Determinantal Quantum Monte Carlo: Algorithm and Measurements

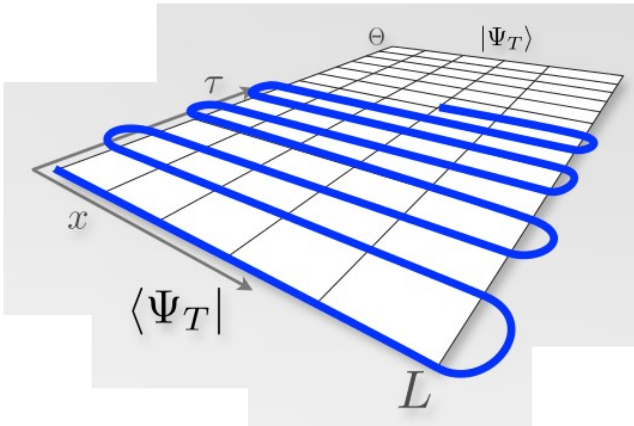
Zi Yang Meng

(孟子杨)

Institute of Physics, Chinese Academy of Sciences

Quantum Monte Carlo

■ Determinantal QMC for fermions



Hubbard model:
- Metal-Insulator transition
- Unconventional superconductivity
- Non-Fermi-liquid
- Interaction effects on topological state of matter

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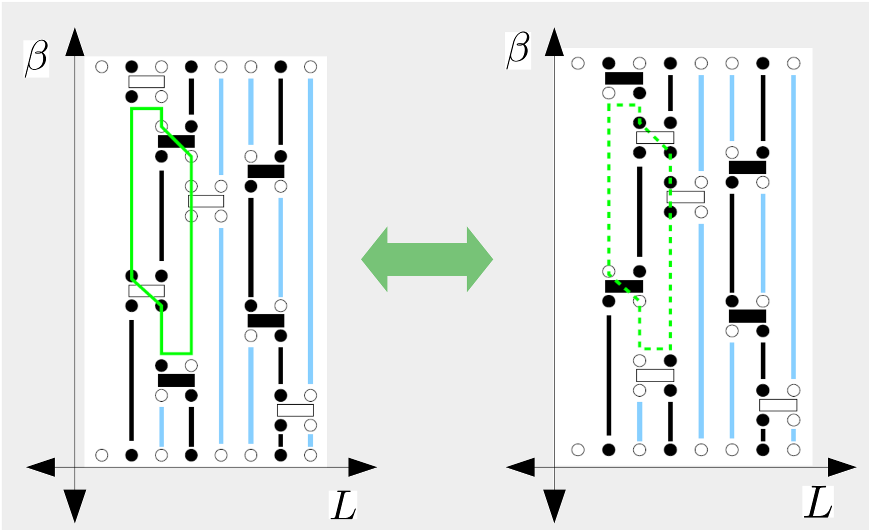
■ World-line QMC for bosons



Heisenberg model:
- Quantum magnetism
- Phase transition and critical phenomena
- Quantum spin liquids
- Quantum spin ice

