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:
$\rightarrow$ neutron matter at low density in the outer crust of neutron star.
$\rightarrow$ proton fraction at low density at the inner core of neutron star.
$\rightarrow$ dilute Fermi gas at low $T$, $^6\text{Li}$, $^{40}\text{K}$, etc.

interaction is ‘tunable’ through Feshbach resonance
temperature as low as $0.05T_F$ achieved
evidence of superfluidity?

Superfluidity expected at low temperature $\rightarrow$ nonzero energy gap $\Delta$.
Importance for the evolution of neutron star.
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 \( i, j, k, \ldots \)
Denote spin \( \downarrow \) particles by \( i', j', k', \ldots \)
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; \( a k_F \)
and effective range,

\[ R_{eff} = 2 \int_0^\infty \left( u_{asymp}^2(r) - u^2(r) \right) dr \]

For example, \( v_0 = 1 \) corresponds to \( a k_F = -\infty \) and \( R_{eff} = \frac{2}{\mu} \).
Work with \( \mu r_0 = 12 \), \( \mu r_0 = 24 \), and we want to approximate \( \mu r_0 \longrightarrow \infty \).
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 $\Psi_i$ 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 $\Psi_0$ by evolution in imaginary time,

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

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

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

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

$$\Psi(\tau) = e^{-(\mathcal{H}-E_T)\tau} \Psi_V(\tau = 0)$$

$$\langle \mathcal{H} \rangle_{\text{mix}} = \frac{\langle \Psi_V | \mathcal{H} | \Psi(\tau) \rangle}{\langle \Psi_V | \Psi(\tau) \rangle} = E_0, \quad \lim \tau \to \infty$$

$E_T$ is updated to keep $\langle \Psi(\tau) | \Psi(\tau) \rangle$ constant $\rightarrow$ *growth estimate*. 
Green’s Function

In general, for any value of \( \tau \) 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,

\[
\mathbf{R} = \{ r_1, r_2, \ldots, r_A \}
\]

Green’s function for short time \( \Delta \tau \),

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

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,

\[
\Psi^n(\mathbf{R}^n) = \int d\mathbf{R}^{n-1} \ldots d\mathbf{R}^0 G(\mathbf{R}^n, \mathbf{R}^{n-1}) \ldots G(\mathbf{R}^2, \mathbf{R}^1) G(\mathbf{R}^1, \mathbf{R}^0) \Psi_V(\mathbf{R}^0)
\]
Short Time Green’s Function

We need analytical expression for,

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

where,

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

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

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

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

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 \(\longrightarrow 0\) for large \(n\) (check by doubling \(n\)).

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

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

\[ \approx e^{-(V(\mathbf{R})+V(\mathbf{R}))-2E_T)\Delta \tau} \frac{\Delta \tau}{2} G_0(\mathbf{R}, \mathbf{R}') \]

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

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

$\longrightarrow$ mixed estimate and exact estimate become equal for large $\tau$,

$$\langle \mathcal{H} \rangle_{mix} = \frac{\langle \Psi_V | \mathcal{H} e^{-(\mathcal{H} - E_T)\tau} | \Psi_V \rangle}{\langle \Psi_V | e^{-(\mathcal{H} - E_T)\tau} | \Psi_V \rangle}$$

$$= \frac{\langle \Psi_V | e^{-(\mathcal{H} - E_T)\tau/2} \mathcal{H} e^{-(\mathcal{H} - E_T)\tau/2} | \Psi_V \rangle}{\langle \Psi_V | e^{-(\mathcal{H} - E_T)\tau/2} e^{-(\mathcal{H} - E_T)\tau/2} | \Psi_V \rangle}$$

$$= \frac{\langle \Psi(\tau/2) | \mathcal{H} | \Psi(\tau/2) \rangle}{\langle \Psi(\tau/2) | \Psi(\tau/2) \rangle} \rightarrow \langle \mathcal{H} \rangle_{exact} \quad \text{for large } \tau$$

In terms of the Green’s functions,

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

where,

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

And,

$$\langle \mathcal{H} \rangle_{mix} \rightarrow E_0 \quad \text{for large enough } n$$
Fermion Green’s Function Monte Carlo

