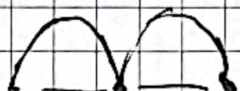
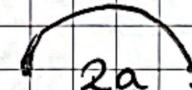


DMRG.

NRG fails of mismatched edge boundary condition.
 当 basis double 时: $| \psi \rangle_{\text{后步}} = | \psi \rangle_{\text{前步}} \otimes | \psi \rangle_{\text{前步}}$

$| \psi \rangle_{\text{前步}}$:  $\Rightarrow | \psi \rangle_{\text{后步}} =$  实际无相互作用
 用语言中为  相差甚大, 截断误差甚大, 而每次增长一个格点误差合适.

DMRG 截断的密度矩阵的特征值 对于等价于做

$$| \psi \rangle = \sum_{m,n} \psi_{mn} | s_m \rangle | e_n \rangle$$

ψ_{mn} 做 SVD 分解, 把新的基下较小的 $m \times n$ system environment 奇异值去掉

$$e_m = \psi_m \psi_m^\dagger = U \Lambda U^\dagger \quad e_n = \psi_n \psi_n^\dagger = V \Lambda V^\dagger$$

$$\psi = \psi_m \otimes \psi_n = \sum_k U_k V_k^\dagger \quad U V \otimes S V^\dagger U^\dagger$$

$$| \psi \rangle = \sum_k S_k | \tilde{l}_k \rangle | \tilde{r}_k \rangle \quad \begin{cases} | \tilde{l}_k \rangle = \sum V_k | s_m \rangle \\ | \tilde{r}_k \rangle = \sum U_k | e_n \rangle \end{cases}$$

$$\text{截 } \rho_m, \rho_n \Rightarrow \rho_m = \left(\sum_{mn} \psi_{mn} \psi_{mn}^\dagger \right) | s_m \rangle \langle s_m |$$

$$\psi_{mn} = U S V \quad \psi \psi^\dagger = U S V V^\dagger S U^\dagger = (U S S^\dagger U^\dagger)$$

$$\Rightarrow \rho_k = U \text{diag}(S_1^2, S_2^2, \dots) U^\dagger \quad \text{截掉奇异值平方即}$$

可即仅仅在 ψ 中截掉 S_k 对应的 basis 就可以了 不必再回到 ρ_l, ρ_r 表象中了.

之于 Kondo 适用 NRG 解法.

$$H = H_0 + H_{fk} = \sum_{m \rightarrow n} H_m$$

$$H_{m+1} = H_m + E_m f_m^\dagger f_{m+1} + t_m (f_m^\dagger f_{m+1} + \text{h.c.})$$

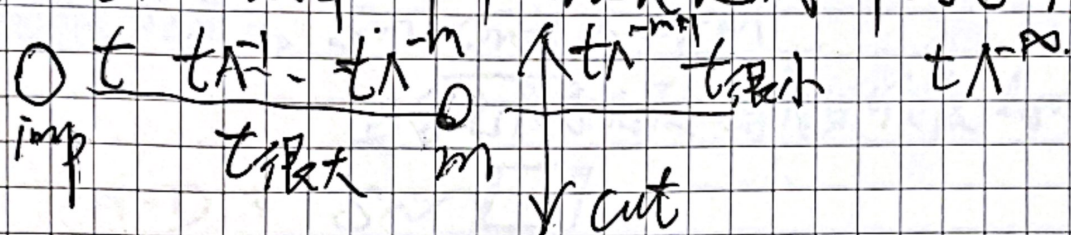
$$H_m: \quad \underbrace{t_V}_{D.H_{\text{imp}}} \quad \underbrace{t_0} \quad \underbrace{t_1} \quad \underbrace{t_2} \quad \underbrace{t_{m-1}} \quad \underbrace{t_m}_{E_m}$$

它把杂质 δ 作为半无限长一维链的增长过程。

全为 f_m^+ 项，而 $t_1 \dots t_{m-1}$ 为随着 m Λ^{-m} 形式。

对于能标 t $t_{m+1} = \Lambda^{-1} t_m$ 我们截断能标 $t \dots t_{ps}$

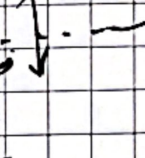
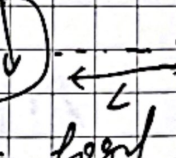
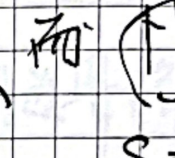
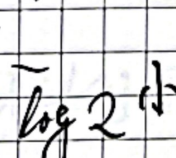
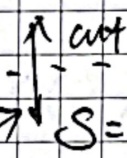
把 $t_{s+1} \dots$ 丢掉 即半无限长链截断到了某个 m ($\sim m$)



"Kordon" 中 "cut" 自然把 "t 很大" 与 "t 很小" 部分给分开了。

截恰到好处。对于 Bond Dimension.

