DIAGRAMMATIC MONTE CARLO: WHAT HAPPENS TO THE SIGN-PROBLEM

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Outline

Ising spins vs Feynman Diagrams: Is there any difference from the Monte Carlo perspective?

Acceptable solution to the sign problem?

Polarons in Fermi systems

Yes! (so far ...)

Many-body implementation for the Fermi-Hubbard model
Feynman Diagrams: graphical representation for the high-order perturbation theory

\[ H = H_0 + H_{\text{int}} \]

\[ \langle A \rangle = \sum \frac{\langle \Psi_n | A e^{-H/T} | \Psi_n \rangle}{\sum_n \langle \Psi_n | e^{-H/T} | \Psi_n \rangle} = \langle A \rangle_0 + \langle AB \rangle_0 + \langle AC \rangle_0 + \ldots \]

\[ \propto H_{\text{int}} \quad \propto H_{\text{int}}^2 \]

explicit graphical representation for all terms and easy rules to convert graphs to math

Diagrammatic technique: explicit summation of geometric series “on-the-go” with self-consistent re-formulation of the diagrams
\[ H = \sum_{k,\sigma} (\varepsilon_k - \mu) a_{k\sigma}^\dagger a_{k\sigma} + \sum_{k\delta q, \sigma\sigma'} \mathcal{U}_q a_{k-q\sigma}^\dagger a_{p+q\sigma}^\dagger a_{p\sigma} a_{k\sigma}, \]

Configuration space = (diagram order, topology and types of lines, internal variables)
Standard Monte Carlo setup:

- configuration space (depends on the model and its representation)

- each cnf. has a weight factor

- quantity of interest $\langle A \rangle = \frac{\sum_{cnf} A_{cnf} W_{cnf}}{\sum_{cnf} W_{cnf}}$

Monte Carlo configurations generated from the prob. distribution $W_{cnf}$
\[ A(y) = \sum_{n=0}^{\infty} \sum_{\xi} \int \int \int \cdots d x_1 d x_2 K d x_n W_n(\xi; x_1, x_2, K x_n, y) = \sum_{\nu} W_{\nu} \]

Monte Carlo (Metropolis-Rosenbluth-Teller) cycle:

\[ R_{acc} \sim \frac{|W_{\nu'}|}{|W_{\nu}|} \frac{1}{P_{\nu \rightarrow \nu'}(\text{new } \{x\})} \]

Collect statistics: \[ A_{\text{counter}}(y) = A_{\text{counter}}(y) + \text{sign}(\nu) \]

sign problem and potential trouble!, but ...
Sign-problem

Variational methods
- universal
- often reliable only at T=0
- systematic errors
- finite-size extrapolation

Determinant MC
- "solves" $n_{i\sigma} + n_{i-\sigma} = 1$ case
- CPU expensive
- not universal
- finite-size extrapolation

Cluster DMFT/DCA methods
- universal
- diagram size extrapolation

Computational complexity
Is exponential: $\exp\{\# \xi\}$

Cluster DMFT
$\xi = \left( \frac{E_F}{T} \right)^L L^D$
linear size

Diagrammatic MC
$\xi = N$
diagram order

for irreducible diagrams
Further advantages of the diagrammatic technique

Calculate **irreducible** diagrams for \( \Sigma \), \( \Pi \), ... to get \( G \), \( \bar{U} \), .... from Dyson equations

\[
G(p, \tau) = \sum G_0(p, \tau) + \cdots
\]

\[
\bar{U} = \pi + \cdots
\]

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

Make the entire scheme **self-consistent**, i.e. all internal lines in \( \Sigma \), \( \Pi \), ... are “bold”
Polaron problem:

\[ H = H_{\text{particle}} + H_{\text{environment}} + H_{\text{coupling}} \rightarrow \text{quasiparticle} \]

\[ E(p = 0), \, m_*, \, G(p, t), \, ... \]

Electrons in semiconducting crystals (electron-phonon polarons)

\[ H = \sum_p \varepsilon(p) a_p^+ a_p + \sum_q \omega(p) (b_q^+ b_q + 1/2) + \sum_{pq} (V_{pq} a_{p-q}^+ a_p b_q^+ + h.c.) \]
Fermi-polaron problem:

\[ H = \frac{p^2}{2m} + H_{\text{Fermi sea}} + \int V(r - r') \, n(r') \, dr' \]

Particle dressed by interactions with the Fermi sea:
cold Fermi gases with population strong imbalance
orthogonality catastrophe, X-ray singularities, heavy fermions,
quantum diffusion in metals, ions in He-3, etc.
Examples:

Electron-phonon polarons (e.g. Frohlich model) = particle in the bosonic environment.

Too “simple”, no sign problem, $N : 10^2$

Fermi–polarons (polarized resonant Fermi gas) = particle in the fermionic environment.

Sign problem! $N_{\text{max}} = 11$
Fermi-Hubbard model: 

\[ H = -t \sum_{<ij>,\sigma} a_{i\sigma} \text{a}_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma} \]

Self-consistency in the form of Dyson, RPA

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

\[ \overline{U} = U + \Pi \]

Extrapolate to the \( N \rightarrow \infty \) limit.
1D

\[ U/t = 4 \]
\[ \mu/t = -0.5 \]
\[ T/t = 0.3 \]

![Graph showing energy versus inverse number of particles for 1D system with different resummation methods.

3D

\[ U/t = 4 \]
\[ \mu/t = 1.5 \]
\[ T/t = 0.5 \]

![Graph showing density versus inverse number of particles for 3D system with different resummation methods.

Better quality than in 1D!
In 3D temperatures are low enough $T/zt < 0.03$ to claim Fermi-liquid properties (using bare propagators so far)
3D: $U=4.0$, $\mu=1.5$

Energy $E_\sigma/tV$ vs. $T/t$ for $T/t = 0$ to $12$.

- Red squares: energy
- Green line: 2nd order high-T series
- Blue line: 8th order high-T series
- Brown line: 10th order high-T series
- Black line: $\propto T^2$ (Fermi-liquid), $\rho(\varepsilon_F)=0.087(3), \rho'(\varepsilon_F)=-0.0113(3)$
Conclusions/perspectives

• **Bold-line Diagrammatic series can be efficiently simulated.**
  - combine analytic and numeric tools
  - thermodynamic-limit results
  - sign-problem tolerant (relatively small configuration space)

• **Work in progress:** bold-line implementation for the Hubbard model and the resonant Fermi-gas (\( G \Gamma \) version) and the continuous electron gas, or jellium model (screening version).

• **Next step:** Effects of disorder, broken symmetry phases, additional correlation functions, etc.