Determinantal Quantum Monte Carlo solver for Cluster Perturbation Theory

Edwin Huang
with: Shuhan Ding, Jiarui Liu, Yao Wang

Phys. Rev. Research **4**, L042015 (2022)

ILLINOIS

UNIVERSITY OF NOTRE DAME

TACC

CLEMSON UNIVERSITY SOUTH CAROLINA 1889

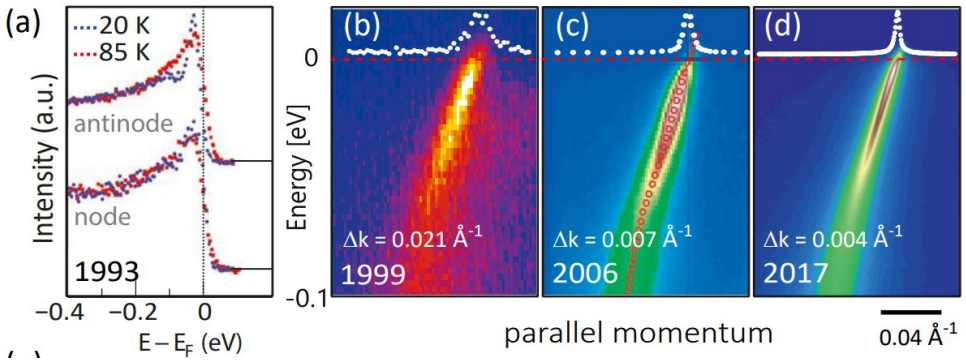
A(k, ω)

$$A^{<}(k,\omega) = \sum_n |\langle n|c_k|G\rangle|^2 \delta(\omega + (E_n - E_G))$$

$$A^{>}(k,\omega) = \sum_n |\langle n|c_k^{\dagger}|G\rangle|^2 \delta(\omega - (E_n - E_G))$$

$$A^{<}(k,\omega) + A^{>}(k,\omega) = A(k,\omega)$$

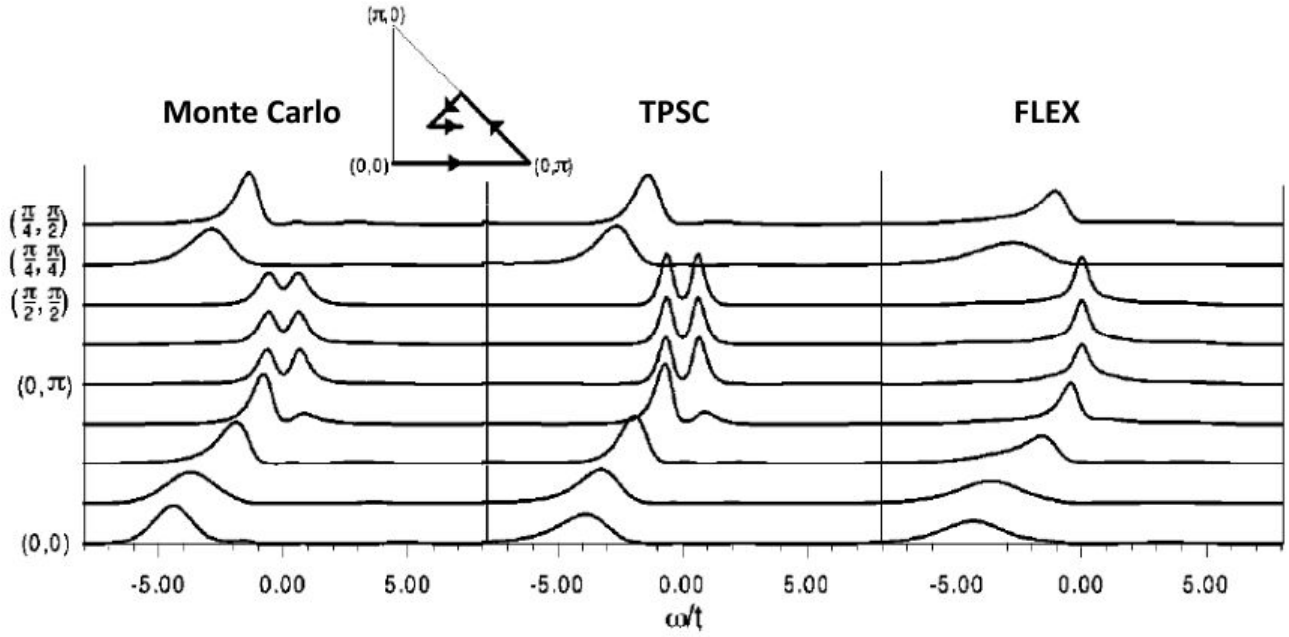
photoemission:



