- Determinant QMC Algorithm

- sign problem & sign problem free

- World-line, sign problem & complexity
  - Metropolis

- other QMC methods,

Hubbard Model

- single band Hubbard Model with nearest-neighbor hopping:

$$\hat{H} - \mu\hat{N} = -t \sum_{\langle i,j\rangle,\alpha} \left(c_{i\alpha}^{\dagger} c_{j\alpha} + \mathrm{h.c.}\right) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) \tag{1}$$

- on a bipartite lattice, at $\mu = U/2$, particle-hole symmetry is possessed by the system, i.e. charge-conjugation operation defined by $\mathscr{C} c_{i\sigma} \mathscr{C}^{-1} = (-1)^i c_{i\sigma}^{\dagger}$ preserves the Hamiltonian, and the system is at half-filling.
- repulsive Hubbard model, at half-filling, and on a two-dimensional honeycomb lattice is a well-studied model exhibiting metal-insulator Mott transition.

SU(N) generalization of the Hubbard model

- at half-filling, Hubbard Hamiltonian is rewritten as $\left(SU(2)\right)\begin{pmatrix} c_{i\uparrow} \\ c_{i\downarrow} \end{pmatrix}$

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

- which motivates a generalization for N spin flavours

$$\hat{H} = -t\sum_{\langle i,j\rangle}\sum_{\alpha=1\cdots N}\left(c^{\dagger}_{i\alpha}c_{j\alpha} + \mathrm{h.c.}\right) + \frac{U}{2}\sum_{i}\left(n_i - \frac{N}{2}\right)^2, \quad (3)$$

in which $n_i = \sum_{\alpha} c^{\dagger}_{i\alpha}c_{i\alpha}$ is the particle number operator on site i

Overview

- an unbiased method for quantum system at finite temperature, calculating observable expectation in the grand canonical ensemble
- first proposed by [Blankenbecler et al., 1981]
- convert an interacting model into a problem of free fermion coupled with classical fields (known as auxillary fields). Integrating out the fermion degree of freedom generally results in determinants that depend on auxillary field configurations.
- the determinant is reinterpreted as weight for a probability distribution, and observable expectation as weighted average. Monte Carlo method is then applied.

Hubbard-Stratonovich Transformation

- in evaluating $Z = \mathcal{T}r\left[\exp(-\beta\hat{H})\right]$ [1], imaginary time β is breaked up into M "time slices". Suzuki-Trotter decomposition is applied to single out the interacting part of the Hamiltonian

$\hat{H} = \hat{H}_0 + \hat{H}_I$

$$Z = \mathcal{T}r\left[\prod_{n=1}^{M} e^{-\Delta\tau\hat{H}}\right] = \mathcal{T}r\left[\prod_{n=1}^{M} e^{-\Delta\tau\hat{H}_0} e^{-\Delta\tau\hat{H}_I}\right] + \boxed{O(\Delta\tau^2)} \quad (4)$$

- Hubbard-Stratonovich (H-S) transformation allows one to introduce auxillary field s, and turn $\hat{H}_I$ into non-interacting Hamiltonians $\hat{b}(s) = c_i^\dagger[b(s)]_{ij}c_j$

$$\exp(-\Delta\tau\hat{H}_I) = \sum_s \exp\left[-\Delta\tau\hat{b}(s)\right] \quad (5)$$

generically, b(s) has the dimension of all single particle sites

[1] chemical potential in the grand canonical ensemble is absorbed by a redefinition of $\hat{H}$, i.e. $\hat{H} - \mu\hat{N} \to \hat{H}$

Schemes of HS Transformations I

S_z Channel

for Hubbard interaction

$$\hat{H}_I = \frac{U}{2}\sum_i (n_{i\uparrow} + n_{i\downarrow} - 1)^2 \tag{6}$$

an exact HS transformation is proposed by [Hirsch, 1985]

$$e^{-\frac{U}{2}\Delta\tau(n_{i\uparrow}+n_{i\downarrow}-1)^2} = \frac{1}{2}e^{-\frac{U\Delta\tau}{2}}\sum_{s_i=\pm 1} e^{-s_i\lambda(n_{i\uparrow}-n_{i\downarrow})}, \tag{7}$$

$n_\uparrow - n_\downarrow = S_z$

in which $\cosh\lambda = e^{U\Delta\tau/2}$, (7) is now known as the HS transformation in S_z channel.

