

Example: $H_b = J \vec{S}_i \cdot \vec{S}_j$ $J > 0$ Square

Basis: $S^Z: \{ \uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow \}$.

$\langle \uparrow\downarrow | H_b | \downarrow\uparrow \rangle = J/2 > 0$ We need $\langle \alpha | -H_b | \alpha' \rangle \geq 0$
 $\langle \downarrow\uparrow | H_b | \uparrow\downarrow \rangle = J/2 > 0$

Basis: $\hat{U} = \prod_{j \in B \text{ (sublattice)}} e^{i\pi S_j^Z}$

$$\hat{U} H_b = S_i^Z S_j^Z + (-1/2) (S_i^+ S_j^- + S_i^- S_j^+)$$

That can fit the condition.

Local Unitary transform to let $\langle \alpha | \hat{H}_b | \alpha' \rangle < 0$

(Heisenberg $J > 0$) on bipartite lattice no sign problem

triangle $\rightarrow$ frustrated. No unitary transform.

Usually sign problem.

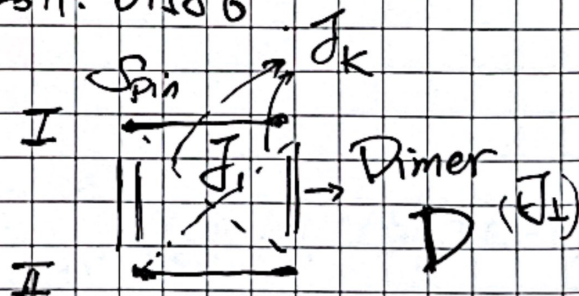
partial frustrate

arXiv: 1511.01586

i) $K_x = J_x$

ii) $K_L = J_L$

iii) $K_L = -J_L$



Basis: $\{ |\uparrow_I \downarrow_{II}\rangle - |\downarrow_I \uparrow_{II}\rangle, |\uparrow_I \uparrow_{II}\rangle, |\downarrow_I \downarrow_{II}\rangle, |\uparrow_I \downarrow_{II}\rangle + |\downarrow_I \uparrow_{II}\rangle \}$

1D fermion, hubbard, NN, OBC, SSE

Basis: $\{1\uparrow \dots L\uparrow, 1\downarrow \dots L\downarrow\}$

hopping $\langle \alpha | -t c_i^\dagger c_j | \alpha' \rangle = 0 \text{ or } -t \text{ (i,j} \in \text{NN)}$

Fermion Determinant:

$$Z = \sum_{\{\uparrow, \downarrow\}} \det(M_\uparrow(s)) \det(M_\downarrow(s))$$

$$M_\delta(s) = \mathbb{I} + B_{L+1}^\delta \dots B_1^\delta$$

$$B_l^\delta(s) = e^{-\Delta_l \tau K} e^{V_l^\delta(s)}$$

sign-free case.

(i) attractive, ($U < 0$). Hubbard.

(ii) repulsive, ($U > 0$). Half-filling, bipartite.

Loh et al (1990). Troyer and Wiese (2005)

Henelius and Sandvik (2000).

Mondani et al (2022).

Phase problem $w(c) \in \mathbb{C}$

$$Z = \sum_c w(c) = \sum_c \text{Re } w(c)$$

$$\begin{aligned} \langle 0 \rangle &= \frac{\sum_c w(c) O(c)}{\sum_c w(c)} = \frac{\sum_c w(c) / \text{Re } w(c) \cdot \text{Re } w(c)}{\sum_c \text{Re } w(c)} \cdot \frac{\sum_c \text{Re } w(c)}{\sum_c \text{Re } w(c)} \\ &= \frac{\langle \text{sgn}(c) \cdot O(c) \rangle_{\text{Re}(w)}}{\langle \text{sgn}(c) \rangle_{\text{Re}(w)}} = \text{sgn } c'' \quad \langle \text{sgn}(c) \rangle_{\text{Re}(w)} \\ &\Rightarrow \frac{Z_w}{Z_{\text{Re}(w)}} \geq \frac{Z_w}{Z_{|w|}} \Rightarrow \frac{Z_w}{Z_{\text{Re}(w)}} \geq \frac{Z_w}{Z_{|w|}} \Rightarrow \frac{Z_w}{Z_{\text{Re}(w)}} \geq \frac{Z_w}{Z_{|w|}} \end{aligned}$$

$$Z(w) \geq Z_{\text{Re}(w)} \geq Z_{\text{Re}(w)} = Z_w \geq 0 \quad Z_{\text{Re}(w)} \geq Z_{|w|}$$