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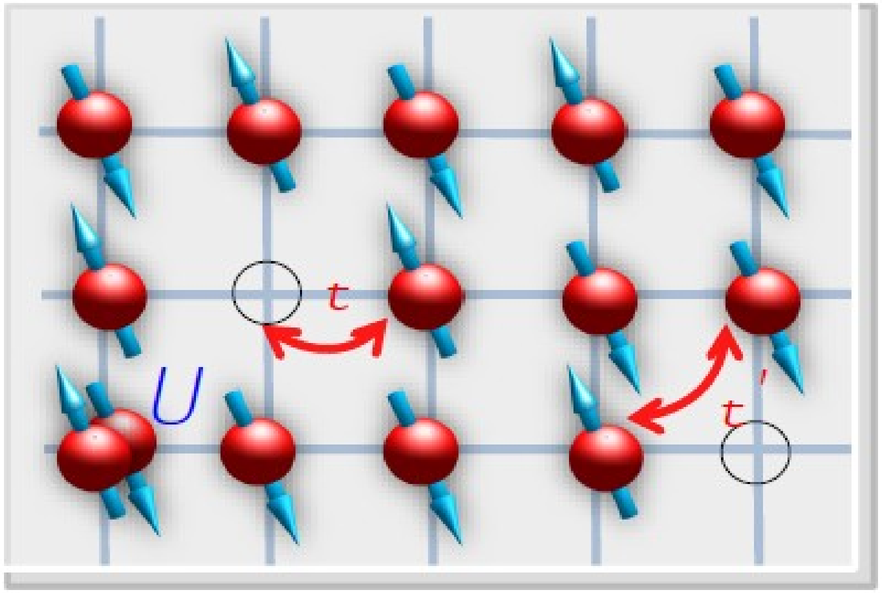
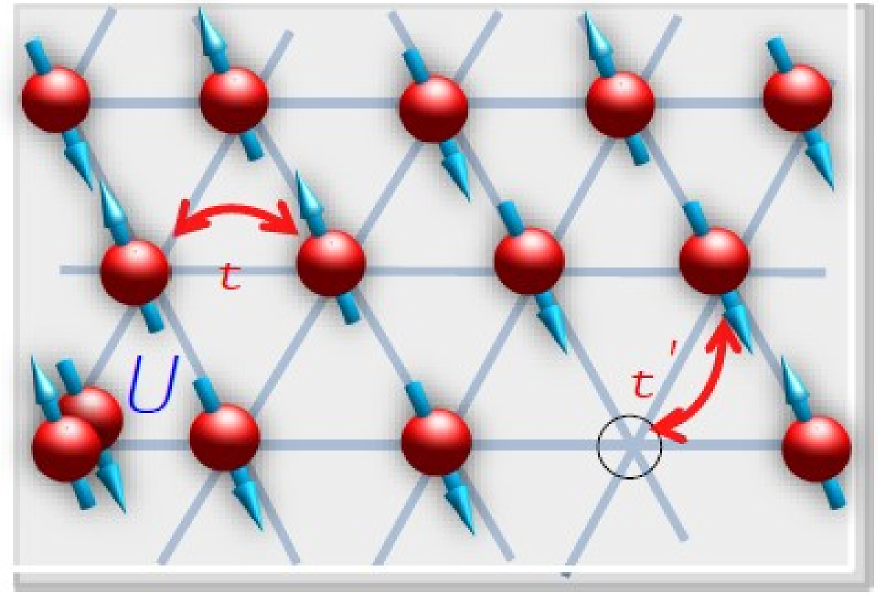
Basic problem





Partition function: $$Z = \mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] = \sum_n \langle n|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle$$

Observables : $$\langle\hat{A}\rangle = \frac{\mathrm{Tr}\left[\hat{A}e^{-\beta(\hat{H}-\mu\hat{N})}\right]}{\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right]} = \frac{\sum_n \langle n|\hat{A}e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle}{\sum_n \langle n|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle}$$

Fock space : $$\{|n\rangle\} \sim e^{N_e \ln(2)}(2^{N_e}) \ \text{ or } \ e^{N_e \ln(4)}(4^{N_e})$$

Determinantal quantum Monte Carlo

$$H = -t \sum_{\langle i,j \rangle, \sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \mathrm{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$

- Path-integral & Trotter-Suzuki decomposition

$$Z = \mathrm{Tr}\big[e^{-\beta \hat{H}}\big] \approx \mathrm{Tr}\big[\prod_{l=1}^{m} e^{-\Delta\tau \hat{H}_t} e^{-\Delta\tau \hat{H}_U}\big] \qquad \Delta\tau = \frac{\beta}{m}, m \to \infty$$