First introduced by J. B. Anderson in 1975.
Integrals evaluated stochastically (Monte Carlo),

\[ \text{path}_i = \{ \mathbf{R}_i^n, \ldots, \mathbf{R}_i^0 \} \]

subscript \( (i) \) = path index

superscript \( (n) \) = time step

\[ P(\mathbf{R}_i^n, \ldots, \mathbf{R}_i^0) = \text{probability used to sample the paths} \]

\[ N_t = \text{total number of sampled paths} \]

then,

\[
\langle \mathcal{H} \rangle = \frac{\sum_{i=1}^{N_t} Np_i}{\sum_{i=1}^{N_t} Dp_i}
\]

where we have defined,

\[ Np_i = \frac{E_L(\mathbf{R}_i^n) \Psi_V(\mathbf{R}_i^n) G(\mathbf{R}_i^n, \mathbf{R}_i^{n-1}) \ldots G(\mathbf{R}_i^1, \mathbf{R}_i^0) \Psi_V(\mathbf{R}_i^0)}{P(\mathbf{R}_i^n, \ldots, \mathbf{R}_i^0)} \]

\[ Dp_i = \frac{\Psi_V(\mathbf{R}_i^n) G(\mathbf{R}_i^n, \mathbf{R}_i^{n-1}) \ldots G(\mathbf{R}_i^1, \mathbf{R}_i^0) \Psi_V(\mathbf{R}_i^0)}{P(\mathbf{R}_i^n, \ldots, \mathbf{R}_i^0)} \]

The path probability (by Kalos) is,

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

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

then path probability becomes,

\[ P(\text{path}_i) = |\Psi_V(\mathbf{R}_i^n)| G(\mathbf{R}_i^n, \mathbf{R}_i^{n-1}) \ldots G(\mathbf{R}_i^1, \mathbf{R}_i^0) |\Psi_V(\mathbf{R}_i^0)| \]
Denominator of the mixed estimate becomes,
\[
\sum_{i=1}^{N_t} N_p_i = \sum_{i=1}^{N_t} \frac{\Psi_V(R_i^n)\Psi_V(R_i^0)}{|\Psi_V(R_i^n)||\Psi_V(R_i^0)|}
\]
\[
= \sum_{i=1}^{N_t} \{ +1 \text{ or } -1 \}
\]

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

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

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

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

This means,
\[
\sum_{i=1}^{N_t} \frac{\Psi_V(R_i^n)\Psi(R_i^0)}{|\Psi_V(R_i^n)||\Psi(R_i^0)|} \rightarrow 0 \text{ for large } N_t
\]

Similarly for the numerator, assuming that \(E_L(R_i^n) \approx E_0\),
\[
\sum_{i=1}^{N_t} Dp_i = \sum_{i=1}^{N_t} \frac{E_L(R_i^n)\Psi_V(R_i^n)\Psi(R_i^0)}{|\Psi_V(R_i^n)||\Psi(R_i^0)|}
\]
\[
\approx E_0 \sum_{i=1}^{N_t} \frac{\Psi_V(R_i^n)\Psi(R_i^0)}{|\Psi_V(R_i^n)||\Psi(R_i^0)|}
\]
\[
\rightarrow 0 \text{ for large } N_t
\]

In the end, the so-called ‘Fermion Sign Problem’ of GFMC,
\[
\langle \mathcal{H} \rangle \rightarrow \frac{0}{0} \text{ for large } N_t
\]

**NOTE:** Bose ground state wave function \(\Psi_{Bose}(R) \geq 0\), hence no sign problem.
**Fixed Node GFMC**

Fermion Sign Problem appears because $\Psi_V(R_i^j)$ can change sign as the time step $j$ increases.

A remedy; ‘Fixed Node’ GFMC.

Let $\Psi_V(R_i^0) > 0$ for the initial time step.

Then constrain the path to the positive domain; $\Psi_V(R_i^j) > 0$ for all $j$.

$$|e^{-(\mathcal{H}-E \tau)\tau}|_{F_N} \Psi_V(R^+, 0) \rightarrow \Psi(R^+, \tau)$$

or

Let $\Psi_V(R_i^0) < 0$ for the initial time step.