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_V \quad V = \lambda \sum_{ij} \phi_{ij} (n_{i\uparrow} + n_{i\downarrow} - 1) V(\phi_{ij})$$

$$\exists T, e^{-\beta \mathcal{H}} = \sum_{\{\phi\}} \prod e^{-\sum_k h_k \phi_k}, \text{ st: } (T^2 = -1)$$

$$[h(\phi_k), \hat{T}] = 0,$$

$$\text{then: } \det [I + \frac{\pi}{1} e^{-\Delta_k} h] \geq 0$$

spinful case: $\hat{T}: "i\delta_y R"$ 与之对易 $(\delta_0, i\delta_x, i\delta_y, i\delta_z)$

Attractive Hubbard: Decouple to δ_0 , No sign problem in density channel, Decouple to $i\delta_z$, No sign problem in spin channel.

It's time-reversal symmetry after H-S transformation, not the hamiltonian itself!

Spinless t - V model: (bipartite).

$$\hat{V} = V \sum_{\langle ij \rangle} (n_i - 1/2) (n_j - 1/2)$$



spinless "time reversal": $\hat{T}_{int} \in \mathbb{C} \quad \hat{T}^2 = -1$ hard to realize.

"Fermion bag Approach"

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int} \quad \text{perturbation.}$$

$$\mathcal{Z} = \text{Tr} \left[e^{-\beta \mathcal{H}_0} T_{\#} \exp \int_0^\beta d\tau \mathcal{H}_{int}(\tau) \right]$$

$$e^{-\beta \mathcal{H}_0} \mathcal{H}_{int} e^{\beta \mathcal{H}_0}$$

$$H = \sum_{\langle ij \rangle} c_i^\dagger M_{ij} c_j + \frac{V}{4} \sum_b (n_i^+ - n_i^-) (n_j^+ - n_j^-)$$

$$M^T = DMD \quad D_{ij} = \delta_i \delta_{ij} \quad \delta_i = \begin{cases} 1 & \text{if } i \text{ is even} \\ -1 & \text{if } i \text{ is odd} \end{cases}$$

$$n_i^+ = c_i^\dagger c_i \quad n_i^- = 1 - n_i^+ = c_i c_i^\dagger$$

$$\text{Hint} = \frac{V}{4} \sum_{\substack{b, s_i, s_j \\ \text{Bond.}}} (s_i n_i^{s_i}) (s_j n_j^{s_j}) \text{ to calculate.}$$

$$\sum_n (-1)^n \int \prod_I dI \cdot \text{Tr} e^{-\beta H_0} \text{Hint}(I_1) \dots \text{Hint}(I_n) \quad I_K > \dots > I_1$$

$$Z = \sum_K \sum_{\{b, s\}} \int [dz] \left(-\frac{V}{4}\right)^K \text{Tr} e^{-\beta H_0} \times \left[s_{2K} n_{2K}^{s_{2K}} s_{2K-1} n_{2K-1}^{s_{2K-1}} \right. \\ \left. \times \dots \times s_2 n_2^{s_2} s_1 n_1^{s_1} \right] (s_i = \pm 1)$$

$$= Z_0 \times \frac{\int \text{Tr} e^{-\beta H_0} \times 0}{\text{Tr} e^{-\beta H_0}} \quad \downarrow \text{关联函数}$$

$$= Z_0 \times \sum_K \sum_{\substack{\text{bond} \\ (ij)}} \int dz \left(-\frac{V}{4}\right)^K \cdot \text{Det} [G_0(b, s, I)] \quad (2K \times 2K)$$

use Wick, know $\langle C_{0q}^\dagger C_{0q'} \rangle = \left(\frac{e^{-zM}}{1 + e^{-\beta M}} \right) (i q, i q')$

$$\langle C_{iq}^\dagger(z) C_{iq'}(0) \rangle = \left(\frac{e^{zMT}}{1 + e^{\beta MT}} \right) (iq, iq')$$

H_0 : particle-conserved. only $\langle C^\dagger C \rangle$ No $\langle CC \rangle$

decouple $\langle n_{ik} n_{ik-1} \dots n_{i2} n_{i1} \rangle_0$ to:

$$\text{For } q < q' \quad [G_0(b, s, I)]_{qq'} = \left(\frac{e^{-(I_q - I_{q'})M}}{1 + e^{-\beta M}} \right) (iq, iq')$$

$$\downarrow q=q' = [G_0(b, s, I)]_{qq'} = -\frac{s_q}{2} \delta_{qq'}$$

only depend on S only depend on S .