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.

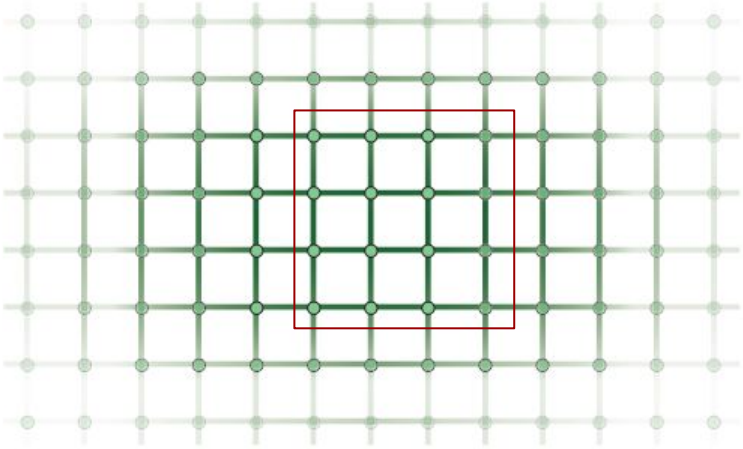


U/t=4, <n>=1, T/t=0.2

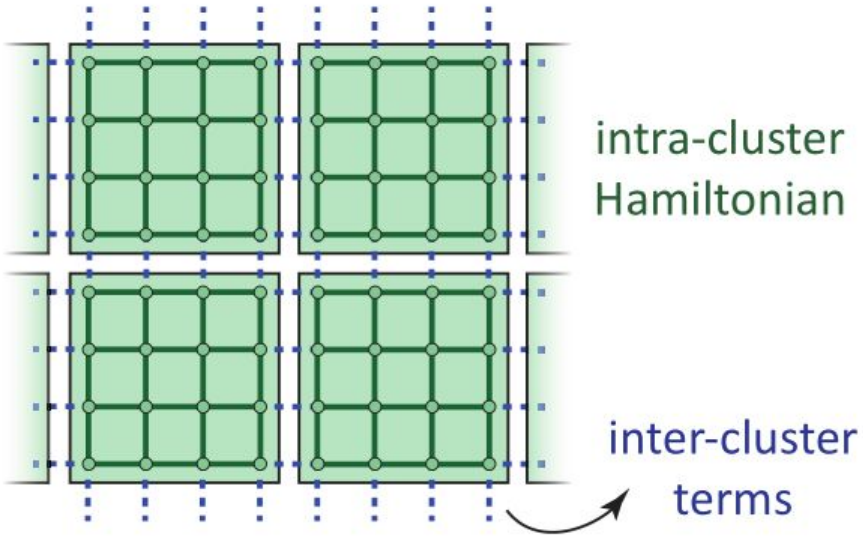
Moukouri et al, PRB 2000

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)



$$\mathcal{H} = \sum_{\mathcal{C}} \mathcal{H}^{\mathcal{C}} + \sum_{ij\sigma} h^{b}_{ij} c^{\dagger}_{i\sigma} c_{j\sigma}$$

[12] S. Pairault, D. Sénéchal, and A.-M. Tremblay, Phys. Rev. Lett. **80**, 5389 (1998).
[13] D. Sénéchal, D. Perez, and M. Pioro-Ladrière, Phys. Rev. Lett. **84**, 522 (2000).
[14] D. Sénéchal, D. Perez, and D. Plouffe, Phys. Rev. B **66**, 075129 (2002).
[15] D. Sénéchal, in *Strongly Correlated Systems* (Springer, 2012) pp. 237–270.

