Квантовые методы Монте Карло в теории коррелированных систем

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LDA+DMFT framework (beginning)

LDA+DMFT V2O3 quasiparticle bands obtained by truncating the self-energies. The left-hand panel gives the eigenvalues of the renormalized Hamiltonian and the right-hand side gives the pure $eg$ black and $a1g$ dashed green band structure (from PhysRevB_76_085127)

A. Lichtenstein, et. al. PRB, 57, 6884 (1998)
Models systems

What is CT-QMC for?

Lattice too complicated

Impurity model

Atom too simple
DMFT impurity problem

\[ S_{imp} = \sum_{\omega, \sigma} (\Delta_\omega - \mu - i\omega) c_{\omega, \sigma}^* c_{\omega, \sigma} + U \int_0^\beta n_{\uparrow \tau} n_{\downarrow \tau} d\tau \]

\[ g_\omega = \sum_k \frac{N^{-1}}{g_\omega^{-1} - \epsilon_k + \Delta_\omega} \]

\[ G_{\omega k} = \frac{1}{g_\omega^{-1} - \epsilon_k + \Delta_\omega} \]
Beyond DMFT

- DMFT is the best local approximation
- Going nonlocal means either cluster flavors of DMFT or expansion around DMFT
- Collective excitations are essentially nonlocal
- Vertex parts (or, equally, many-particle Green's function) of the impurity problem needed

**Dual ladder diagram for magnons**

Annals of Physics 327 1320 (2012)
Mathematics behind Monte-Carlo methods

In Monte-Carlo methods, statistical and/or quantum average is replaced with an average over Markov random walk

\[ \langle G \rangle = \frac{G_K w_K}{w_K} \]

Here random walk is performed over certain ensemble of auxiliary systems \( \{K\} \); we should be able to calculate \( G_K \) and prove the above equality.

For classical Metropolis Monte-Carlo \( \{K\} \) is an ensemble of possible coordinates \( \{x\} \).

For world-line Monte-Carlo \( \{K\} \) is an ensemble of imaginary-time trajectories \( \{x(\tau)\} \).

For Hirsch-Fye scheme \( \{K\} \) is an ensemble of auxiliary spins

Algorithms can differ in the ensemble \( \{K\} \) and in the Markov matrix.
Optimal sampling

Averages are estimated stochastically

\[
\langle G \rangle = \frac{\sum_K w_K G_K}{\sum_K w_K} = \frac{w_K G_K p_K^{-1}}{w_K p_K^{-1}}
\]

Minimization of the variance

\[
(w_K (G_K - \langle G \rangle) p_K^{-1})^2 = \min, \quad \sum_K p_K = 1
\]

Gives

\[
p_K \propto |w_K (G_K - \langle G \rangle)|
\]

The most known is so-called importance sampling

\[
p_K \propto |w_K|
\]
Elementary moves satisfy

1) Detailed balance
   (if one tries to go from $K$ to $K'$, he also tries moves from $K'$ to $K$)

2) Metropolis acceptance criterion

\[
p_{K \rightarrow K'} = \min \left( \frac{p'_K}{p_K}, 1 \right)
\]

Normally, $K$ and $K'$ are ``similar''.

+ easy calculation of $p_{K \rightarrow K'}$
+ good acceptance rate
- autocorrelations

\[
\delta G \approx \sqrt{\frac{D^2(G') N_{\text{autocorr}}}{N}}
\]
Fermionic algorithms prior to CT-QMC

Hubbard-Stratonovich transformation:
  - R. L. Stratonovich, 1957
  - J. Hubbard, 1959

Discrete transformation:

\[ e^{-\delta \tau U \hat{n}_\uparrow \hat{n}_\downarrow + \hat{A}} \approx \frac{1}{2} \sum_{s=\pm 1} e^{s \sqrt{\delta \tau U} (\hat{n}_\uparrow - \hat{n}_\downarrow) - \delta \tau U (\hat{n}_\uparrow + \hat{n}_\downarrow) + \hat{A}} \]

No time discretisation:
Interaction expansion

The series always converges for a finite fermionic system at finite temperature.