- Free fermion (Slater) determinant

$$\mathrm{Tr}\Big[e^{-\sum_{i,j} c_i^{\dagger} A_{i,j} c_j}\Big] = \mathrm{Det}\Big[\mathbf{1} + e^{-\mathbf{A}}\Big]$$

Determinantal quantum Monte Carlo

$$H = -t \sum_{\langle i,j \rangle,\sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$

- Path-integral & Trotter-Suzuki decomposition

$$Z = \mathrm{Tr}\{e^{-\beta \hat{H}}\} \approx \mathrm{Tr}\Big[\prod_{l=1}^{m} e^{-\Delta\tau \hat{H}_t} e^{-\Delta\tau \hat{H}_U}\Big] \qquad \Delta\tau = \frac{\beta}{m}, m \to \infty$$

- Discrete Hubbard-Stratonovich transformation

$$e^{-\Delta\tau U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})} = C \sum_{s_1,\ldots,s_N = \pm 1} e^{\alpha \sum_{i=1}^{N} s_i (n_{i,\uparrow} - n_{i,\downarrow})}$$

$$(C, \alpha)(U, N, \Delta\tau)$$

$$\int_{-\infty}^{\infty} dx \; e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}$$

- Blankenbecler et. al., Phys. Rev. D 24, 2278 (1981)
- Hirsch, Phys. Rev. B 28, 4059(R) (1983)
- Hirsch, Phys. Rev. B 31, 4403 (1985)
- Assaad and Evertz, Lec. Notes. In Phys. 739 (2008)

$$\int_{-\infty}^{\infty} dx \; e^{-\frac{a}{2}x^2 + bx} = \int_{-\infty}^{\infty} dx \; e^{-\frac{a}{2}(x - \frac{b}{a})^2 + \frac{b^2}{2a}} = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}}$$

Determinantal quantum Monte Carlo

$$H = -t \sum_{\langle i,j\rangle,\sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \mathrm{h.c.}) + \frac{U}{2} \sum_{i=1}^{N} (n_{i,\uparrow} + n_{i,\downarrow} - 1)^2$$

- Path-integral & Trotter-Suzuki decomposition

$$Z = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right] \approx \mathrm{Tr}\left[\prod_{l=1}^{m} e^{-\Delta\tau \hat{H}_t} e^{-\Delta\tau \hat{H}_U}\right] \qquad \Delta\tau = \frac{\beta}{m}, m \to \infty$$

- Discrete Hubbard-Stratonovich transformation

$$e^{-\Delta\tau \frac{U}{2}(n_{i,\uparrow}+n_{i,\downarrow}-1)^2} = \frac{1}{4} \sum_{s_1, s_2, \cdots, s_N = \pm 1, \pm 2} \gamma(s_i) e^{i\sqrt{\Delta\tau \frac{U}{2}}\eta(s_i)(n_{i,\uparrow}+n_{i,\downarrow}-1)} + O[(\Delta\tau)^4]$$

$$\int_{-\infty}^{\infty} dx\ e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}$$

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- Assaad, Phys. Rev. B 71, 075103 (2005)
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$$\int_{-\infty}^{\infty} dx\ e^{-\frac{a}{2}x^2+bx} = \int_{-\infty}^{\infty} dx\ e^{-\frac{a}{2}(x-\frac{b}{a})^2+\frac{b^2}{2a}} = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}}$$

