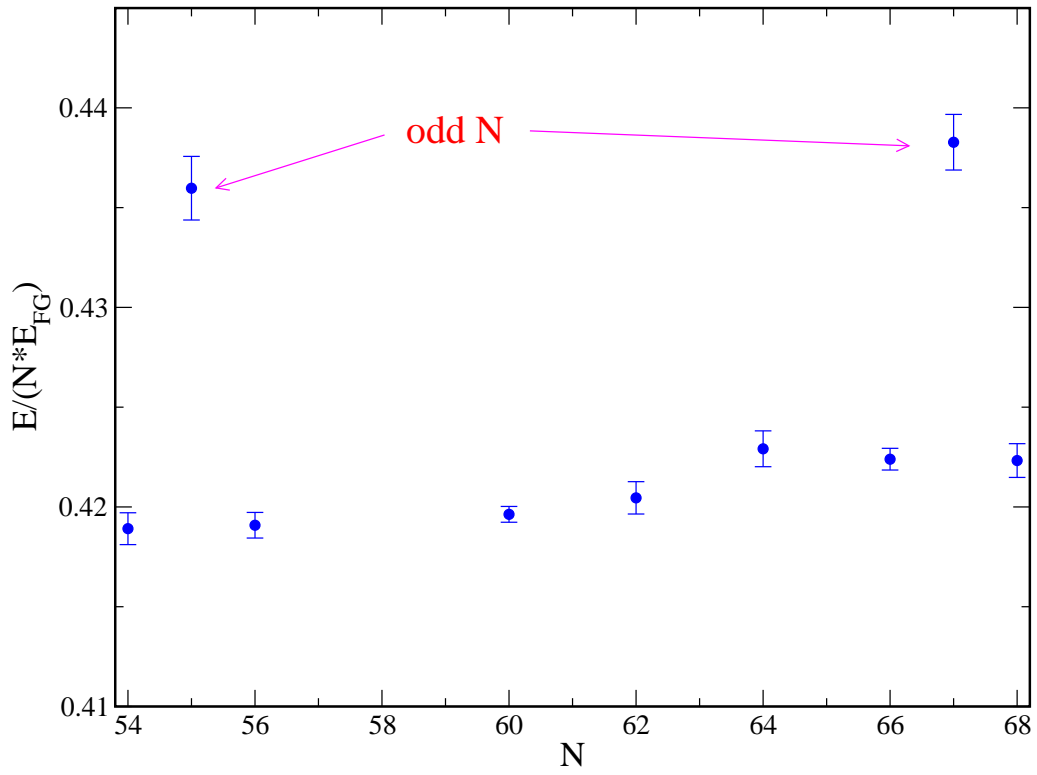
Gap Energy

Gap energy is obtained from,

$$\Delta(2n + 1) = E(2n + 1) - \frac{1}{2}(E(2n) + E(2n + 2))$$



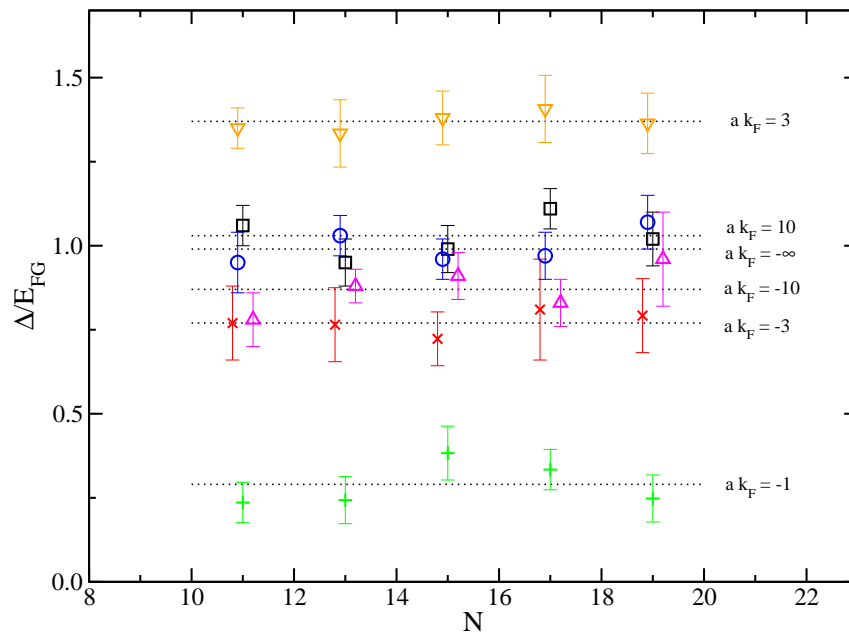