Idea of algorithm is to perform a random walk in the space of \{k, (arguments of integrals)\}.

Optimizing the average sign

"Trivial" sign problem:

Idea of solution:

For real-time evolution, no solution of the sign (phase) problem is known.
Random walk in K-space

Call state K the set

\[ K = k, t_1 \ldots t_k, r_1 \ldots r_k \]

and perform a random walk with probability density

\[ p(K) \propto Z_K = SpTW_0(\tau_1, r_1) \cdots W_0(\tau_k, r_k) \]

Trace here can be explicitly calculated from the Wick theorem \((H_0 \text{ is Gaussian!})\)

\[ \langle Tc_1^\dagger \cdots c_k^\dagger c_k \rangle = \det ||g_{ij}|| \]

It is possible to prove that for such an ensemble

\[ G = \overline{g_0}, \text{ or } \langle Tc^\dagger(\tau)c(\tau') \rangle \geq \langle Tc^\dagger(\tau)c(\tau') \rangle_0 \]
Random walk in K-space

Call state $K$ the set

$$K = k, t_1 ... t_k, r_1 ... r_k$$

and perform a random walk with probability density

$$p(K) \propto Z_k = \text{Sp}TW_0(\tau_1, r_1)...W_0(\tau_k, r_k)$$

Trace here can be explicitly calculated from the Wick theorem ($H_0$ is Gaussian!)

$$< Tc_1^{\dagger}c_1...c_k^{\dagger}c_k = \det ||g_{ij}||$$

It is possible to prove that for such an ensemble

$$G = \bar{g}_0, \text{ or } < Tc^{\dagger}(\tau)c(\tau') >= < Tc^{\dagger}(\tau)c(\tau') >_0$$
**Strong-coupling expansion**

\[ S = S_{at} + \Delta_{\tau-\tau'}s_{s's'} c_{s\tau}^\dagger c_{s'\tau'} \]

The idea is to expand in hybridization.

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"Метод интегрирования по траекториям ... фактически никогда не был полезен при рассмотрении вырожденных Ферми-систем"

Р. Фейнман, А.Хиббс

Квантовая механика и интегралы по траекториям
Calculation with different CT-QMC schemes
Optimum sampling

\[ w_K = 0 \]

\[ w_K G_K \neq 0 \]

Recall

\[ < G >= \frac{\sum_K w_K G_K}{\sum_K w_K} = \frac{w_K G_K p_K^{-1}}{w_K p_K^{-1}} \]

Importance sampling

\[ p_K \propto |w_k(G_K - < G >)| \approx |w_k| \]

Better take

\[ p_K \propto |w_k(G_K - < G >)| \approx |w_k| \sqrt{G_K^2 + 1} \]
**Speeding up:**

**Fast updates**

\[
(A + x \cdot y)^{-1} = A^{-1} - \frac{A^{-1}x \cdot yA^{-1}}{1 + (yA^{-1}x)}
\]

**Krylov method**
DMFT phase diagram of Hubbard model
DF calculation of "paramagnetic" pseudogap in Hubbard model
Applications

DF calculation of Fermi arcs in doped Hubbard model

\[ b=80 \quad U=2 \quad t=0.25 \quad t'=-0.3t \quad \text{doing 10\%} \]
Studies of a Kondo lattice model

The single-particle excitation spectrum for $J = 0.3$ and $n_c = 0.9$ at (a) $T = 0.25$ and (b) $T = 0.0025$

Real materials, multiorbital models

Momentum resolved spectral function calculated for BaFe$_2$As$_2$

Applications

DF calculation of Fermi arcs in doped Hubbard model

\[ b=80 \ U=2 \ t=0.25 \ t'=-0.3t \] doing 10%
Main problems at the moment:
- more effective multiorbital algorithms
- real-time CT-QMC

For a review:
E. Gull, A.J. Millis, A.I. Lichtensten, A.N. Rubtsov, M.Troyer, Ph. Werner
Continuous-time Monte Carlo methods for quantum impurity models
Reviews Of Modern Physics – 2011 – V.83 P.349