Cluster perturbation theory (CPT)

$$\mathcal{H} = \sum_{\mathcal{C}} \mathcal{H}^{\mathcal{C}} + \sum_{ij\sigma} h^b_{ij} c^\dagger_{i\sigma} c_{j\sigma}$$

$$\mathbf{G}(z) = \frac{\mathbf{G}^c(z)}{\mathbf{I} - \mathbf{h}^b \mathbf{G}^c(z)}$$

- Exact at U=0.

$$\mathbf{G}^c(z) = \frac{1}{z - \mathbf{h}^c}$$

$$\mathbf{G}(z) = (z - \mathbf{h}^c - \mathbf{h}^b)^{-1} = \frac{1}{z - \mathbf{h}}$$

- Exact at t=0.

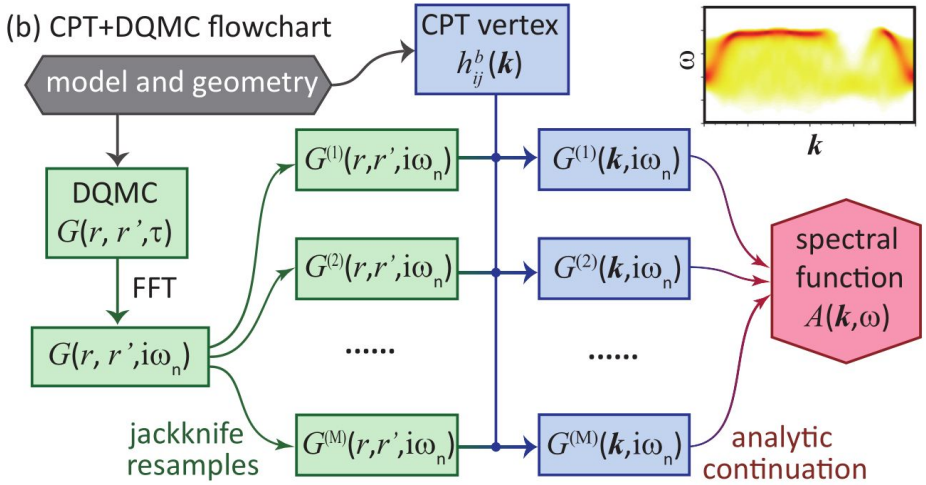
Solving H^c to obtain G^c

- 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: $G^{c}_{rr'}(\tau) = -\left\langle c_{r\sigma}(\tau) c^{\dagger}_{r'\sigma} \right\rangle$