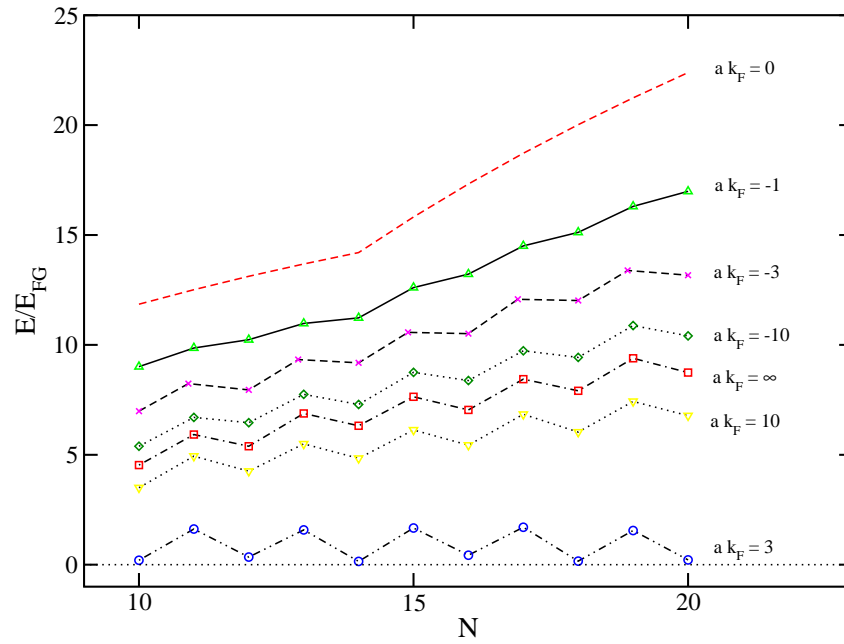
Result for $ak_F = -\infty$



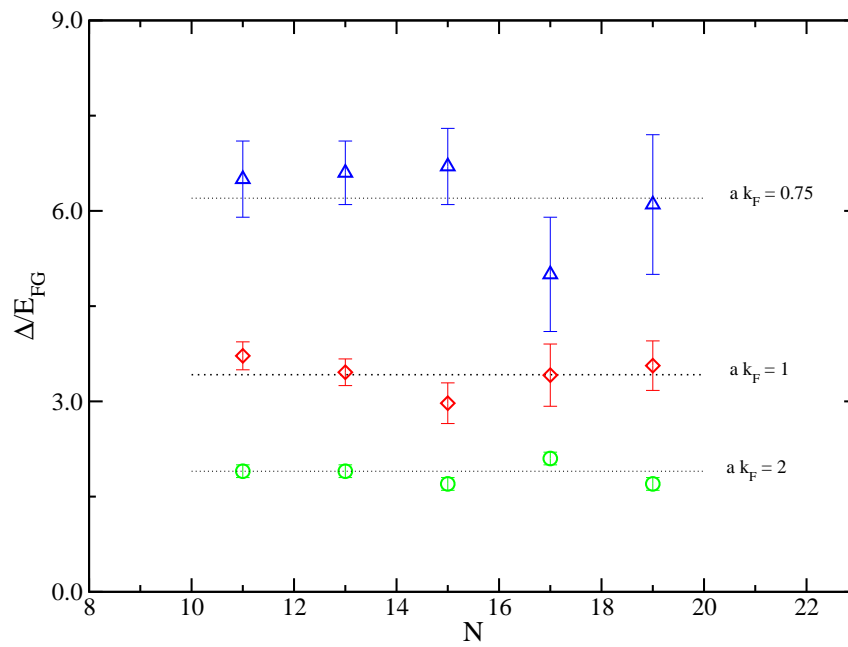
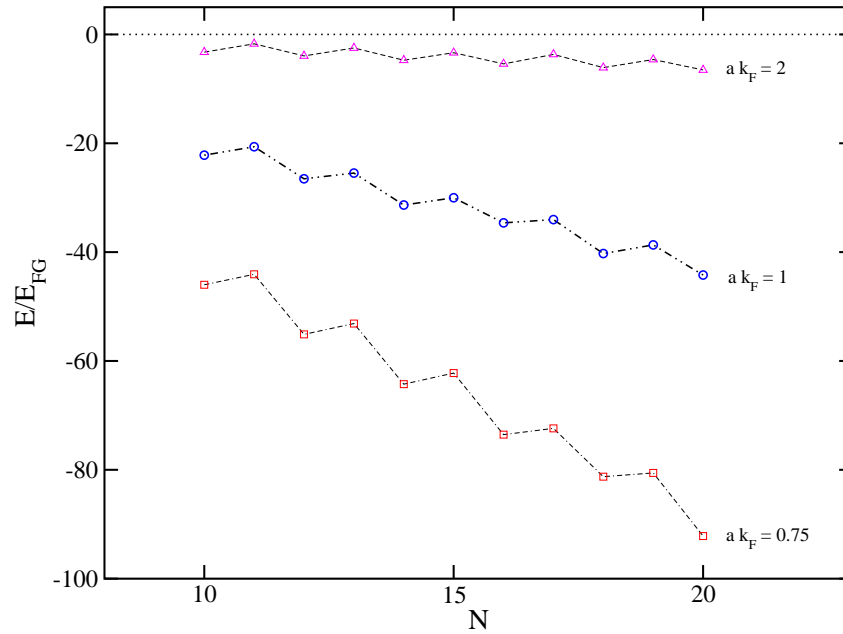
Result for $ak_F = -\infty$; Energy per particle for large N.