± 1

S_z, S_x, S_y

$+$

$C_\alpha \quad \sigma_{\alpha\alpha'} \quad C_{\alpha'}$

Schemes of HS Transformations II

$\hat{O} = c_i^{+} O_{ij} c_j$

Charge Channel

for repulsive Hubbard in the generalized SU(N) case, the transformation can be done at a cost of introducing complex numbers and more auxillary-field components

$$e^{-\frac{U}{2}\Delta\tau\hat{O}^2} = \frac{1}{4}\sum_{l=\pm1,\pm2,\dots}\gamma(l)e^{i\eta(l)\hat{O}} \tag{8}$$

utilizing the fact that $\hat{O} = n_i - \frac{N}{2}$ has only discrete eigenvalues, the transformation can be done exactly, using $2\left\lceil\frac{N+2}{4}\right\rceil$ component auxillary fields.

$i, j \cdots 1 \cdots N_{sites}$

$\left(\sum b_{ij} c_i^{+} c_j\right)^2$ $\qquad$ $\hat{H}_I = \sum V_{ijkl}\, c_i^{+} c_j^{+} c_k c_l$ $\qquad$ N_s^2

$(ik, jl) = N_s^2$

DQMC for SU(2N) Hubbard Model

- We now focus on the SU(2N) case, where the grand canonical partition function is carried out as

$$
\begin{aligned}
Z &= \mathcal{T}r\, e^{-\beta \hat{H}} \\
&= \left(\frac{1}{4}\right)^{N_{\text{sites}} M} \sum_{\{s\}} \Bigg[\left(\prod_{i,l} \gamma(s_i(l)) \right) \\
&\mathcal{T}r \left(\prod_{l=M}^{1} \prod_{\sigma=1}^{2N} e^{-\Delta\tau \sum_{i,j} c_{i\sigma}^{\dagger} K_{ij} c_{j\sigma}} e^{-\Delta\tau \sum_i V_i(l)\left(c_{i\sigma}^{\dagger} c_{i\sigma} - \frac{1}{2}\right)} \right) \Bigg]
\end{aligned} \tag{9}
$$

under particle-hole $\mathscr{E} \cdot \mathscr{E}^{-1}$

in which

$$
V_i(l) = -\frac{\mathrm{i}}{\Delta\tau} \eta(s_i(l)) - \mu \tag{10}
$$

$c^{+} K c \rightarrow K$

$c^{+}c - 1/2 \rightarrow -(c^{+}c - 1/2)$

chemical potential is included in the interacting part, such that kinetic term is invariant under particle-hole transformation.

Proof of

sign-problem-free at half-filling

- using the identity

$$Tr\prod_l e^{c^\dagger_{i\sigma}h_{ij}(l)c_{j\sigma}} = \det\left[1+\prod_l e^{h(l)}\right] \tag{11}$$

H. Yao, SC Zhang et al. → $\boxed{\text{sign-problem-free}}$

which leads to [2]

Classification of non-interacting Hamiltonian by symmetry

$$Z = \sum_{\{s\}}\left(\gamma(\{s\})\left[e^{-\mathrm{i}\frac{1}{2}\sum_{i,l}\eta(s_i(l))}\det\left(1+B_M B_{M-1}\cdots B_1\right)\right]^{2N}\right)$$
$$\equiv \sum_{\{s\}}\gamma(\{s\})\left[\underline{v(\{s\})}\right]^{2N} \equiv \sum_{\{s\}} w(\{s\}) \tag{12}$$

$$\det\left(I+\begin{bmatrix} B_M\cdots B_1 & & \\ & \ddots & \\ & & B_M\cdots B_1\end{bmatrix}\right)$$

2N spin flavour

where $B_l \equiv e^{-\Delta\tau\mathbf{K}}e^{-\Delta\tau\mathbf{V}(l)}$.At half-filling, $w(\{s\})$ remains positive for arbitrary configuration $\{s\}$

C

[2] This result requires that spin-orbital coupling is absent and HS transformation is symmetric with respect to all spin flavours.