Therefore: $G[b, s, z] = \begin{pmatrix} D_0[s] & A[b, z] \\ \text{Diag.} & \text{Non-Diag.} \end{pmatrix}$

$$\sum_{\{s\}} \text{Det} \cdot G =$$

$$\sum_{\{s\}} d\bar{\psi} d\psi e^{-\bar{\psi} (D_0[s] + A[b, z]) \psi}$$

行列式可写为 Grassman 数 Berezin 积分.

$$\Rightarrow \sum_{\{s\}} e^{-\bar{\psi} D_0(s) \psi} = \prod_{q, s_q = \pm 1} \left(1 + \frac{s_q}{2} \bar{\psi} \psi \right) = 4^K$$

$$\Rightarrow Z = Z_0 \times \sum_{K, [b]} \int [d\tau] \cdot (-V)^{K/2} \times \text{Det} [A(b, z)]$$

A : Real. $A^T = -\hat{D} A \hat{D} \quad (\hat{D})_{ij} = \delta_{ij} \cdot \text{sig} = \delta_{ij} \cdot \delta_{i, q, 2q}$

$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ A : 实反对称阵, 则 $\det[A \hat{D}] \neq 0$
而 $\det(\hat{D}) = (-1)^K$

$$\Rightarrow Z = Z_0 \times \sum_{K, [b]} \int [d\tau] \times V^{K/2} \times \text{Det}(A \hat{D})$$

Fermion bag: $[s]$: part to fermion degree of freedom that can be summed out independently.

$[b, \tau] \neq 0$. sample bond.

Majorana Representation: $\mathbb{R}$ (李自新).

$$c_i = \frac{1}{2} (\gamma_i^1 + i \gamma_i^2)$$

$$c_i^\dagger = \frac{1}{2} (\gamma_i^1 - i \gamma_i^2)$$

$$H_0 = \frac{1}{2} (\gamma_i^1 \gamma_j^2 - \frac{i}{2} \gamma_i^2 \gamma_j^1) \quad X$$

Gauge transform first: $C_i \rightarrow i C_i$, @

$$H_0 \rightarrow -i C_i^\dagger C_j + h.c. \rightarrow -\frac{i}{2} \gamma_i^1 \gamma_j^1 - \frac{i}{2} \gamma_i^2 \gamma_j^2$$

$$H_{int} \rightarrow H_{int} \text{ (No change)} \rightarrow -\frac{V}{4} \sum_{ij} (i \gamma_i^1 \gamma_j^1) (i \gamma_i^2 \gamma_j^2)$$

$$\xrightarrow{\text{H.S.}} e^{V_0 \pi / 4 \cdot (i \gamma_i^1 \gamma_j^1) (i \gamma_i^2 \gamma_j^2)} = \frac{1}{2} e^{-\frac{V_0 \pi}{4} \sum_{\phi_j = \pm 1} \frac{1}{2} \lambda \phi_{ij} i I_5} e^{\frac{1}{2} \gamma_i^1 \gamma_j^1 + \frac{1}{2} \gamma_i^2 \gamma_j^2}$$

$$\cosh \lambda = e^{V_0 \pi / 2}$$

majorana 1 and 2 couple the same auxiliary field.

$$W(\{\phi_i\}) = \text{Tr} \frac{1}{11} \sum_{l=1}^2 e^{\frac{1}{4} \gamma^a h_{(l)}^a \tilde{\gamma}^a}$$

$$h_{(l)}^a = i [t_{0l} \delta_{ij} + \lambda \phi_{ij} (l) \delta_{0j}]$$

$$W_2(\{\phi_i\}) \xrightarrow[\text{Method}]{\text{Pfaffian}} \left\{ \det \left[\mathbb{1} + \frac{1}{11} \sum_{l=1}^2 e^{h_{(l)}^a} \right] \right\}^{1/2}$$

$$W[\{\phi_i\}] = W_1(\{\phi_i\}) W_2(\{\phi_i\})$$

Time Reversal: $\gamma = UK$ $U: \gamma_i^1 \rightarrow (-1)^i \gamma_i^2$
if satisfy this symmetry: on Bipartite.