2. Fourier transform: $G^{c}_{rr'}(i\omega_n) = \int_0^\beta \mathrm{d}\tau \, e^{i\omega_n \tau} G^{c}_{rr'}(\tau)$

3. Jackknife resample.

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

5. MaxEnt $G(k, i\omega_n) = \int \mathrm{d}\omega \, \frac{A(k,\omega)}{i\omega_n - \omega}$

Benchmarking: attractive Hubbard model, SC phase

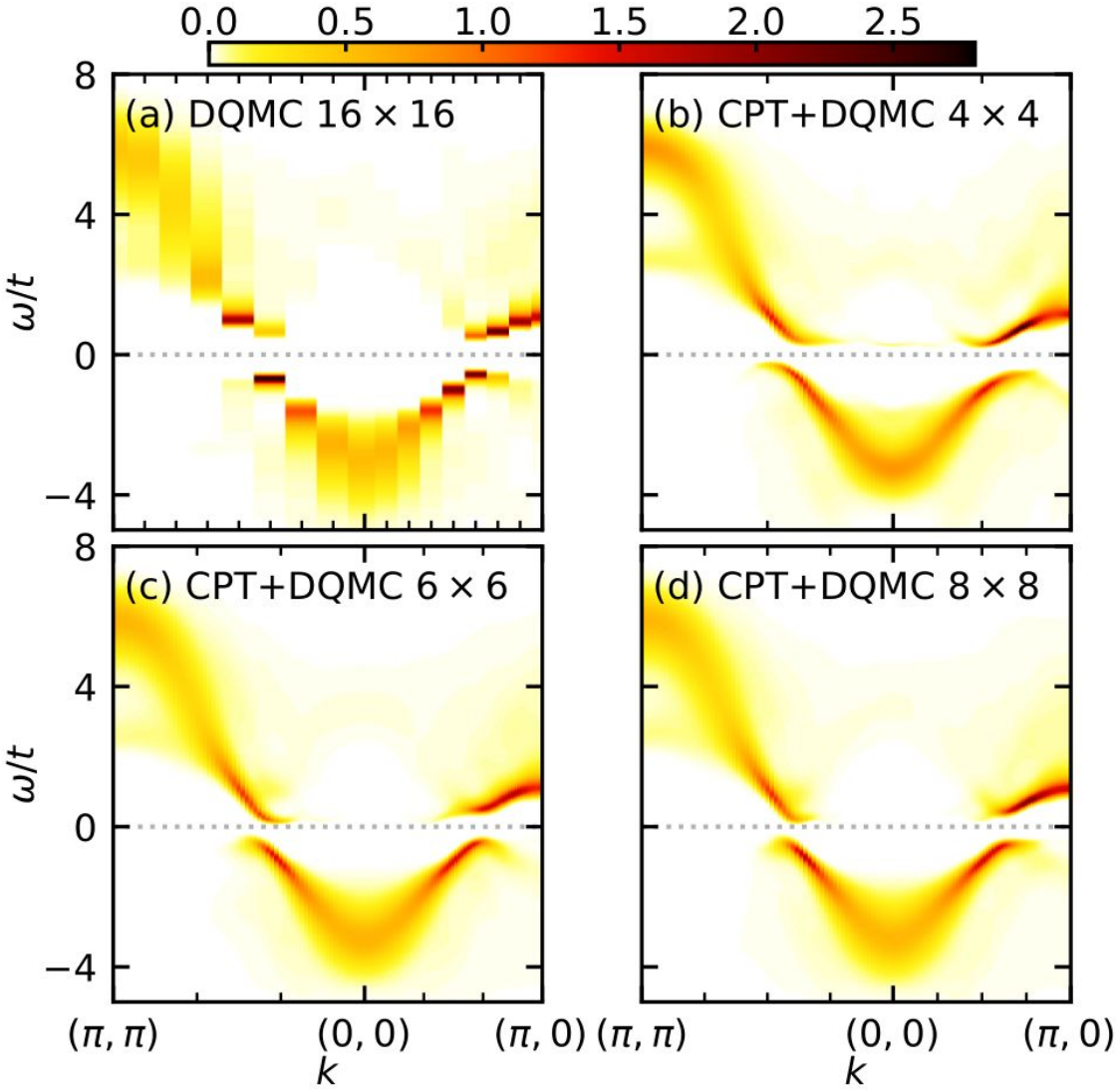
- Sign-free DQMC simulations.
- *s*-wave SC with KT transition at $T_c/t \approx 0.14$ for $U/t = -4$, $\langle n \rangle = 0.6$