Evaluation of Observables

- for arbitrary observable $\hat{O}$, define

$$O(\{s\}) = \frac{\mathcal{T}r\left(\hat{O}\prod_{l=M}^{1}\prod_{\sigma=1}^{2N} e^{-\Delta\tau\sum_{i,j} c_{i\sigma}^{\dagger}K_{ij}c_{j\sigma}} e^{-\Delta\tau\sum_{i} c_{i\sigma}^{\dagger}V_i(l)c_{i\sigma}}\right)}{\mathcal{T}r\left(\prod_{l=M}^{1}\prod_{\sigma=1}^{2N} e^{-\Delta\tau\sum_{i,j} c_{i\sigma}^{\dagger}K_{ij}c_{j\sigma}} e^{-\Delta\tau\sum_{i} c_{i\sigma}^{\dagger}V_i(l)c_{i\sigma}}\right)} \tag{13}$$

- ensemble average is written as an weighted average on the configuration space

$$\left\langle \hat{O} \right\rangle = \frac{1}{Z}\cdot\sum_{\{s\}}\left[O(\{s\})w(\{s\})\right] \tag{14}$$

$$\frac{tr(\hat{O}e^{-\beta\hat{H}})}{tr(e^{-\beta\hat{H}})}$$

$$Z = \sum w(c)$$

$\to c$

$$\langle c_i c_j^{\dagger}\rangle_c = \left[(1+B_m\cdots B_1)^{-1}\right]_{ij}$$

$$\langle \hat{O} \rangle = \boxed{\frac{\sum O(c)\, W(c)}{\sum W(c)}} \qquad \epsilon \qquad \frac{1}{\epsilon^2}.$$

$$\langle c_i c_j c_k^\dagger c_l^\dagger \rangle = \sum \langle c_1 c_2 c_3^\dagger c_4^\dagger \rangle_c \, W(c)$$

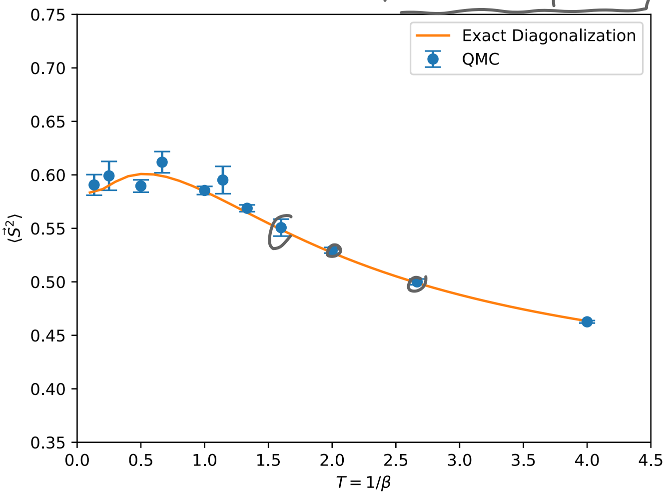
$$= \sum \Big[\langle c_1 c_3^\dagger \rangle \langle c_2 c_4^\dagger \rangle + \underline{\langle c_1 c_4^\dagger \rangle} \langle c_2 c_3^\dagger \rangle + \cdots \Big] W(c)$$

$$c \sim \boxed{W(c)}$$

$$c \downarrow O(c)$$

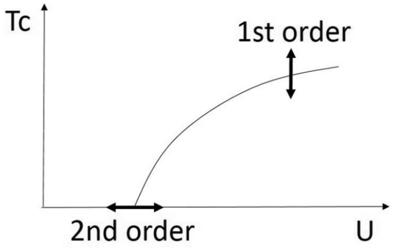
$\langle\sigma_x\rangle^2 + \langle\sigma_y\rangle^2 + \cdots \quad \langle\sigma_z^2\rangle = \langle(c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow)^2\rangle$

$= \langle c_\uparrow^\dagger c_\uparrow c_\downarrow^\dagger c_\downarrow\rangle.$



- 6 sites chain $+ \cdots$
- PBC
- local momentum $S^2 = \frac{1}{N}\sum_i(\mathbf{S}_i)^2$
- reproduction of FIG.4 in [Hirsch, 1985]

Phase Diagram of SU(2N) Hubbard Model at half-filling



- putative phase diagram of the Dirac semimetal-to-insulator phase transition of SU(2N) Hubbard Model on the honeycomb lattice [Zhou et al., 2016]
- gap opens at U_c, $U_c/t \propto N$ is expected.