Kondo singlet



$S \sim \log L$ 甚小.

Bond Dimension: $| \Psi \rangle = \sum A^{s_1} A^{s_2} \dots A^{s_N} | s_1 \dots s_N \rangle$

$A^{s_1}: (1 \times d) \dots A^{s_{L/2}}: (d^{1/2} \times d^{1/2+1}) A^N: (d \times 1)$

A 维度 $\propto$ 保留的 A 维度 Bond Dimension.

Bond Dimension 决定保留低能态数量.

$$d_{i-1} \times d_i = d_{i+1} \times d_{i+2} \quad A^{s_{i+1}} = \text{dim} [X_i \cdot d_{i+1} \cdot X_{i+1}]$$

site link site Bond Dimension.

$$A^{s_i} \quad A^{s_{i+1}} \quad \sqrt{S \leq \log d}$$

① 做无限DMRG到 L 自然扩大 Bond Dimension.

② 只有几个 site 也有几个 Bond Dimension.

关联甚强时. J 为大. 似乎引入 $\gamma = 3$ 等等.

更多件. 相互作用. 极大增加了 ~~系统~~ 自由度.

$$i(s_i) \otimes (i-j) [s_i \otimes s_j], \quad S \leq \log x \text{ (下页)}$$

"Link" 的自由度因相互作用太大了; 一个 s_i 与多 site



奇异值一样. $S_{\max} = \log M \rightarrow$ 矩阵维度.

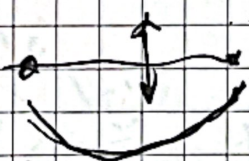
$S \sim \log(d^{1/2}) = \frac{1}{2} \log d$ (1-D). $S \propto$ A-B 边界长度

而低能态 $S \sim \text{const} \times \log M$

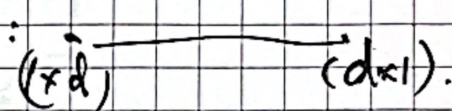
与系统尺寸无关 与系统维度 $\log M$

2-D: $S \sim$  $L \times \log L$

PBC:



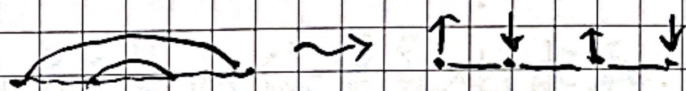
OBC:



"纠缠均匀分布" $x_L = \dots = x_N$ 无法利用边界降低
计算复杂度. 全都是 $x_{\max}$.

Disentangler. 通过 Unitary transformation. 可以把
 $(| \uparrow \downarrow \rangle - | \downarrow \uparrow \rangle) / \sqrt{2} \rightarrow | \uparrow \downarrow \rangle$.

similar, 也可以把态. 降低纠缠通过 disentangler.



通过走一条量子线路做构造 Unitary Matrix.

2-D 设计 Disentangler.

$$\text{Finite } T: |\varphi\rangle = e^{-\beta H} |\varphi_{\max \text{ entangle}}\rangle = |\varphi_T\rangle$$

$$= (e^{-\delta_1 H})^N |\varphi_{\max \text{ ent}}\rangle$$

$$= (e^{-\delta_1 H}) \dots (e^{-\delta_N H}) |\varphi_{\text{ent}}\rangle$$

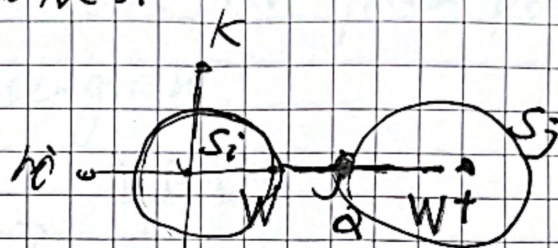
DMRG cutoff until truncation error

张量网络

① 两分量函数可以用张量网络表示

2-D Ising:

