Determinantal Quantum Monte Carlo solver for Cluster Perturbation Theory

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\[ A(k, \omega) = \sum_n |\langle n | c_k | G \rangle|^2 \delta(\omega + (E_n - E_G)) \]

\[ A^< (k, \omega) = \sum_n |\langle n | c_k^\dagger | G \rangle|^2 \delta(\omega - (E_n - E_G)) \]

\[ A^< (k, \omega) + A^> (k, \omega) = A(k, \omega) \]

photoemission:

Sobota, He, Shen, RMP 2021
How to calculate?

- Semi-analytical/perturbative methods (e.g. FLEX)
  - Low computational cost, high momentum resolution, low temperatures.
  - Approximate. Questionable validity for intermediate/strongly interacting systems.
- Finite cluster methods (e.g. DQMC, ED)
  - Exact.
  - High computational cost. Limited cluster size/momentum resolution, limited temperatures.

Moukouri et al, PRB 2000

\[
\begin{align*}
U/t=4, \langle n \rangle = 1, T/t=0.2
\end{align*}
\]
How to calculate?

- **Semi-analytical/perturbative methods (e.g. FLEX)**
  - Low computational cost, high momentum resolution, low temperatures.
  - Approximate. Questionable validity for intermediate/strongly interacting systems.

- **Finite cluster methods (e.g. DQMC, ED)**
  - Exact.
  - High computational cost. Limited cluster size/momentum resolution, limited temperatures.

- **Embedding methods (e.g. CDMFT, DCA, CPT)**
  - “Exact at short-range, approximate at long-range”
Cluster perturbation theory (CPT)

\[ \mathcal{H} = \sum_{\mathcal{C}} \mathcal{H}^C + \sum_{ij\sigma} h_{ij}^b c_{i\sigma}^\dagger c_{j\sigma} \]

Cluster perturbation theory (CPT)

\[ \mathcal{H} = \sum_c \mathcal{H}^c + \sum_{ij\sigma} h^b_{ij} c^\dagger_{i\sigma} c_{j\sigma} \]

\[ G(z) = \frac{G^c(z)}{I - h^b G^c(z)} \]

- Exact at U=0.

\[ G^c(z) = \frac{1}{z - h^c} \]

\[ G(z) = (z - h^c - h^b)^{-1} = \frac{1}{z - h} \]

- Exact at t=0.
Solving $H^c$ to obtain $G^c$

- **Exact diagonalization (ED):**
  - Limited to ~16 site clusters.
  - Zero temperature. Finite temperature limited to fewer sites.

- **Time-dependent DMRG (Yang, Feiguin, PRB 2016):**
  - Restricted to narrow ladder geometries

- **DQMC:**
  - Larger system sizes (~100s) possible.
  - Finite temperature
  - Possible to handle problems difficult for ED (e.g. Holstein model)
DQMC solver for CPT (CPT+DQMC)

1. DQMC: \[ G_{r,r',t'}^c(\tau) = -\left< c_{r\sigma}(\tau) c_{r',\sigma}^\dagger \right> \]

2. Fourier transform: \[ G_{r,r',i\omega_n}^c(i\omega_n) = \int_0^\beta d\tau \ e^{i\omega_n \tau} G_{r,r',t'}^c(\tau) \]


4. CPT. \[ G(k, z) = \frac{1}{N_c} \sum_{r,r'} e^{-ik(r-r')} \left[ \frac{G_c^c(z)}{I - \tilde{h}^b G_c^c(z)} \right]_{r,r'} \]

5. MaxEnt \[ G(k, i\omega_n) = \int d\omega \ \frac{A(k, \omega)}{i\omega_n - \omega} \]
Benchmarking: attractive Hubbard model, SC phase

- Sign-free DQMC simulations.
- $s$-wave SC with KT transition at $T_c/t \approx 0.14$ for $U/t = -4$, $\langle n \rangle = 0.6$
Benchmarking: attractive Hubbard model, SC phase

$U/t = -4$

$\langle n \rangle \approx 0.63$

$T/t = 1/12$
Benchmarking: half-filled repulsive Hubbard model

U/t = 8
<n> = 1
T/t = 1/16

(a) DQMC 12 x 12

(b) CPT+DQMC 4 x 4

(c) CPT+DQMC 8 x 8
Doped repulsive Hubbard model: $A(k, \omega = 0)$

$U/t = 8$
$\langle n \rangle \approx 0.94$
Summary

● Advantages over DQMC:
  ○ Continuous momentum resolution
  ○ Smaller clusters
    ■ Reduced sign problem
    ■ Lower computational cost

● Advantages over CPT+ED:
  ○ Larger system sizes/reduced finite-size effects
  ○ Temperature dependence
  ○ Handles multi-orbital models, el-ph models, etc more easily

Next steps:

● Pseudogap
● Apply better methods of analytic continuation
● Apply to more models