Benchmarking: attractive Hubbard model, SC phase

U/t = -4

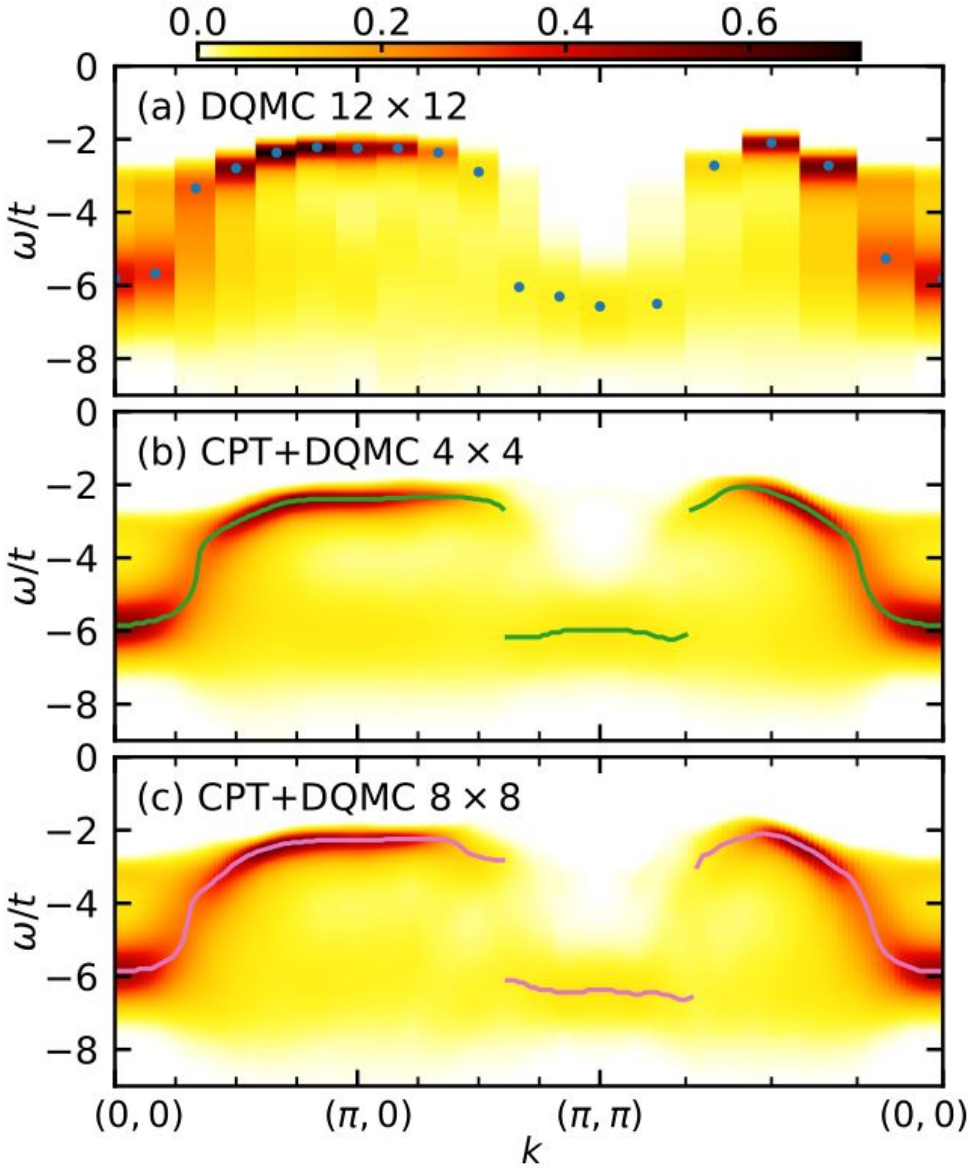
<n> ≈ 0.63

T/t = 1/12



Benchmarking: half-filled repulsive Hubbard model