$$E/N = 0.422(4) E_{FG}$$

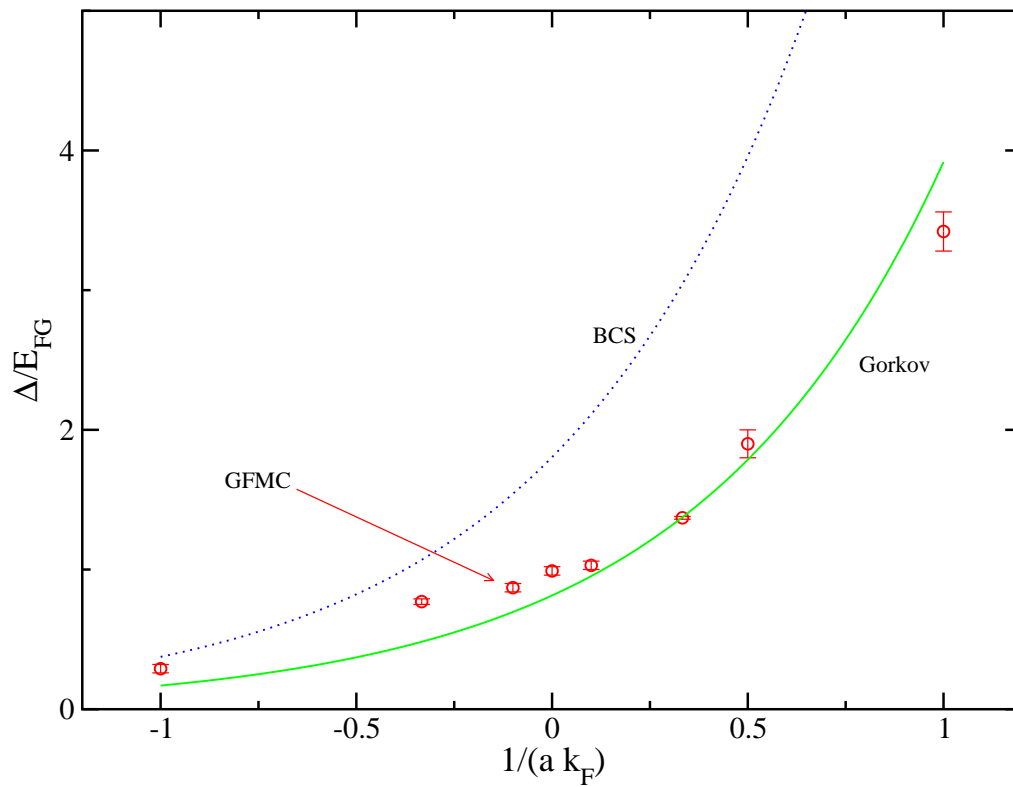
Results: $E > 0$ for various ak_F



Results: $E < 0$ for various ak_F



Comparison of Gap: GFMC, BCS and Gorkov



$$\Delta_{BCS} = \frac{8}{e^2} \epsilon_F e^{\pi/(2k_F a)}$$

$$\Delta_{Gorkov} = \left(\frac{2}{e}\right)^{7/3} \epsilon_F e^{\pi/(2k_F a)}$$

Comparison with LOCV

LOCV was first used in 1970s to study neutron matter.

LOCV is used to study unstable Bose gases.

Comparison of results: ‘cosh’ potential with δ potential.

Given a Hamiltonian of the form,

$$\mathcal{H} = -\frac{\hbar^2}{2m} \sum_{n=1}^A \nabla_n^2 + \sum_{i,j'} v(r_{ij'})$$