Determinantal quantum Monte Carlo

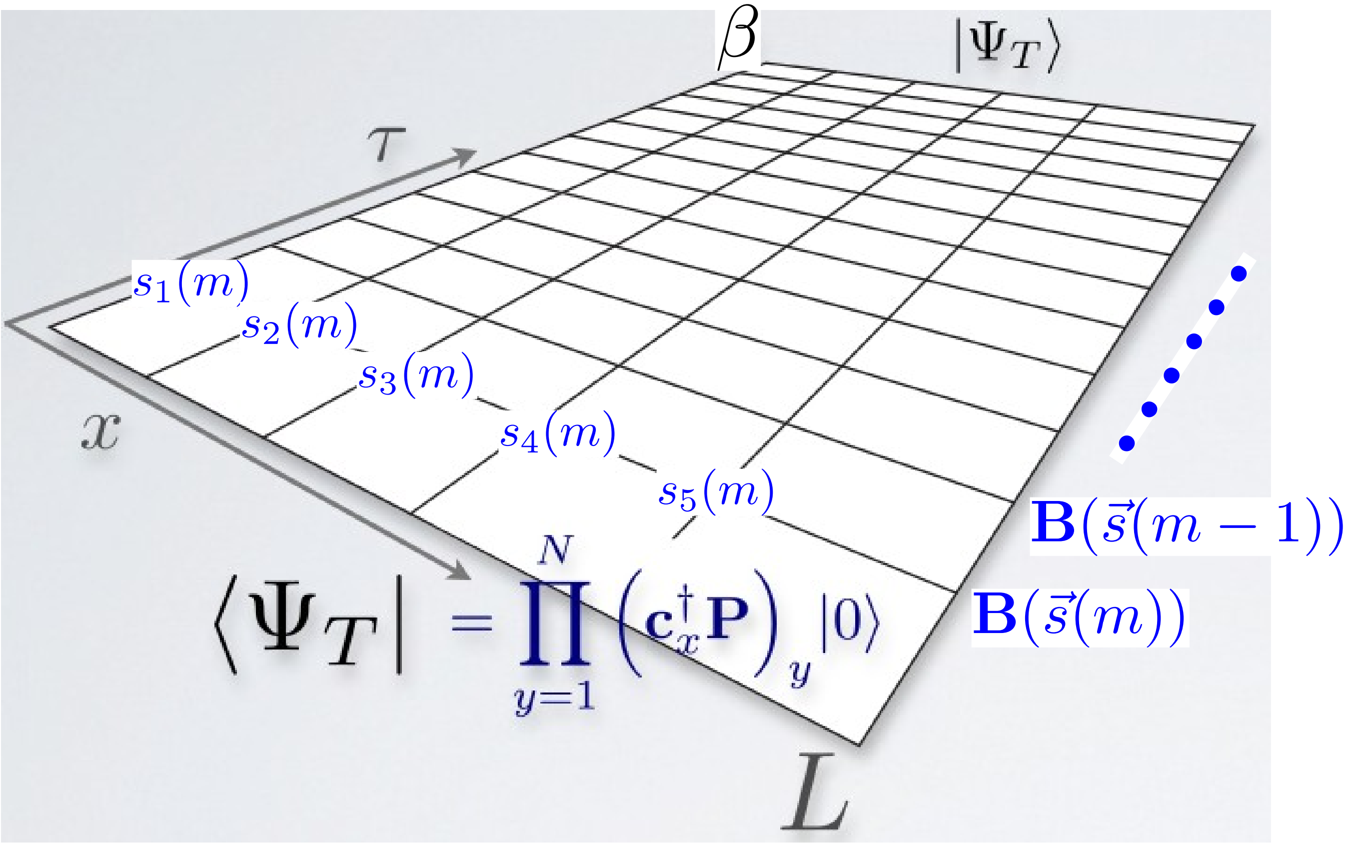
- Write Path-integral into determinant

$$Z = \mathrm{Tr}\left[\prod_{l=1}^{m} e^{-\Delta\tau \hat{H}_t} e^{-\Delta\tau \hat{H}_U}\right] = C^m \sum_{\vec{s}_1,\vec{s}_2,\ldots,\vec{s}_m} \det[\mathbf{1} + \mathbf{P}^\dagger \mathbf{B}_m \mathbf{B}_{m-1} \ldots \mathbf{B}_1 \mathbf{P}]$$

$$\mathbf{B}_l = e^{-\Delta\tau \mathbf{H_t}} e^{-\Delta\tau \mathbf{H_U}(\vec{s}(l))}$$