$$Z = \sum_{\{S_i\}} \prod e^{-\beta S_i \cdot S_j}$$



$$= \sum W_{S_i, a}^i W_{S_i, b}^i W_{S_j, c}^{j\dagger} W_{S_j, d}^{j\dagger}$$

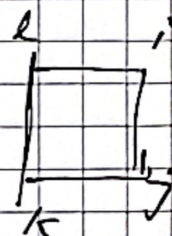
$$\text{Tr} \left[A_{\text{site}}^{\text{Link 1, 2, 3, 4}} \times A_{\text{Link 1, 2, 3, 4}}^{\text{site } i+1} \right]$$

张量缩并为求 Tr.

$$e^{\beta J S_i S_j} = e^{\beta J / 2 (\delta_{ij} + \delta_{jk} + \delta_{kl} + \delta_{li})}$$

site index

Bond Index



因此

$$Z = \sum_{\{S_i\}} \prod e^{-\beta H \{S_i\}}$$

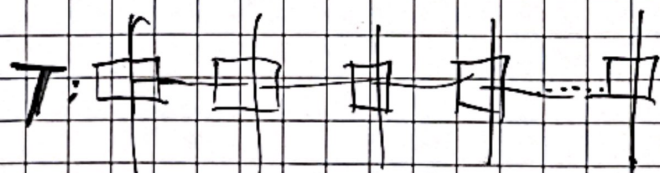
Link 由 Tr 缩并

$$= \text{Tr} (A^{S_1} A^{S_2} \dots A^{S_N})$$

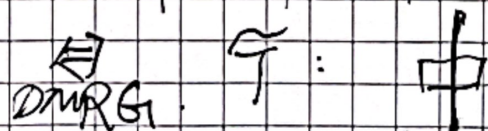


② 张量网络重整化求和.

1) DMRG



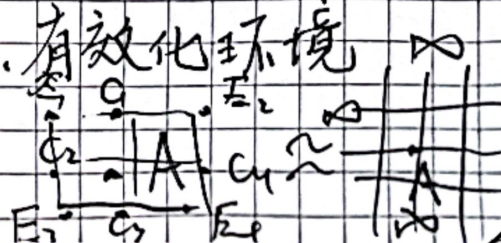
Tr index 指数增加.
DMRG 截断有限 index



$$2) \text{CTMRG} \quad Z = \text{Tr} (T A e T e)$$

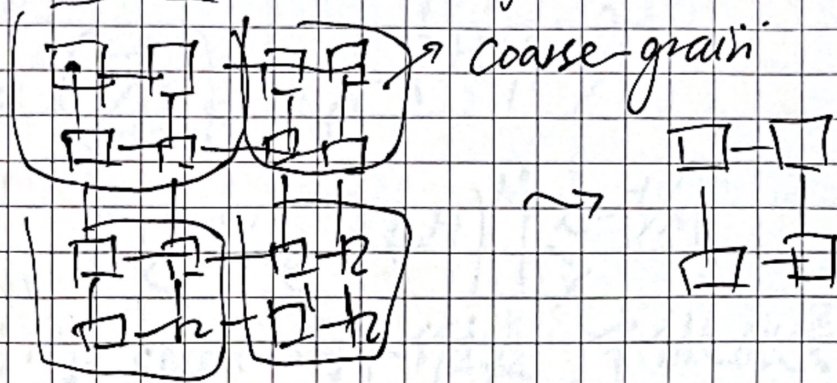
A 为一个 site; e 为 site 外的环境. 有效化环境

$$T e \sim \{C_1, C_2, C_3, C_4, E_1, E_2, E_3, E_4\}$$

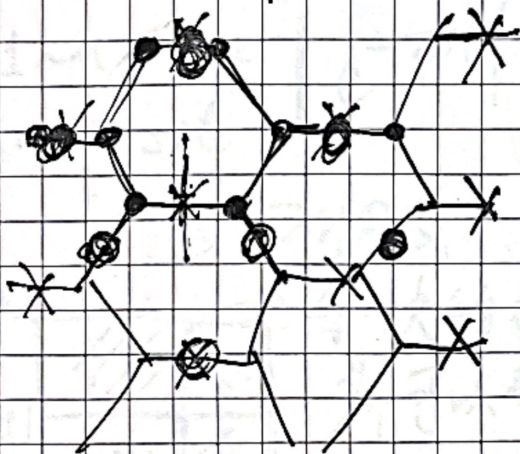


3) Coarse graining - graining TRG.