Single Particle Gap

- consider the imaginary-time Green's function

$$G(i,j,\tau) = \sum_{\alpha} \left\langle c_{i,\alpha}(\tau) c^{\dagger}_{j,\alpha}(0) \right\rangle \tag{15}$$

- at Dirac point $\mathbf{K}, \mathbf{K}'$ of the Brillouin Zone

$$G(\mathbf{K},\tau) = \frac{1}{N_s} \sum_{i,j} G(i,j,\tau) e^{\mathrm{i}\mathbf{K}\cdot(\mathbf{r}_i - \mathbf{r}_j)} = \sum_{\alpha} \left\langle c_{\mathbf{K},\alpha}(\tau) c^{\dagger}_{\mathbf{K},\alpha}(0) \right\rangle \tag{16}$$

  in which $c_{\mathbf{k},\alpha}(\tau) = c_{i,\alpha}(\tau) e^{i\mathbf{k}\cdot\mathbf{r}_i}$

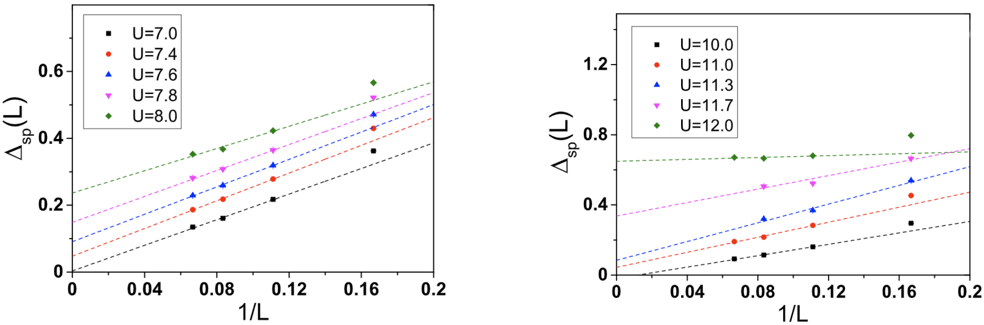
- Lehmann representation gives [Zhang, 2020]

  $G(\mathbf{k},\tau) = \frac{1}{Z} \sum_{n,m,\alpha} e^{-\beta E_n} e^{(E_n - E_m)\tau} \left| \left\langle m \middle| c^{\dagger}_{\mathbf{k},\alpha} \middle| n \right\rangle \right|^2$, therefore

$$G(\mathbf{K},\tau) \approx e^{-\Delta_{sp}\tau} \tag{17}$$

  Δ_{sp} can be extracted from the slope of $\log[G(\mathbf{K},\tau)] - \tau$ at large enough β

projector



finite-size scaling result. For SU(4) and SU(6) Hubbard Model, the quantum critical point U_c is estimated to be 7.0, and 10.0.

projector QMC

行列式蒙卡能够给出有限温的无偏结果，但对于研究基态问题来说就略显笨重。对于多体系统的基态研究，常用的算法是投影量子蒙卡方法（Projector QMC）[10]，其基本想法是，任何一个量子态 $|\psi_T\rangle$，只要其与基态的内积非零，就可以使用投影算符 $\exp(-\Theta\widehat{H})$，选取一个充分大的 Θ，使得 $\exp(-\Theta\widehat{H})|\psi_T\rangle$ 任意接近物理的基态，这里的初始波函数 $|\psi_T\rangle$ 也称为试探波函数。算符 $\widehat{O}$ 的基态期望值成为

$$\left\langle\widehat{O}\right\rangle=\frac{\langle\psi_T|\, e^{-\Theta\widehat{H}}\widehat{O}e^{-\Theta\widehat{H}}\,|\psi_T\rangle}{\langle\psi_T|\, e^{-2\Theta\widehat{H}}\,|\psi_T\rangle} \tag{2.9}$$

类似与行列式蒙卡中的操作，投影算符也可以在 Trotter 分解、引入辅助场后写成某个“无相互作用”投影算符 $U_{\{s\}}(\Theta,0)$ 对辅助场构型求和

$$e^{-\Theta\widehat{H}}=\sum_{\{s_n\}}\left(\prod_n e^{-\Delta\tau\widehat{H}(n)}\right)\equiv\sum_{\{s\}}U_{\{s\}}(\Theta,0) \tag{2.10}$$