- Monte Carlo sampling in configuration space

$$\mathbf{H_U}(\vec{s}(l)) \propto \alpha \vec{s}(l)$$



Quantum Monte Carlo

- Hubbard-Stratonovich Transformation

$$\exp\{-\Delta\tau\frac{U}{2}(n_{i,\uparrow}+n_{i,\downarrow}-1)^2\}=\frac{1}{4}\sum_{s_i=\pm1,\pm2}\gamma(s_i)e^{i\sqrt{\Delta\tau\frac{U}{2}}\eta(s_i)(n_{i,\uparrow}+n_{i,\downarrow}-1)}+O[(\Delta\tau)^4]$$

$$\exp\{-\Delta\tau\frac{J}{8}(D_{i,j}-D^\dagger_{i,j})^2\}=\frac{1}{4}\sum_{t_{i,j}=\pm1,\pm2}\gamma(t_{i,j})e^{i\sqrt{\Delta\tau\frac{J}{8}}\eta(t_{i,j})(D_{i,j}-D^\dagger_{i,j})}+O[(\Delta\tau)^4]$$

- QMC measurements

$$\langle H\rangle=\langle H_{KM}\rangle+\langle H_U\rangle+\langle H_J\rangle \qquad G(k,\tau)\propto Z_{sp}(k)e^{-\Delta_{sp}(k)\tau} \qquad k=K,M$$

$$\frac{S^{xy}(Q_{AF})}{L^2}=m_S^2+\frac{a_1}{L}+\frac{a_2}{L^2}+\cdots \qquad S^{xy}(k,\tau)\propto Z_S(k)e^{-\Delta_S(k)\tau} \qquad k=Q_{AF}=\Gamma$$

Quantum Monte Carlo

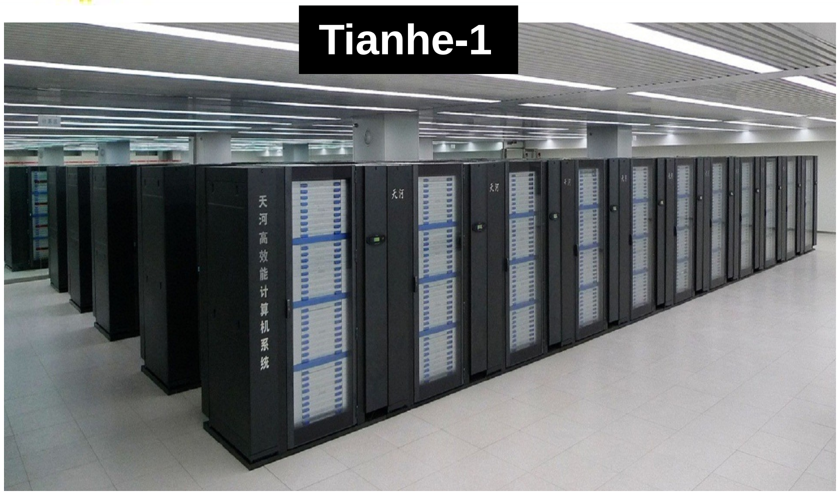
- Computation effort scales linearly with βN^3