Do SVD-based scale transformation. till fixed point.



每次 coarse-graining 总能把 $\times$ 大到 1 个 site 就是天
做 local SVD 直接按谱切断至 $1/4$ 类似 NRG 忽略环
境纠缠的作用。



Finite temperature RG.

cooling ① Trotter Decomposition:

$$Z = \left(\sum_{\{I\}} e^{-\beta H} \right)^M$$

$$= \langle (e^{-\beta H})^M \rangle_{Z^{-1/M}}$$

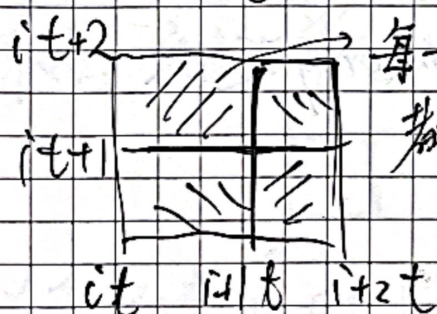
有: 虚时间. site i 两个维度. 中做张量缩并 Tr .

$$H(i, i+1) \sim H(\{i, i+1\}, \{i+1, i+2\}, \{i, i+1\}, \{i+1, i+2\})$$

$$\Rightarrow Z = \sum_{\{I\}} e^{-\beta H} \Rightarrow Z_{MN}$$

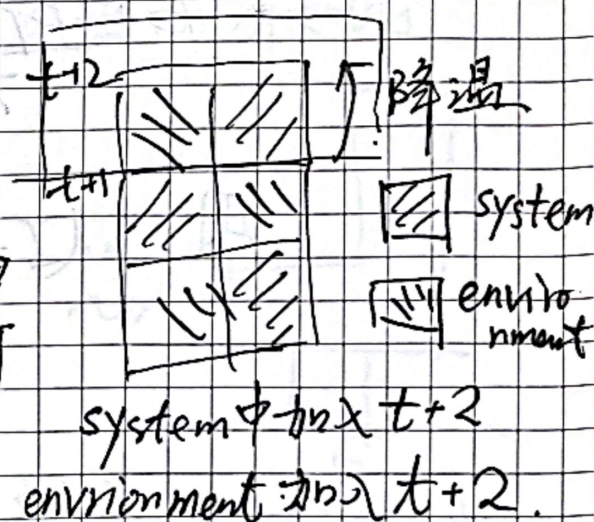
$$\left\langle \sum_{1 \sim N \text{ site}} e^{-\beta H} \right\rangle$$

② DMRG



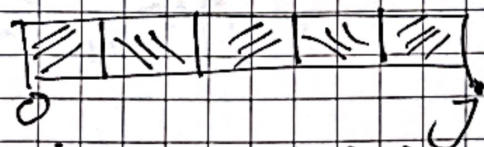
每一块的张量缩并
都可以给出

加一个



得 reduced density matrix. 做截断.

$T \rightarrow \infty$ $t=0$

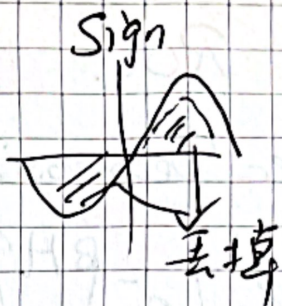


MPS 已知.

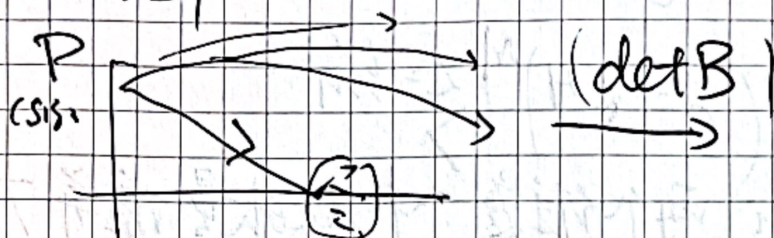
(基本 Random setup)

在若干步虚时间后也需要空
间做 sweep 保证精确.