$$W_1(\{\phi_i\}) = W_2^*(\{\phi_i\}) \Rightarrow W \geq 0$$

Further can proof W_2 itself.

$$\det \left[\mathbb{1} + \frac{1}{11} \sum_{l=1}^2 e^{h_{(l)}^a} \right] \geq 0$$

These Results show on bipartite, spinless t-V model (half-filling) has No sign problem.

split orthogonal group. (Lei's Wang)

if $M \in O(n, n)$. $2n \times 2n$. real. The Group satisfies:

$$M^T \eta M = \eta \quad \eta = \begin{pmatrix} 1 & & \\ & \ddots & \\ & & 1 & \\ & & & -1 & \\ & & & & \ddots & \\ & & & & & -1 \end{pmatrix} \begin{matrix} n \\ \\ n \end{matrix}$$

then:

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} : |\det(M_{11})| \geq 1 \quad |\det(M_{22})| \geq 1$$

separate group to $O^{\pm, \pm}(n, n)$ subgroup.

we can prove: for $M \in O^{++}(n, n)$. $\det(I + M) \geq 0$

For spinless t-V model: H.S.

$$e^{-\sum V (n_i - 1/2)(n_j - 1/2)} \xrightarrow[\text{channel}]{\text{hopping}} \frac{1}{2} e^{-\frac{V \sum \lambda \phi_{ij}}{4}} \frac{(c_i^\dagger c_j - c_j^\dagger c_i)}{2} = \hat{A}$$

$$\cosh \lambda = \frac{1}{2} e^{V \sum / 2}$$

The $\hat{A}$ satisfies: $\eta \hat{A}_i \eta = -\hat{A}_i^T$. Then. $\det(\hat{I} + \prod_i e^{\hat{A}_i}) \geq 0$

Fermion Bag. $\hat{O}_b = (c_i^\dagger c_j + c_j^\dagger c_i)$ $\begin{cases} \hat{O}_b^4 = \hat{O}_b^2 = n_i + n_j \\ \hat{O}_b^3 = \hat{O}_b = -2n_i n_j \end{cases}$

Let: $\hat{U}_{ij} = V(n_i n_j - \frac{n_i + n_j}{2}) - T_{(I \neq 0)}$

Then: $-\hat{U}_{ij} = \frac{T}{2} \sum_{\phi_{ij} = \pm 1} e^{\phi_{ij} \lambda} (c_i^\dagger c_j + c_j^\dagger c_i)$

Fermion Bag: $\dots H(I_k) H(I_{k-1}) \dots$
 $= n_i n_j \dots n_i n_j$

$= \dots e^{\lambda (c_i^\dagger c_j + c_j^\dagger c_i)} \times e^{\lambda \dots}$

still satisfy

No sign problem.

orthogonal Group.

$$SSE: e^{\lambda \hat{O}_b^1} = \frac{1}{\sinh \lambda} \sinh \lambda \hat{O}_b^1 + (\cosh \lambda - 1) \hat{O}_b^1{}^2$$

$$H = \frac{-t}{\sinh \lambda} \sum_{b=1}^{N_b} e^{\lambda \hat{O}_b^1} + \text{const.}$$

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \text{Tr}(H^n)$$

$$= \sum_{n=0}^{\infty} \left(\frac{t}{\sinh \lambda} \right)^n \frac{\beta^n}{n!} \sum_{b_1 \dots b_n} \text{Tr}(e^{\lambda \hat{O}_{b_1}} \times \dots \times e^{\lambda \hat{O}_{b_n}})$$

关联函数可直接求出

$$\text{Still split orthogonal Group.} = \det(\mathbb{1} + \pi e^{A_i})^n \geq 0$$

① split orthogonal Group

② Majorana - Time - Reversal

③ Fermion Bag

} Not Restricted to
spinless t-V model.