Use trial wave function of the form,

$$\begin{aligned} |\Psi\rangle &= \prod_{i,j'} f_{ij'} |\Phi\rangle \\ |\Phi\rangle &= \text{ground state of free fermions} \end{aligned}$$

Do the cluster expansion of $\langle \mathcal{H} \rangle$.

Include up to two-body terms.

‘healing distance’ d is defined such that,

$$f(|r| > d) = 1 \quad \text{and} \quad \frac{df}{dr}(|r| = d) = 0$$

After Euler-Lagrange minimization of energy, we have LOCV equation,

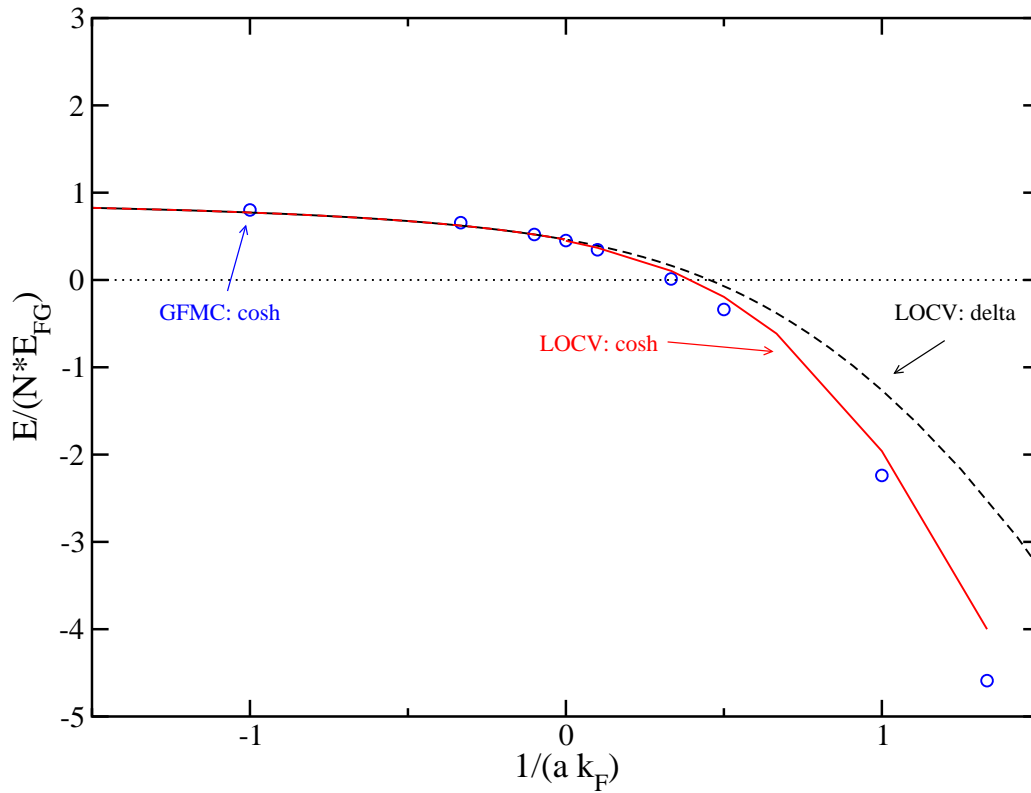
$$-\frac{\hbar^2}{m} \nabla^2 f(r) + v(r) f(r) = \lambda f(r)$$