限制路径. AFQMC
向DMC: 符号问题



DMC过程中



所有路径中一旦概率掉到零. 直接丢掉这条路径.

所谓 $\sum P \times \det(I+B)$ 只在此处近似

$$B = B_1 \times \dots \times B_l \times B_{l+1} \times \dots \times B_N$$

Throw!

Find $p =$

用

$$\left(I + \sum_{l=1}^N B_l \right)$$

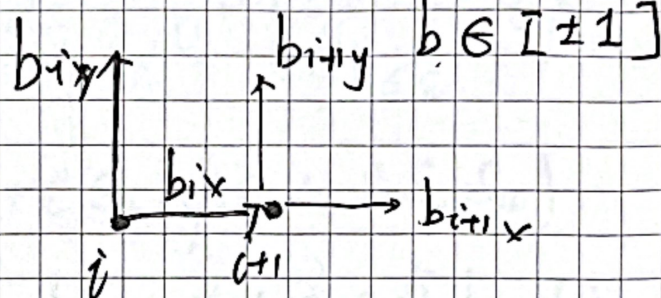
Here 做 only 近似

Ising Model. 蠕虫蒙特卡.

$$H = -J \sum_{\langle i,j \rangle} \delta_i \delta_j = -J \sum_{\langle i,j \rangle} b_{ij} \mu_i \mu_j$$

在 bond 表来写出 Ising.

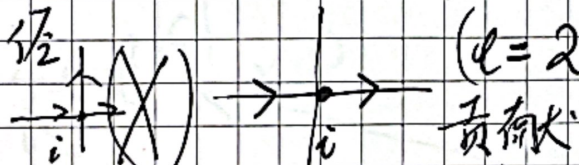
$$Z = \sum_{\{n_b\}} \frac{J^{n_b}}{n_b!} \sum_{\{b_i\}} b_i^{n_b} P_i$$



用 "closed Loop" 表示 Z.

$$Z = 2^N \sum_{\{n_b\}} \left(\frac{J^{n_b}}{n_b!} \right) W_{\{n_b\}}$$

对于格点 i , 有偶数个 bond 属于 "Loop" 可以存在. 才为闭合路径.



开始. 产生小单元. 增加小单元

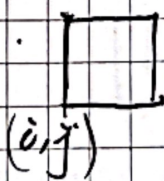


关联函数同时生成

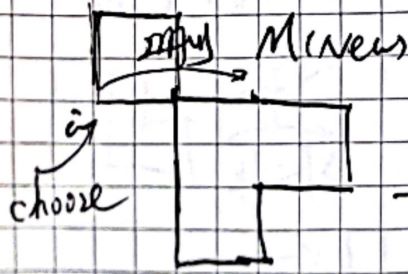
$$\langle \delta_i \delta_j \rangle = \frac{\sum_{\{n_b\}} W_{\{n_b\}} A_{i,j}}{\sum_{\{n_b\}} W_{\{n_b\}}}$$

断开 $\{n_b\}$ 路径在 i,j 处的 w

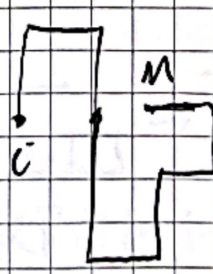
更新.



closed for contain loop.
 $\therefore \therefore 1 \rightsquigarrow -1$ 减一线



删除接收数据



直到 $i \sim m$ 重新同一点

$$Z = (\cos \beta J)^{N_b} \sum_{\{S_i\}} \prod_{\langle ij \rangle} (\tan(\beta J) \cdot S_i \cdot S_j + 1)$$