如果依然希望将算符期望值整理成对辅助场构型空间概率分布求期望形式 $\left\langle\widehat{O}\right\rangle=\sum P_{\{s\}}O(\{s\})$，则容易发现

$$P_{\{s\}}\propto\langle\psi_T|\,U_{\{l\}}(2\Theta,0)\,|\psi_T\rangle,\quad O(\{s\})=\frac{\sum_s\langle\psi_T|\,U_s(2\Theta,\Theta)\widehat{O}U_s(\Theta,0)\,|\psi_T\rangle}{\sum_s\langle\psi_T|\,U_s(2\Theta,0)\,|\psi_T\rangle} \tag{2.11}$$

如果选择试探波函数有 Slater 行列式的形式

$$|\psi_T\rangle=\prod_j\left(\sum_i c_i^\dagger Q_{i,j}\right)|vac\rangle \tag{2.12}$$

其中 i 是晶格格点、自旋的（也即单粒子可能状态）的标号，j 则为体系中实际的电子数的标号，于是 Q 一般而言为一个非方形的矩阵。进一步的计算将表明前述的“无相互作用”投影算符在 Slater 行列式上的作用是可以严格给出的，于是也成为了一个可以用蒙特卡洛采样方法解决的问题。本文使用的行列式蒙卡得到的结果将与用此投影方法给出的结果进行比对，以确保程序的正确。

Sign Problem

$w(c) \geq 0$ $\qquad q(x)$

configuration weight $w(c)$ is generically not a positive number, if this is the case, underlying configuration weight can be altered via importance sampling

$\langle f \rangle_p = \int f(x) \cdot p(x)\, dx$

$= \int \boxed{f(x) \cdot \frac{p(x)}{q(x)}} \cdot q(x)\, dx$

$$\left\langle \hat{O} \right\rangle_{c\sim\omega(c)} = \frac{\sum_c \omega(c) O(c)}{\sum_c \omega(c)} = \frac{\sum_c O(c)\text{sign}(c)|\omega(c)| / \sum_c |\omega(c)|}{\sum_c \text{sign}(c)|\omega(c)| / \sum_c |\omega(c)|} = \frac{\left\langle \hat{O} \right\rangle_{c\sim|\omega(c)|}}{\langle \text{sign} \rangle_{c\sim|\omega(c)|}} \tag{18}$$

$\text{sign}(c) \cdot |w(c)| = w(c)$

if $|\langle \text{sign} \rangle| < 1$, the complexity for estimating $\left\langle \hat{O} \right\rangle$ to a given precision ε is $O\left(N_{\text{sites}}^{2+p} M \frac{1}{\varepsilon^2 \cdot |\langle \text{sign} \rangle|^2}\right)$, exponential decaying $|\langle \text{sign} \rangle|$ leads to the sign problem.

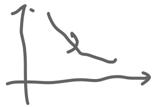
polynomial complexity not guaranteed even if $\langle \text{sign} \rangle = 1$

$\langle \hat{O} \rangle$

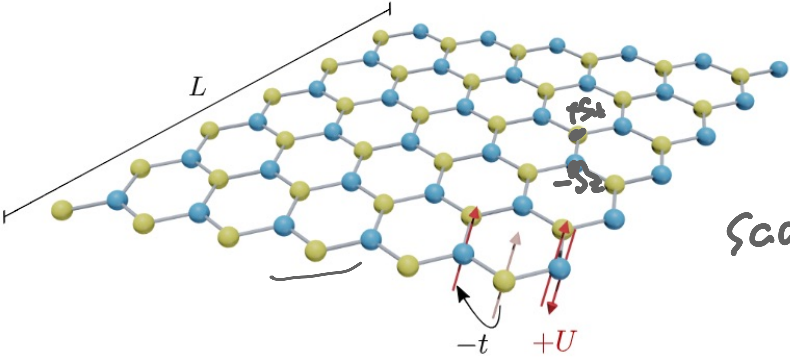
$N_{site} \to +\infty$, $\beta \to +\infty$