Allow correlation between closest pair by imposing constraint,

$$\frac{\rho}{2} \int_0^d f^2(r) d^3r = 1$$

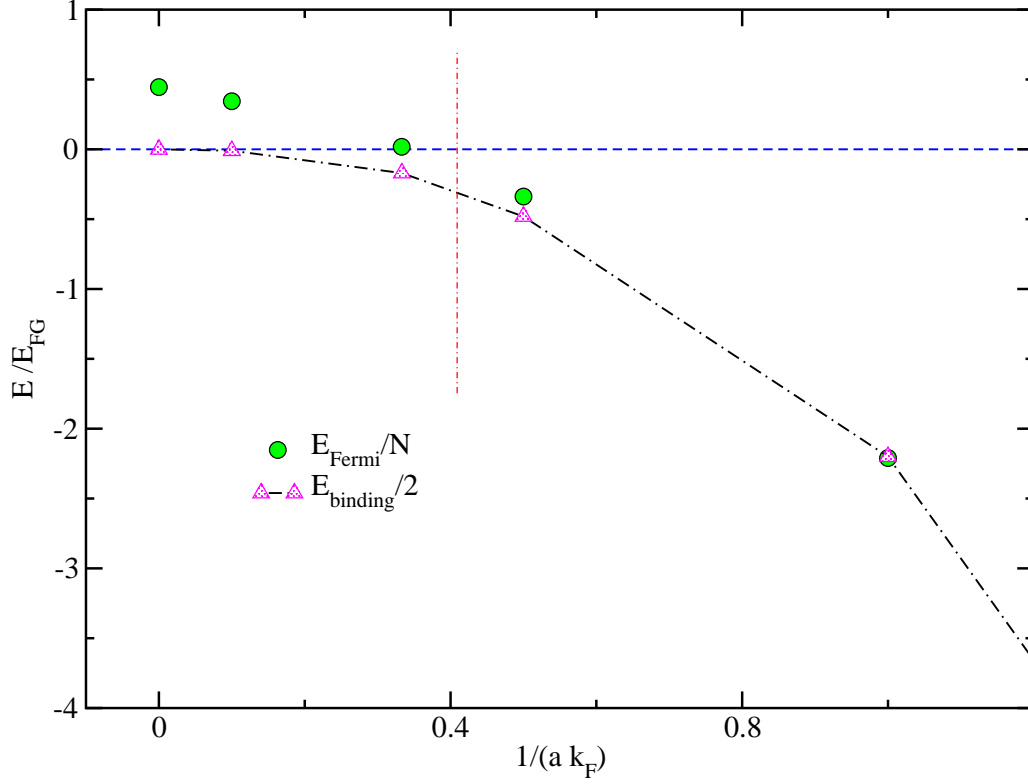