Then constrain the path to the negative domain; $\Psi_V(R_i^j) < 0$ for all $j$.

$$|e^{-(\mathcal{H}-E \tau)\tau}|_{F_N} \Psi_V(R^-, 0) \rightarrow \Psi(R^-, \tau)$$

When the constraint is imposed with the nodal surface of the exact $\Psi_0(R)$, we get the exact $E_0$.

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

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

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

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

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

We minimize variationally Fixed Node $\langle \mathcal{H} \rangle_{mix}$. 
**Trial Wave Function $\Psi_V$**

$\Psi_V$ is used as:

$\rightarrow$ Initial guess of $\Psi_0(\mathbf{R})$.

$\rightarrow$ Importance function $I(\mathbf{R}) = |\Psi_V(\mathbf{R})|$.

$\rightarrow$ 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,

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

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

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,

$$
\Psi_{BCS} = \prod_i (u_i + v_i a_{k_i \uparrow} a_{-k_i \downarrow}^\dagger) |0\rangle
$$

$$
|u_i|^2 + |v_i|^2 = 1
$$

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

This common form of $\Psi_{BCS}$ 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 \( \Psi_{BCS} \) is given by,

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

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

**NOTE:** \( \Psi_{BCS} = \Psi_{JS} \) when \( \alpha_i = \{1, 1, \ldots, 1, 1, 0, 0, 0, \ldots \} \).

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

\[
\phi(\mathbf{r}) = \tilde{\beta}_bc(\mathbf{r}) + \sum_{i \leq i_c} \alpha_i e^{i\mathbf{k}_i \cdot \mathbf{r}}
\]

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

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

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

\[
\rightarrow \quad \Psi_{BCS} = \text{Determinant of }
\begin{pmatrix}
\phi(r_{11'}) & \phi(r_{12'}) & \ldots & \phi(r_{1(N+d)'}) & \psi_{1\uparrow}(r_1) & \psi_{2\uparrow}(r_1) \\
\phi(r_{21'}) & \phi(r_{22'}) & \ldots & \phi(r_{2(N+d)'}) & \psi_{1\uparrow}(r_2) & \psi_{2\uparrow}(r_2) \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
\phi(r_{(N+u)1'}) & \phi(r_{(N+u)2'}) & \ldots & \phi(r_{(N+u)(N+d)'}) & \psi_{1\uparrow}(r_{N+u}) & \psi_{2\uparrow}(r_{N+u}) \\
\psi_{1\downarrow}(r_1') & \psi_{1\downarrow}(r_2') & \ldots & \psi_{1\downarrow}(r_{(N+d)'}) & 0 & 0 \\
\psi_{2\downarrow}(r_1') & \psi_{2\downarrow}(r_2') & \ldots & \psi_{2\downarrow}(r_{(N+d)'}) & 0 & 0 \\
\psi_{3\downarrow}(r_1') & \psi_{3\downarrow}(r_2') & \ldots & \psi_{3\downarrow}(r_{(N+d)'}) & 0 & 0
\end{pmatrix}
\]

Variational parameters: \( b, c, \) and \( \{\alpha_0, \alpha_1, \ldots, \alpha_{i_c}\} \).

**STRATEGY:**

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

\[
\rightarrow \quad \text{best overlap with the nodal structure of the true ground state.}
\]
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 $\delta$ 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,

$$|\Psi\rangle = \prod_{i,j'} f_{ij'} |\Phi\rangle$$

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

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 $\delta$ 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 $\Delta$ with LOCV?
Bosonization

\begin{tabular}{cccccccc}
\hline
$1/a k_F$ & $\Delta$ & $E_{GFMC}/N$ & $E_{pair}/2$ & $\sqrt{<r^2>/r_0}$ & $R_{eff}/r_0$ & $R_{eff}/\sqrt{<r^2>}$ \\
\hline
0 & 0.9 & 0.44 & 0 & $\infty$ & 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 & 0.74 & 0.20 \\
1.0 & 3.4 & -2.20 & -2.22 & 0.38 & 0.37 \\
1.3 & 6.2 & -4.60 & -4.63 & 0.28 & 0.43 \\
2.0 & 14.4 & -12.8 & -12.9 & 0.19 & 0.53 \\
\hline
\end{tabular}
2-body radial wave function
(not normalized)
2-body radial solution $R(r)^2$ vs pair correlation function $g(r)$.

(both normalized)