$e^{-N\beta\alpha}$

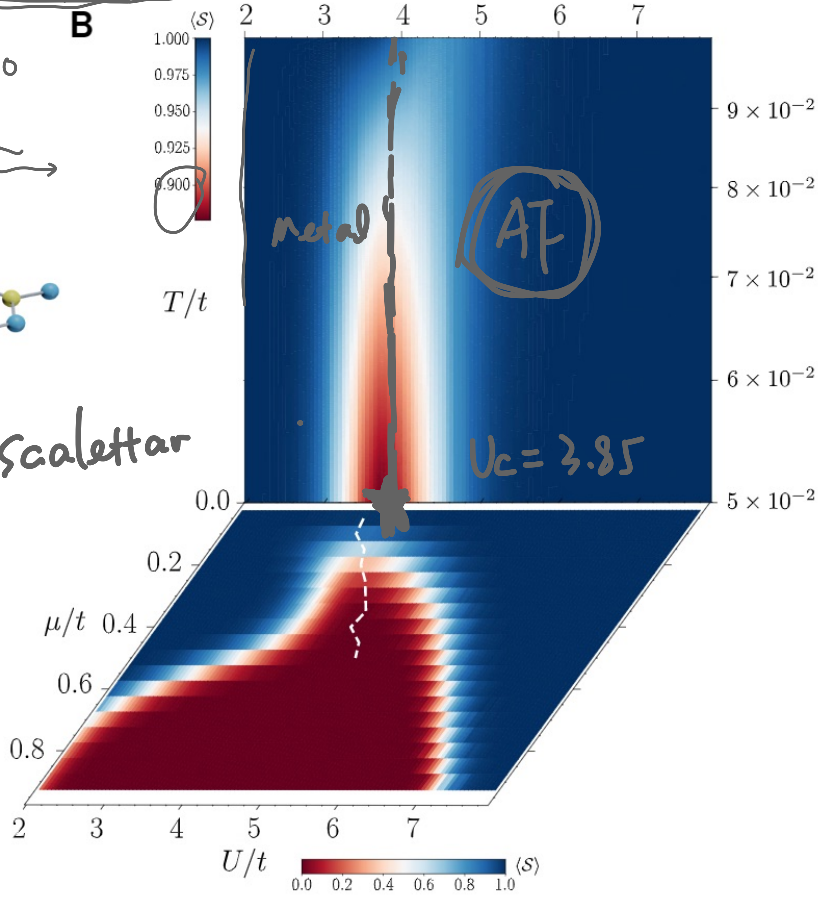
$|\langle sign \rangle| \to 0$



A



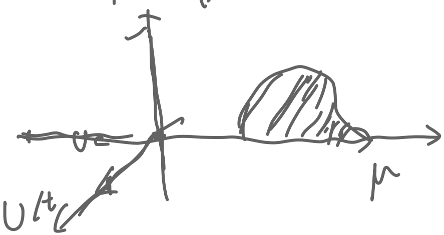
B



Scalettar

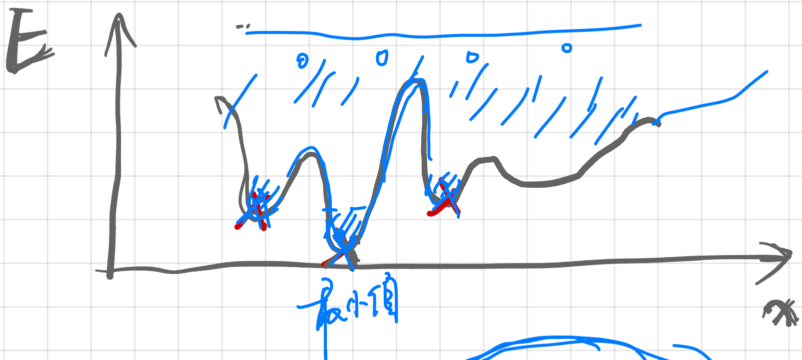
Mott

$T = 1/\beta$



"local minima"

e.g. simulated annealing



$$p(x) \propto e^{-E(x)/kT}$$

tunneling time $\propto$ $\exp(aN)$

e.g. Traveling Sales Man

1777. MC for π

after WWII, ~1948

MANIAC.

Metropolis. Ulam

Von Neumann.

1953 $e^{-E/kT}$

potential not fully discovered

1965. Hasting

1990s. PCs

世界线 QMC 多应用于这样的情况，即体系 Hilbert 空间 $\mathcal{H}$ 的一组完备基，不妨记为 $\{|s\rangle\}$，以及哈密顿量在这组基上的表示是容易得到的，例如 Ising 模型的完备基可以取为一个 $|s\rangle = |01\cdots\rangle$ 的 0-1 比特串，表示每一格点自旋在 Z 方向基上的本征值. 这一方法不像 DQMC 那样依赖于哈密顿量特有的结构，在例如计算复杂性的问题上会更便于理论分析.