The energy per particle is given by,

$$E_{LOCV} = E_{FG} + \frac{\lambda}{2}$$

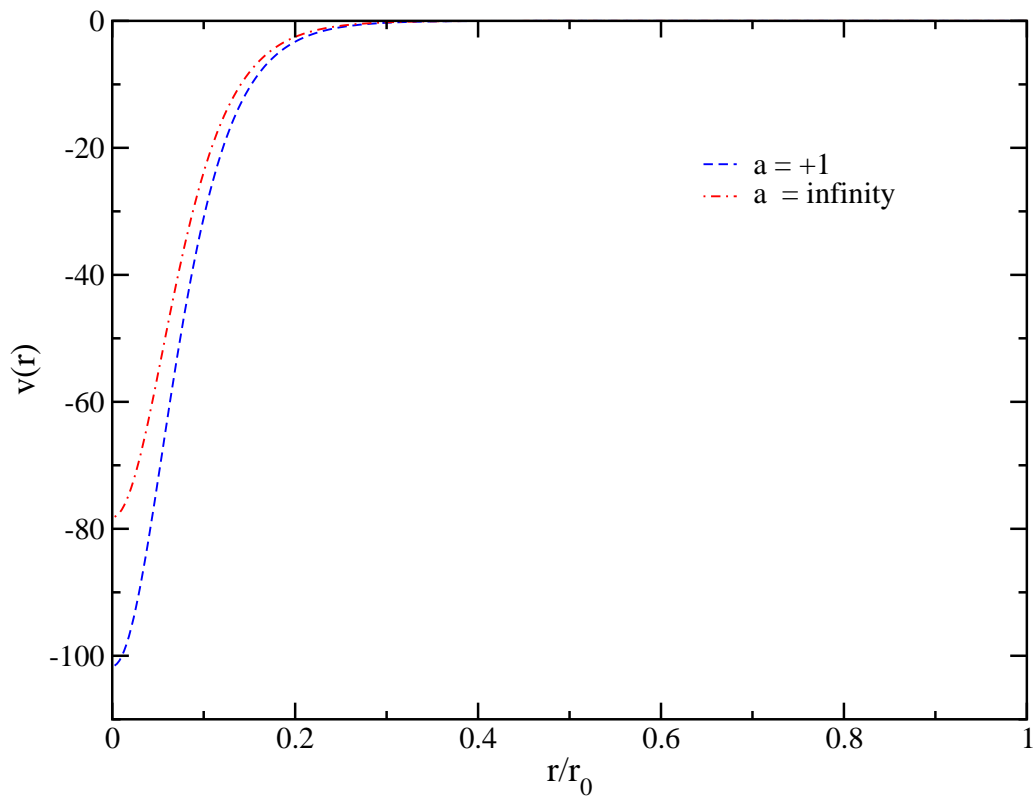
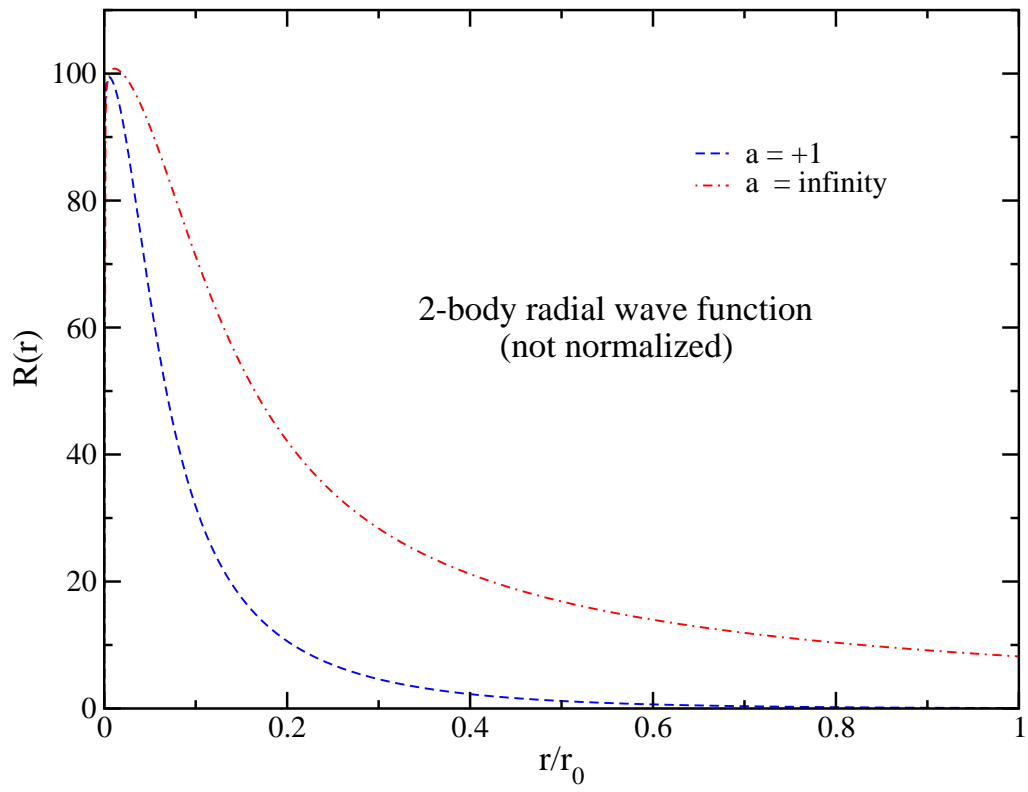