而:

$$\prod_{\langle ij \rangle} (1 + t S_i \cdot S_j) = \sum_{E \subseteq \text{edge}} t^{|E|} \prod_{\langle ij \rangle \in E} S_i \cdot S_j$$

$$(1 + t S_1 S_2)(1 + t S_1 S_3)(1 + t S_2 S_4)(1 + t S_3 S_4)$$

$$= t^1 (\text{方格子中只有1条 bond}) + t^2 (\text{有2条 bond})$$

而 $\sum_{S_i = \pm 1} - \text{一条 bond} = 0 \dots \dots$ 只有某些项非零
即每个 i 处都连接2个 bond 的构型

$$Z = \sum_{\{C\}} t^{|C|} \times 2 = (2)^{\sum_{\{C\}} |C|}$$

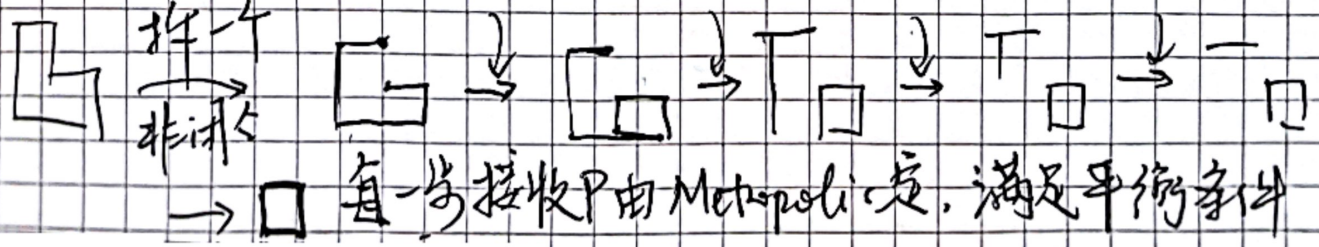
该构型包含的 bond 数目为 C

闭合路径构型
构型中只包含

$$Z = \sum_{3 \times 3} (t^4 \times 2 \times 4 + t^6 \times 2 \times 2 + t^6 \times 2 \times 2 + t^8 \times 2 \times 1 + \dots)$$

$\{C\} = \square$ 4个 $\{C\} = \square$ $\{C\} = \square$ $\{C\} = \square$

从某个构型出发 随机 直至遍历所有构型



关键是让“端点”遍历所有闭合 Loop 空间。

通过 local update (足够多) + global update 遍历所有拓扑构型。接收概率 $p(c_1 \rightarrow c_2) = \frac{t^{c_1 - c_2}}{N_{\text{paths}}}$ 满足细致平衡条件。若 c_1 已知，构型已知，可得各物理量了。

通过非闭合路径计算关联函数。

$$Z_{ij} = \sum_{c \in P_{ij}} t^{|c| + P_{ij}} \text{ 从 cloud } i \text{ 打开 } P_{ij}$$

$$\langle S_i S_j \rangle \propto \sum_{P_{ij}} (\text{Probability } P_{ij} \text{ 接收}) \times t^{P_{ij}}$$

$$G(i, j) = \langle S_i S_j \rangle = \frac{1}{Z} \sum_{S, k, l} S_i S_j e^{-\beta H}$$

$$= \frac{1}{Z} \sum_{\{S\}} t^{|\mathcal{L}|} \underbrace{\sum_{\{S, k\}} S_i S_j}_{\text{关联}} \underbrace{\sum_{\langle k, l \rangle \in E} S_k S_l}_{\text{closed}}$$

现在是求 $\sum_{\{S, k\}} S_i S_j \sum_{\langle k, l \rangle \in E} S_k S_l$

现在非零条件为 (i, j) 处有奇数个 Bond 其它为偶数个闭合 Loop，故 G_{ij}

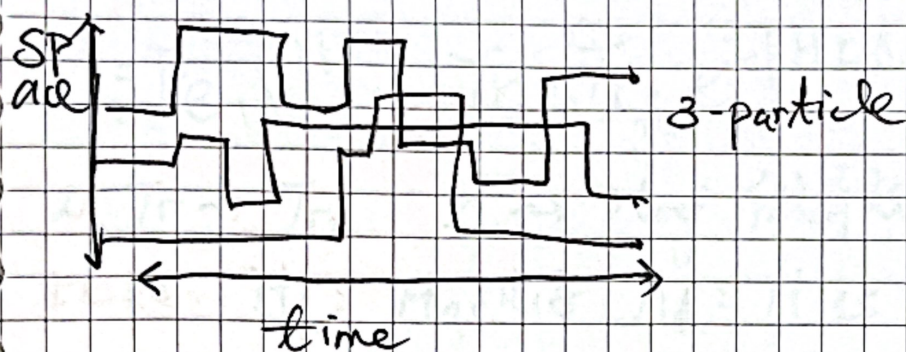
$$G_{ij} = \left(\right) \times \begin{array}{|c|c|} \hline \bullet & \bullet \\ \hline \end{array} \begin{array}{|c|c|} \hline \bullet & \bullet \\ \hline \end{array}$$

$$\left(\begin{array}{|c|} \hline \bullet \\ \hline \end{array} + \begin{array}{|c|c|} \hline \bullet & \bullet \\ \hline \end{array} + \dots \right)$$