  System sizes: $N_s = 2 \times L^2 \quad L = 3, 6, 9, 12, 15, 18$

  Time discretization: $\beta t \propto L, \Delta\tau t = 0.05$

  Parallelization: ~ 10^3 CPUs, ~ 10^6 CPU hours

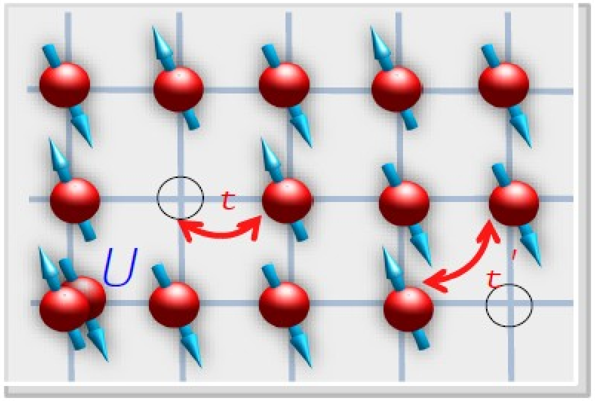
NSCC 国家超级计算天津中心 National Supercomputer Center in Tianjin

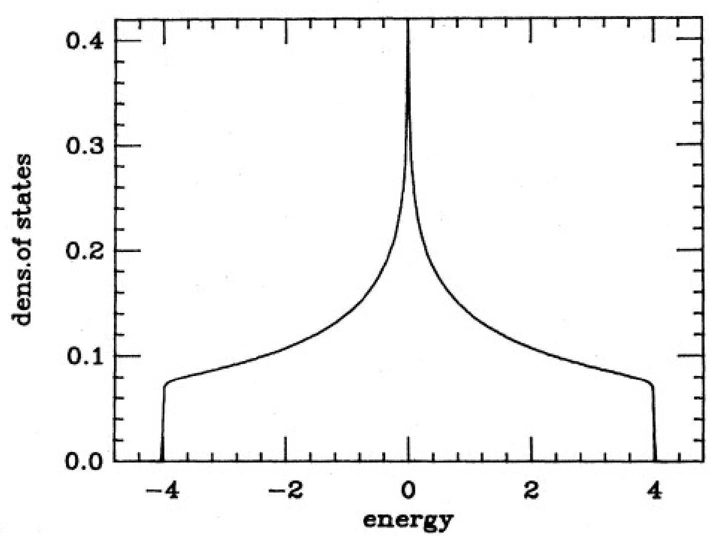


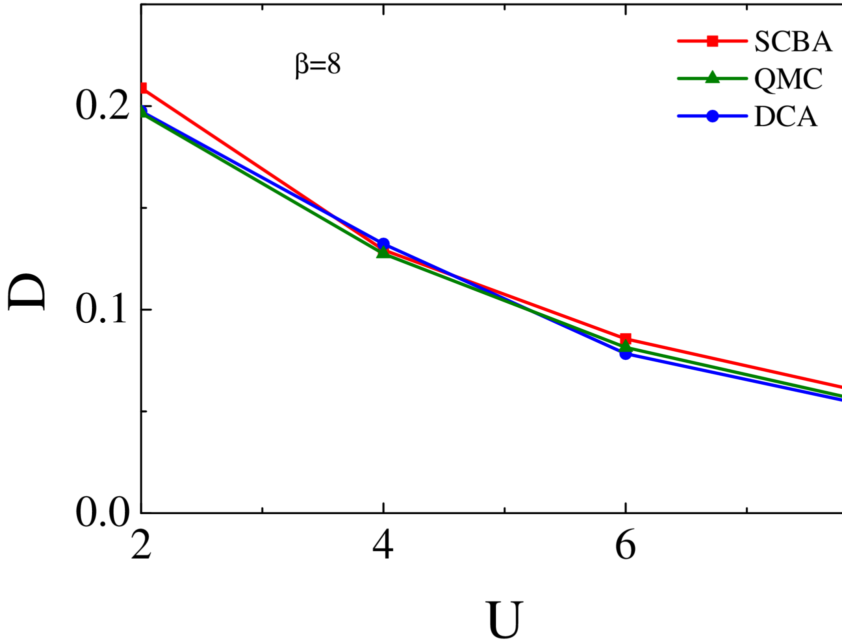
国家超级计算广州中心 NATIONAL SUPERCOMPUTER CENTER IN GUANGZHOU

