DIAGRAMMATIC MONTE CARLO APPLICATIONS

Polarons

Path-integrals

Resonant fermions & Neutron stars

Fermi Hubbard model

Frustrated Quantum magnetism

Tallahassee, NHMFL (January 2012)
Lattice path-integrals for bosons and spins are “diagrams” of closed loops!

\[
Z = \text{Tr} \ e^{-\beta H} \equiv \text{Tr} \ e^{-\beta H_0} \ e^{\int_0^\beta H_1(\tau) \ d\tau} \\
= \text{Tr} \ e^{-\beta H_0} \left\{ 1 - \int_0^\beta H_1(\tau) \ d\tau + \int_0^\beta \int_0^\beta H_1(\tau) \ H_1(\tau') \ d\tau \ d\tau' + \ldots \right\}
\]
Simulating Bose-Hubbard model “as is” and comparing to experiments: (in this example, $N \approx 300000$)

Nature Physics, 6, 998–1004, (2010)
It is realistic to do about 2,000,000 or more particles at temperatures relevant for the experiment.

\[ U/zt = 4 \]
\[ T/t = 2.4 \]
\[ V/t = 0.0033 \]
Path-integrals in continuous space; He-4 case

\[ Z_{WA} = \iiint dR_1 \ldots dR_P \exp \left\{ - \sum_{i=1}^{P=\beta/\tau} \left( \frac{m(R_{i+1} - R_i)^2}{2\tau} + U(R)\tau \right) \right\} + G \]

\[ R_i = (r_{i,1}, r_{i,2}, \ldots, r_{i,N}) \]
Superfluid density: 2D & 3D He-4

\[ \rho_s = \frac{T\langle W^2 \rangle}{Ld} \]

Ceperley, Pollock '87

2D @ \((n = 0.0432 \, A^{-2})\)

\[ T_C = 0.65(1) \]
$T_C^{Aziz} = 2.193 \quad \text{vs} \quad T_C^{\text{exp}} = 2.177$
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-phononon polarons)

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

\( \text{electron} \quad \text{phonons} \quad \text{el.-ph. interaction} \)
$$H = \sum_p \varepsilon(p) a_p^+ a_p + \sum_q \omega(p)(b_q^+ b_q + 1/2) + \sum_{pq} \left( V_{q} a_{p-q}^+ a_p b_q^+ + h.c. \right)$$

**electron**

$$e^{-\varepsilon(p_i)(\tau'_1 - \tau_1)}$$

**phonons**

$$e^{-\omega(q)(\tau'_1 - \tau_1)}$$

**el.-ph. interaction**

$$V_{q_i}$$

**Green function:**

$$G(p, \tau) = \langle a_p(0) a_p^+ (\tau) \rangle = \langle a_p e^{-\tau H} a_p^+ e^{\tau H} \rangle$$

= Sum of all Feynman diagrams

Positive definite series in the \((p, \tau)\) representation
Analysing data: \( G(p, \tau \to \infty) \to Z_p e^{-E(p)\tau} \)

\[ Z_p = |C_p|^2 \quad \text{probability of getting a bare electron} \]

\[ |E_p\rangle = C_p a_p^\dagger |0\rangle + \sum_q C_{p,q} b_q^\dagger a_{p-q}^\dagger |0\rangle + \sum_{q_1q_2} C_{p,q_1,q_2} b_{q_1}^\dagger b_{q_2}^\dagger a_{p-q_1-q_2}^\dagger |0\rangle + \ldots \]

\[ \ln G_p(\tau) \]

\[ Z_p^{(2)} = \sum_{q_1,q_2} |C_{p,q_1,q_2}|^2 \quad \text{probability of getting two phonons in the polaron cloud} \]
FIG. 4. Bottom of the polaron band $E_0$ as a function of $\alpha$. The error bars are much smaller than the point size.

