Diagrammatic Monte Carlo

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Extensive configurational space

Complexity $\propto e^{V/V_0}$

$V$ is the configuration volume

$V_0$ is the correlation volume

$V/V_0 \sim 10^2$

Diagrams (intensive configurational space)

Complexity $= C (N!)^m$

$N \leq 10$ is the diagram order

$m \sim 1, \quad C \sim 1$

$C$ can be significantly reduced by partial summation
The issue of summability: Can an asymptotic series be regularized?

Dyson’s argument: The perturbative series has **zero convergence radius** if changing the sign of interaction renders the system pathological.

**BUT**

1. Fermions can be put on a lattice…

2. Bosons can be represented as pairs of fermions…
Feynman’s Diagrams

Generic structure of diagrammatic expansions:

\[ Q(y) = \sum_{m=0}^{\infty} \sum_{\xi_m} \int D(\xi_m, y, x_1, x_2, \ldots, x_m) \, dx_1 \, dx_2 \cdots dx_m \]

These functions are visualized with diagrams.

Example:

\[
\begin{align*}
\text{\begin{tikzpicture}
    \draw[green!70!black] (0,0) -- (4,0);
    \draw[green!70!black] (4,0) .. controls (4.5,0.5) .. (5,1);
    \draw[green!70!black] (5,0) .. controls (5.5,-0.5) .. (6,-1);
    \draw[green!70!black] (6,0) -- (0,0);
\end{tikzpicture}} & = \begin{tikzpicture}
    \draw[green!70!black] (0,0) -- (4,0);
    \draw[green!70!black] (4,0) .. controls (4.5,0.5) .. (5,1);
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    \draw[green!70!black] (6,0) -- (0,0);
\end{tikzpicture} + \begin{tikzpicture}
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\end{tikzpicture}
\end{align*}
\]
General principles of Diagrammatic Monte Carlo

Take a diagrammatic series, say the one for polaron Green’s function,

\[ \ldots \]

and interpret it as a partition function for an ensemble of graphical objects (diagrams). Introduce a Markov process generating ensemble, and calculate corresponding histograms/averages.

The Markov process is organized in the form of pairs of complementary updates. In such a pair, A-B, the update A creates a new graphical element with corresponding continuous variables, while the update B removes the element. For example, A creates a new propagator, while B removes it:
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\[ \text{= } + \text{ + } + \text{ ...} \]

and interpret it as a partition function for an ensemble of graphical objects (diagrams).
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Balancing diagrammatic Markov process by (generalized) Metropolis-Hastings algorithm

Acceptance ratios for complementary updates A-B

\[
R_A(\tilde{X}) = \frac{\text{New Diagram}}{\text{Old Diagram}} \frac{1}{W(\tilde{X})}
\]

\[
R_B(\tilde{X}) = \frac{\text{New Diagram}}{\text{Old Diagram}} W(\tilde{X})
\]

Arbitrary distribution function for generating particular values of new continuous variables in the update A.
Numerical counterpart of analytic bold-line trick: Bold(-line) Diagrammatic Monte Carlo

\[ G = G^{(0)} + G^{(0)} \Sigma G + \cdots \]

Dyson equation

\[ G = G^{(0)} + G^{(0)} \Sigma G \]

Self-consistent determination of \( G \)

The Monte Carlo process is *asymptotically* Markovian
Model of Resonant Fermions

Good for both ultracold atoms and neutron stars!

No explicit interactions—just the boundary condition:

\[ \forall i, j \text{ at } |\mathbf{r}_{i\uparrow} - \mathbf{r}_{j\downarrow}| \to 0: \quad \Psi(\mathbf{r}_{1\uparrow}, \ldots, \mathbf{r}_{N\uparrow}, \mathbf{r}_{1\downarrow}, \ldots, \mathbf{r}_{N\downarrow}) \to \frac{A}{|\mathbf{r}_{i\uparrow} - \mathbf{r}_{j\downarrow}|} + B, \quad \frac{B}{A} = c = \text{const} \]

\[ c \gg n^{1/3} \sim k_F \implies \text{BCS regime} \]

\[ |c| \ll n^{1/3} \sim k_F \implies \text{unitarity regime} \]

\[ -c \gg n^{1/3} \sim k_F \implies \text{BEC regime} \]

(In two-body problem, the parameter \( c \) defines the s-scattering length.)
Resonant Fermipolaron:

Sign alternating divergent series


Diagram elements:

- $G^{(0)}_{\downarrow}$
- $\Gamma$

$G_{\uparrow} (k > k_F)$

$G_{\downarrow} (k < k_F)$

a polaron diagram

a molecule diagram
Summability of the divergent series

Energy as a function of cutoff parameter for various summation schemes

$k_F a = 1.0$

Energy as a function of cutoff parameter for various summation schemes

bare data
Answers for fermipolaron

Energy

Effective Mass

\[ E / \xi_F \text{ vs } k_F a \]

\[ m/m \text{ vs } k_F a \]

- **Polaron**
- **Molecule**
Fermipolaron Energy by Bold Diagrammatic Monte Carlo

- Polaron lines are bold, molecule lines are not.
- Both polaron and molecule lines are bold.

Prokof’ev and Svistunov, PRB, 2008.
Observation of Fermi Polarons in a Tunable Fermi Liquid of Ultracold Atoms

André Schirotzek, Cheng-Hsun Wu, Ariel Sommer, and Martin W. Zwierlein
Department of Physics, MIT-Harvard Center for Ultracold Atoms, and Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

arXiv: 0902.302
Hubbard model

\[ H = -t \sum_{<ij>} a_{\sigma i}^+ a_{\sigma j} + U \sum_i n_{\uparrow i} n_{\downarrow i}, \quad n_{\sigma i} = a_{\sigma i}^+ a_{\sigma i} \]
Some Results for the Hubbard Model

1D

$t = 1.0$
$U = 4.0$
$\mu = -0.5$
$T = 0.3$

![Graphs showing 1D results](image)

3D

$t = 1.0$
$U = 4.0$
$\mu = 1.5$
$T = 0.5$

![Graphs showing 3D results](image)
Energy per lattice site

2D: $U = 4.0, \ \mu = -0.15$

$E_0/tV$ vs $T/t$

- Red squares: DiagMC
- Green circles: DMFT
Fermi surface

3D: $U = 4.0$, $\mu = 4.0$
Resonant Fermions at unitarity: Equation of State

\[ \frac{\mu}{E_F} \text{ vs } \frac{T}{T_F} \]

- Free fermions
- Virial expansion (order 2 in fugacity)
- Determinant MC (Burovski et al.)
- DiagMC

\[ \frac{\mu}{E_F} \text{ vs } \frac{T}{T_F} \]