Square lattice Hubbard model

$$H = -t \sum_{\langle i,j \rangle,\sigma}^{N} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \mathrm{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$



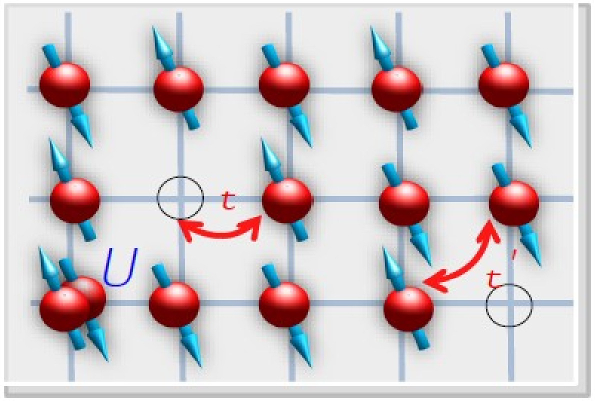


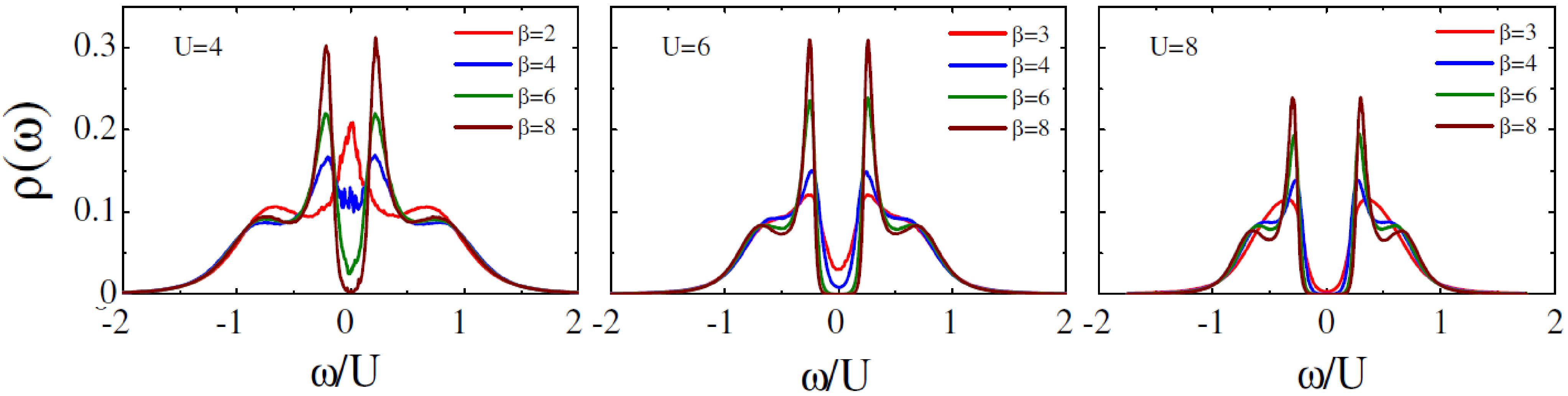


- C. Chen, Bachelor Thesis (2016)

Square lattice Hubbard model

$$H = -t \sum_{\langle i,j \rangle,\sigma}^{N} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + \mathrm{h.c.}) + U \sum_{i=1}^{N} (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2})$$