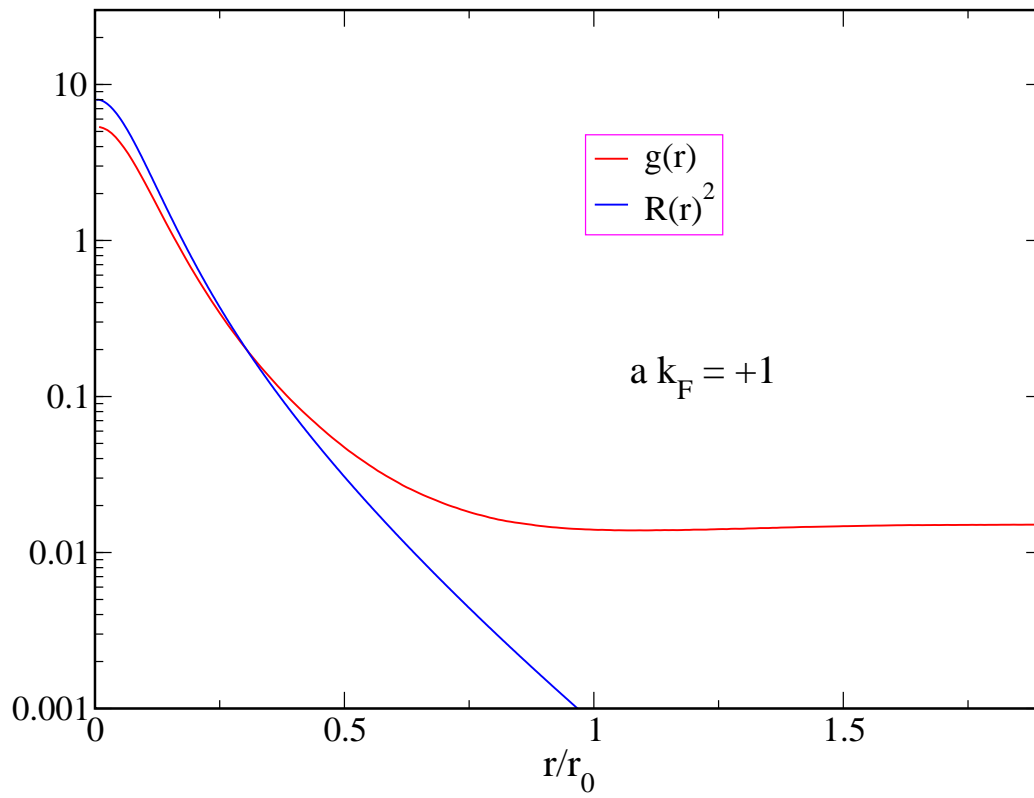
1. 'cosh' and δ potentials are almost the same for $\frac{1}{a k_F} < 0$, but they differ when $\frac{1}{a k_F} > 0$.
2. LOCV energies with 'cosh' potential are in good agreement with GFMC energies.
3. How to calculate Δ with LOCV ?

Bosonization



| $1/ak_F$ | Δ | E_{GFMC}/N | $E_{pair}/2$ | $\sqrt{\langle r^2 \rangle}/r_0$ | R_{eff}/r_0 | $R_{eff}/\sqrt{\langle r^2 \rangle}$ |
|----------|----------|--------------|--------------|----------------------------------|---------------|--------------------------------------|
| 0 | 0.9 | 0.44 | 0 | ∞ | 0.17 | |
| 0.1 | 1.0 | 0.34 | -0.01 | 3.69 | 0.16 | |
| 0.3 | 1.4 | 0.02 | -0.17 | 1.21 | 0.16 | |
| 0.5 | 1.9 | -0.34 | -0.48 | <i>0.74</i> | | <i>0.20</i> |
| 1.0 | 3.4 | -2.20 | -2.22 | <i>0.38</i> | | <i>0.37</i> |
| 1.3 | 6.2 | -4.60 | -4.63 | <i>0.28</i> | | <i>0.43</i> |
| 2.0 | 14.4 | -12.8 | -12.9 | <i>0.19</i> | | <i>0.53</i> |





2-body radial solution $R(r)^2$ vs pair correlation function $g(r)$.
(both normalized)