2^N

为计算该系统的配分函数，我们进行 Trotter 分解，将虚时分为 m 份，$\beta = m\Delta\tau$，并将完备基 $\sum|s\rangle\langle s| = \mathbb{1}$ 插入到其中

$$
\begin{aligned}
Z &= \sum_{s_1,\cdots s_m, s_{m+1}=s_1} \langle s_1|e^{-\Delta\tau\hat{H}}|s_2\rangle\cdots\langle s_m|e^{-\Delta\tau\hat{H}}|s_1\rangle \\
&= \sum_{c\in\Lambda} \langle s_1|\mathbb{1}-\Delta\tau\hat{H}|s_2\rangle\cdots\langle s_m|\mathbb{1}-\Delta\tau\hat{H}|s_1\rangle + O(\Delta\tau^2)
\end{aligned}
\tag{2.1}
$$

进一步将式(2.1)写作 $Z = \sum_c \omega(c)$，其中对构型空间全体元素 $c \in \Lambda \subset [\dim\mathcal{H}]^{\times(m+1)}$ 求和，并可以期望在 Trotter 分解步长足够小时收敛到正确的结果. 可观测量 $\hat{O}$ 的期望值写为

w $\{s_1, s_2 \cdots s_m\}$

$$
\begin{aligned}
\langle\hat{O}\rangle &= \mathrm{Tr}\left(\hat{O}e^{-\beta\hat{H}}\right)/Z \\
&= \sum_c O(c)\omega(c)/Z
\end{aligned}
\tag{2.2}
$$

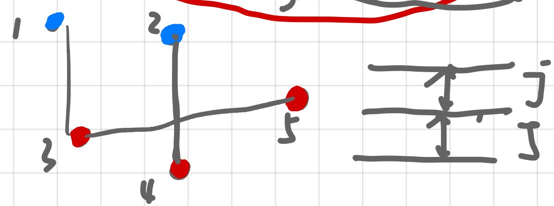
$w \geq 0$

(2.2)式中在 Trotter 分解过程中插入 $\hat{O}$ 的操作，只有 $\hat{O}$ 在 Hilbert 空间这组基下是对角时显然成立，而 $\hat{O}$ 形式复杂时的修补方案可能会引入额外的问题，这一部分与本文的讨论并没有很强的联系所以不作讨论，可以参考[8]。

Sign Problem is NP-hard?

MAX-CUT Problem

$$\hat{H} = -J_{ij}\sum_{i,j\in E}(1 - z_i z_j)$$



$$\langle\hat{H}\rangle < E_0 + \frac{J}{2} \quad \text{for } \beta J \geq N\ln 2$$

"stoquastic"

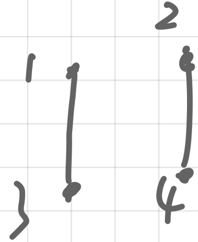
$$\hat{H} = \begin{bmatrix} x & - & - & - & - \\ & x & - & - & - \\ & & x & - & - \\ & & & x & - \\ & & & & x \end{bmatrix}$$

e.g.

$H = -\sum J_{ij} z_i z_j - \sum h_i X_i$, $e^{-\beta\hat{H}}$ $\forall\beta>0$

toric code Hamiltonian

. . . .



$\langle s_1 | I - \Delta\tau \hat{H} | s_2 \rangle$

$$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{pmatrix} - \Delta\tau \begin{pmatrix} & & \\ & & \\ & & \end{pmatrix}$$

$\boxed{(1 - z_i z_j)}$

+1	+1
−1	−1
1	−1

$\boxed{\langle \hat{O} \rangle} \Longleftrightarrow$ HS

① Hubbard sign problem free

$$\begin{cases} \sum e^{-i(n_\uparrow + n_\downarrow)\cdot\square} & \checkmark \\ \sum e^{-(n_\uparrow - n_\downarrow)\square} & \checkmark \end{cases}$$

② $\langle \underline{c c c c c^\dagger c^\dagger c^\dagger} \rangle = \sum_c w(c) \boxed{\underline{(g_{ij}\, g_{kl} \cdots\cdots)}}$

$$\underbrace{\langle \text{sign} \rangle}_{\text{HS}} = \sum_{c} w(c) \boxed{\text{sign}\left(\det(g_{ij}) \right)}$$