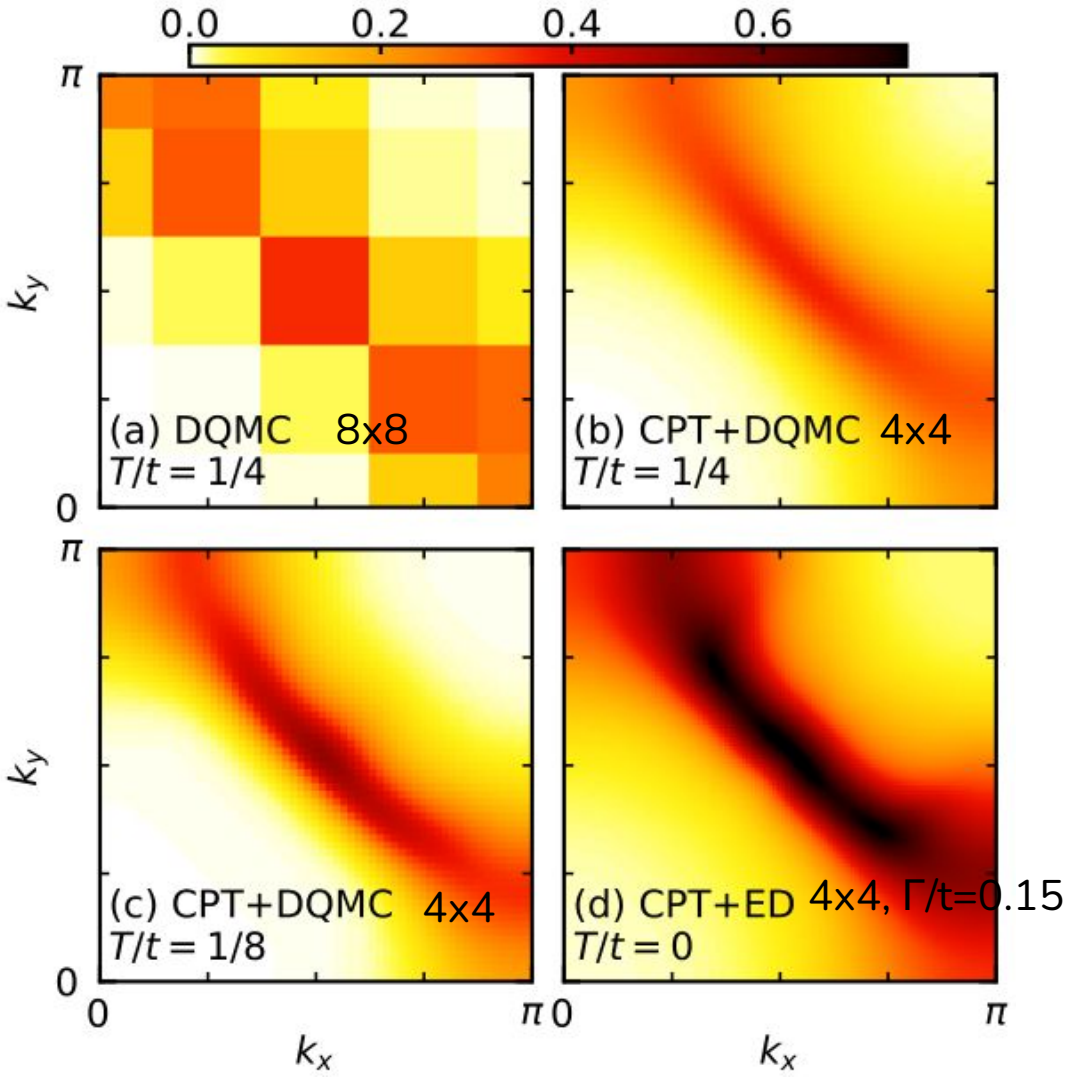
U/t = 8
<n> = 1
T/t = 1/16



Doped repulsive Hubbard model: A(k, ω =0)

U/t = 8

<n> ≈ 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