FIG. 8. The average number of phonons in the polaron ground state as a function of $\alpha$. Filled circles are the MC data (calculated to the relative accuracy better than $10^{-3}$), the dashed line is the perturbation theory result (4.1), and the solid line is the parabolic fit for the strong coupling limit.
Fermi-polaron = particle dressed by interactions with the Fermi sea; orthogonality catastrophe, X-ray singularities, heavy fermions, quantum diffusion in metals, ions in He-3, etc
Cold resonant Fermi gases: resonant interaction

Fermionic quasiparticle (polaron)
\[ E_p(k) = E_p + \frac{k^2}{2m_p} \]
+ quasiparticle residue

Bosonic quasiparticle (molecule)
\[ E_M(k) = E_M + \frac{k^2}{2m_M} \]
+ quasiparticle residue
Resonant Fermions

Universal results in the zero-range, $k_F r_0 \to 0$, and thermodynamic limit
Build diagrams using ladders:

(contact potential)

$$\Gamma^{(0)} \rightarrow U \rightarrow G^{(0)}$$

$$\Sigma = \quad + \quad +$$

$$\Pi = [ \quad - \quad ] \quad + \quad +$$

In terms of “exact” propagators

Dyson Equations:

$$\rightarrow = \rightarrow + \Sigma$$

$$\rightarrow = \rightarrow + \Pi$$
For the rest:

- develop an ergodic algorithm sampling diagrams for $\Sigma_\downarrow$ and $\Sigma_{\text{mol}} = \Pi$ which are proper self-energies for polarons and molecules (an appropriate Worm Algorithm does the job)

- calculate self-energies to higher and higher order (up to 11-th)
$k_F a = 1.0$

Riesz, $\delta = 4$

Riesz, $\delta = 2$

Cesaro

homemade
Polaron spectrum from the \( G_{\downarrow}(p, \omega) \) pole: \( \omega - p^2 / 2m - \Sigma(p, \omega) = 0 \)

In imaginary time representation: \( E - p^2 / 2m - \int_0^\infty \Sigma(\mu_{\downarrow}, p, \tau)e^{(E-\mu_{\downarrow})\tau}d\tau = 0 \)

\[
E_p, E_M = -\frac{1}{ma^2} - \epsilon_F + \frac{2\pi a_{M\uparrow}}{(2/3)m}n_{\uparrow} \quad (k_F a \ll 1)
\]

\( a_{M\uparrow} = 1.18a \) \quad Skorniakov, Ter-Martirosian ‘56
Unpolarized system at unitarity: BCS-BEC crossover

Unitary gas: \( k_F a_S \rightarrow \infty \) when \( k_F \) and \( \varepsilon_F \) are the only length/energy scales
Answering Weinberg’s question: cold atoms solve neutron stars

MIT group: Martin Zwierlein, Mark Ku, Ariel Sommer, Lawrence Cheuk, Andre Schirotzek

Uncertainty due to location of the $\alpha_s = \infty$ resonance $B = 834 \pm 1.5 \, G$

BDMC results
Kris Van Houcke, Felix Werner, Evgeny Kozik, Boris Svistunov, NP

Ideal Fermi gas

Virial expansion (3d order)
Before resummation the data are not nice looking!
Extrapolation to the infinite diagram order for density ($\beta \mu = 1$)

- First order – Haussmann, Zwerger
- Including 3rd order (fully dressed)
- Controls contributing diagram orders
  (the left-most point is effectively order 9 – millions of skeleton diagrams)
Popov-Fedotov trick

Heisenberg model: \( H = \sum_{ij} J_{ij} S_i \cdot S_j = \sum_{ij} J_{ij} \left( f_{i\alpha}^{\dagger} \sigma_{\alpha\beta} f_{i\beta} \right) \cdot \left( f_{j\alpha}^{\dagger} \sigma_{\gamma\delta} f_{j\beta} \right) \)

- Dynamically, physical config. remains physical at all times

- Empty and doubly occupied sites decouple from physical sites and each other

- Projecting out unphysical Hilbert space in statistics of \( Z = Tr_f e^{-H_f/T} \)

\[
Z_S = Tr_f e^{-\frac{H_f}{T}} = \sum_{ij} J_{ij} \left( \int d\tau f_{i\alpha}^{\dagger} \sigma_{\alpha\beta} f_{i\beta} \right) \cdot \left( \int d\tau f_{j\alpha}^{\dagger} \sigma_{\gamma\delta} f_{j\beta} \right) - \mu \sum_{n_{i\tau}} \left( n_{j\alpha} - 1 \right)
\]

with complex \( \mu = i\pi T / 2 \)

Now: \( Z_S = Tr_f e^{-\frac{H_f}{T}} \), i.e. one number does the job!