S_z : $\langle \text{sign} \rangle = 1$

S_x, S_y $\to 0$

Free Energy Argument

Sign problem is often briefly explained by a free energy based argument

$$\langle \text{sign} \rangle_{|\omega(c)|} = \frac{\sum_c \omega(c)}{\sum_c |\omega(c)|} = \frac{\mathcal{T}r\left(e^{-\beta \hat{H}}\right)}{\mathcal{T}r\left(e^{-\beta \hat{H}'}\right)} = \frac{Z}{Z'} \qquad S' \tag{19}$$

$$= \frac{e^{-N\beta f}}{e^{-N\beta f'}} = e^{-N\beta \Delta f} \to 0$$

$Z \sim \exp(-N\beta f)$

$Z' \sim \exp(-N\beta f')$

therefore an exponential decaying feature is a "trivial" one.

construction of reference systems:

$$Z = g \cdot e^{-\beta E_g} \Longleftarrow \beta \to +\infty$$

$$Z = \sum p(c) \, D(c) = \langle D \rangle$$

$$\langle D \rangle \leq \langle |D| \rangle \leq \sqrt{\langle |D|^2 \rangle}$$

$$\Rightarrow \quad \frac{g_D e^{-\beta E_D}}{\sqrt{g_{|D|^2} e^{-\beta E_{|D|^2}}}} \leq \langle \mathrm{sign} \rangle \leq 1$$

bypass sign problem :

fix node Diffusion Monte Carlo

$$\psi(x_1, x_2, x_3 \cdots x_N)$$

$$e^{-\tau \hat{H}} \psi = \sum_c e^{\square \frac{d^2}{dx^2}} \cdot e^{\square V(x_1 \cdots x_N)} \cdots$$

$$\hat{H} = \sum_i -\frac{\hbar^2}{2m} \nabla_i^2 + V(x_1 \cdots x_N)$$

$$E_g = \frac{\langle \psi_T | \hat{H} e^{-\tau \hat{H}} | \psi_0 \rangle}{\langle \psi_T | e^{-\tau \hat{H}} | \psi_0 \rangle}$$

$$\langle \psi_T | \simeq \langle \psi_G |$$

Sign Ease : $\begin{cases} \text{Back Propagation,} \\ \min \|H_7\|_1 \text{ via basis rotation} \end{cases}$ (already NP-complete)

---

is $\langle sign \rangle$ physical ?

Spin Resolved Sign I

[Mondaini et al., 2021, Scalettar et al., 2022] introduced "Spin resolved Sign", for S_z channel HS transformation explicitly.
Denote $(I + B^{\sigma}_{M} B^{\sigma}_{M_1} \cdots B^{\sigma}_{1})$ by M_σ, the configuration weight is

$$w(c) = \det M_{\uparrow}(c) \det M_{\downarrow}(c) \tag{20}$$

at half-filling, particle-hole symmetry gives $\text{sign}(\det M_{\uparrow}) \equiv \text{sign}(\det M_{\downarrow})$ [Hirsch, 1985], which motivates one to define

$$\langle \mathcal{S}_\sigma \rangle = \frac{1}{Z} \sum_{c} w(c) \text{sign}(\det M_\sigma) = \frac{\langle \text{sign}(c) \cdot \text{sign}(\det M_\sigma) \rangle_{c \sim |w(c)|}}{\langle \text{sign}(c) \rangle_{c \sim |w(c)|}} \tag{21}$$

free energy argument also applies to this quantity.

Proof of identities in DQMC, see:
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classification of sign-problem-free QMCs:
- Li, Zi-Xiang, and Hong Yao. "Sign-problem-free fermionic quantum Monte Carlo: Developments and applications." arXiv preprint arXiv:1805.08219 (2018).

a History of metropolis algorithm
- Hitchcock, David B. "A history of the Metropolis–Hastings algorithm." The American Statistician 57.4 (2003): 254-257.

local minimum in Monte Carlo Sampling & is sign problem an NP problem?
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Free energy argument of sign problem
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construction of reference system in free energy argument (DQMC)
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Bypass sign problem by sacrificing the "unbiased" property
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- Qin, Mingpu, et al. "Absence of superconductivity in the pure two-dimensional Hubbard model." Physical Review X 10.3 (2020): 031016.
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