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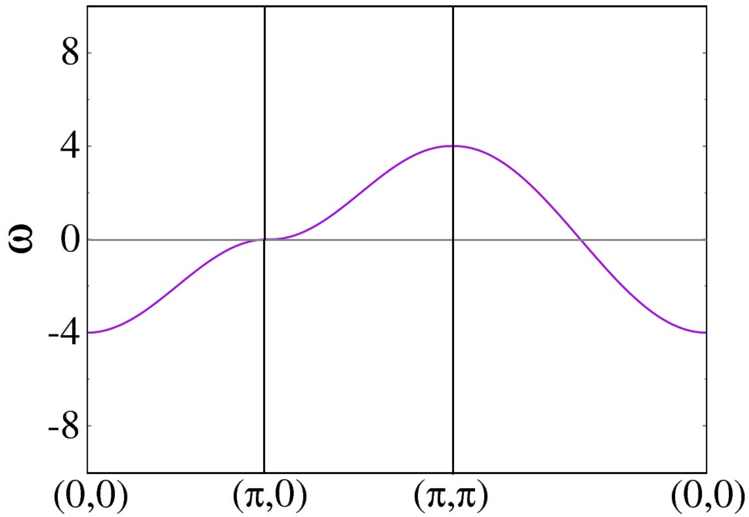
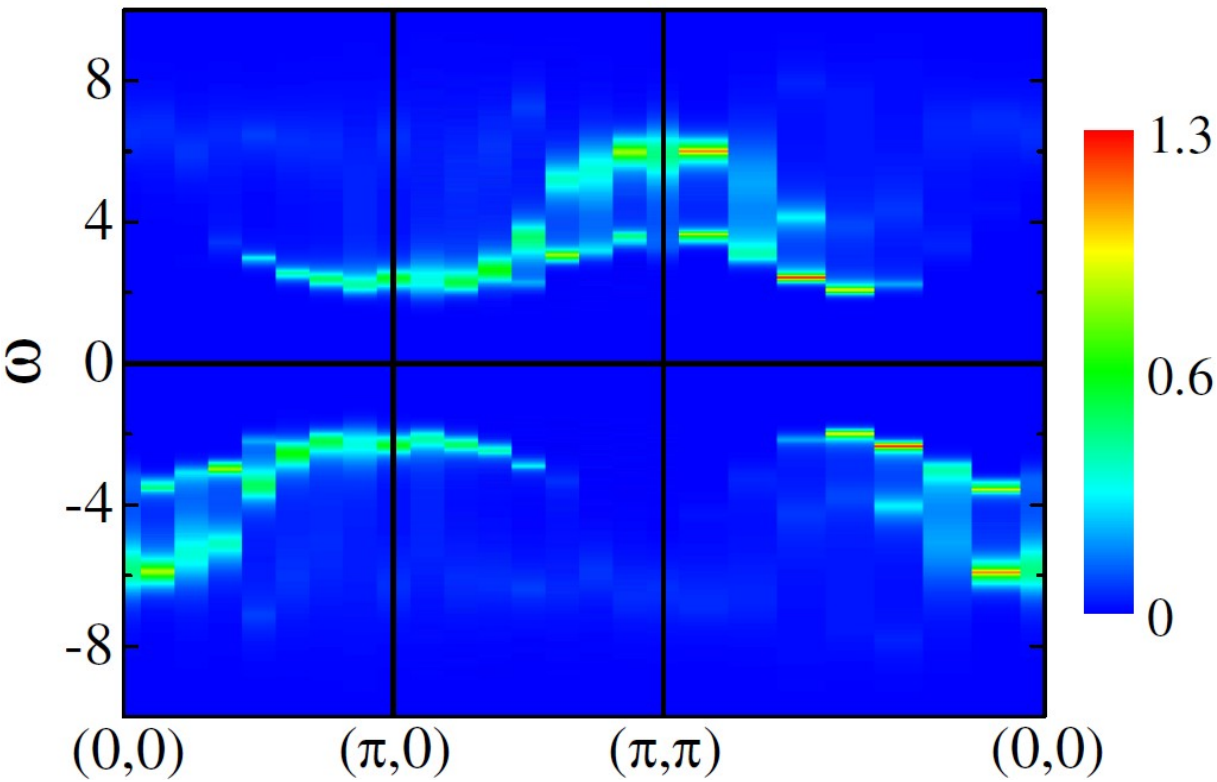
Square lattice Hubbard model





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