Auxiliary gauge field \( \varphi_{i\tau} \)
Proof of \( Z_S = Tr_f e^{-H_f/T} \)

\[
Tr_f e^{-H_f/T} = Z_S + \sum_{K=0}^{N} C^K \sum_{\xi_K} Z_S^{(\xi_K)}
\]

Number of unphysical sites with \( n=2 \) or \( n=0 \)

Partition function of the unphysical site

Configuration of unphysical sites

\[
C = \sum_{n=0,2} e^{\mu(n-1)/T} = e^{-i\pi/2} + e^{i\pi/2} = 0
\]

\[
H_f = H_0 + H_{\text{int}} = -\frac{i\pi T}{2} \sum_{j\alpha} (n_{j\alpha} - 1) + \sum_{ij} J_{ij} \left( f_{i\alpha}^\dagger \sigma_{\alpha\beta} f_{i\beta} \right) \cdot \left( f_{j\alpha}^\dagger \sigma_{\gamma\delta} f_{j\beta} \right)
\]
Main quantity of interest is magnetic susceptibility

\[ \chi = \frac{\mathcal{H}}{1 + \mathcal{Y} g \mathcal{H}} \]
Preliminary data; BDMC up to order 4 for triangular lattice Heisenberg anti-ferromagnet.

1. Sign-blessing works
2. Self-consistency prevents divergence
3. Careful cooling is required for $T \ll T_{MF}$

= linked cluster expansion
Rigol, Bryant, Singh ‘07
Generalizations: Arbitrary spin model
Arbitrary lattice boson model with \( n < \text{MAX} \)
Diagrammatics with expansion on \( t \), not \( U \)!

Prise to pay: diagrammatic elements with many “legs”

If nothing else, definitely good for Nature cover!
Diagrammatic Monte Carlo in the generic many-body setup

1. Stochastic summation of connected Feynman diagrams for self-energy
   \( \xi(\ ) \) controls the typical diagram order

\[ G^{\uparrow}(p,\tau) \quad U(q) \quad G^{\downarrow}(p,\tau) \]

2. Self-consistent feed-back in the form of Dyson, T-matrix, RPA, etc. Eqs.

\[ G^{\downarrow} = G^{(0)} + G^{(0)} \sum \] e.g.

3. Extrapolation to \( \xi \rightarrow \infty \) (asymptotic and divergent series can be dealt with)
Bare series convergence:
yes, after order 4

\[ E(T) - E(0) = \left( \rho_F + \rho_F E_F \right) \frac{\pi^2 T^2}{6} \]

\[ n(T) - n(0) = \rho_F \frac{\pi^2 T^2}{6} \]
2D Fermi-Hubbard model in the Fermi-liquid regime

Comparing DiagMC with cluster DMFT (DCA implementation)

\[ U/t = 4 \]
\[ \mu/t = 3.1 \rightarrow n \approx 1.2 \]
\[ T/t \geq 0.4 : \quad E_F / 10 \]

\[ \Sigma(\omega_0 = \pi T, p_x = p_y) \]
3D Fermi-Hubbard model in the Fermi-liquid regime

\[ U / t = 4 \]
\[ (\mu - nU) / t = 1.5 \rightarrow n \approx 1.35 \]
\[ T / t \geq 0.1 : E_F / 50 \]

DiagMC vs high-T expansion in \( t / T \)
(up to 10-th order)
Conclusions/perspectives

The crucial ingredient, the sign blessing phenomenon, is present in all models (so far)

BDMC for skeleton graphs works all the way to the critical point in strongly correlated Fermi systems

"Higher-level" self-consistent formulations; 3-point vertex to begin with

New models & broken phases, i.e. nothing is off the table ...