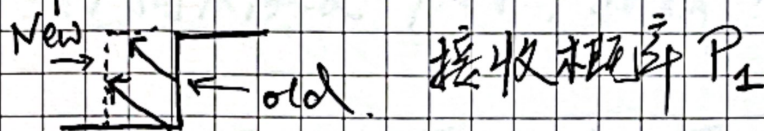
仍然遍历构型，得到 Z_{ij}

量子. 蠕虫算法. 路径积分 + 1维.

一个 World-Line 构型.



Type 1 update: Time Shift

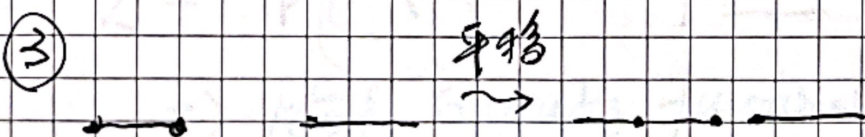
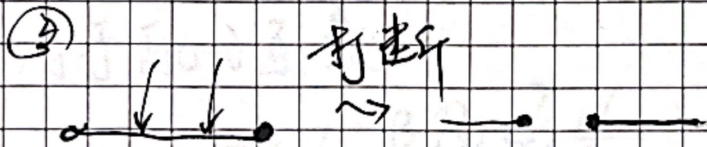
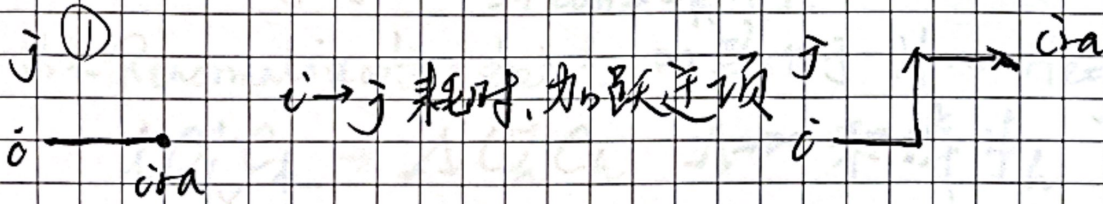


Type 2 update: 一对 'Kink'



Type 1 + Type 2 生成所有构型

在蠕虫中. 加入一组新开世界线. 三种更新



产生蠕虫首末时. 该对时间平移. 空间跳跃.

可以生成所有构型. 格林函数从建程中产生 $G(j, z)$

ED

回顾Boson型的Lindhard Formula. 分子上 $\langle n | A_q^\dagger | m \rangle$
等式子用imaginary time 投影 $e^{-\beta E_n}$ 在 $\beta \rightarrow \infty$ 到基态.
因此考虑零温 (磁) 激发:

$$\frac{1}{d} \sum_m \left[\langle 0^d | \hat{A}_q \frac{1}{i\omega + E_0 - \hat{H} + i\eta} A_q^\dagger | 0^d \rangle \right. \\ \left. \pm \langle 0^d | A_q^\dagger \frac{1}{i\omega - E_0 + \hat{H} + i\eta} A_q | 0^d \rangle \right] = G_A^R(q, \omega)$$

回顾ED. 选择Basis. 考虑好量子数 ($S_{\text{tot}}^z, S_{\text{tot}}^2, \text{spin-rotation symmetry, translation symmetry}$).

$$[\hat{T}_i, H] = 0 \quad \hat{T}_i |\psi(\vec{k})\rangle = e^{i\vec{k} \cdot \vec{r}_i} |\psi(\vec{k})\rangle$$

Lanczos $\forall |V_0\rangle$ 起始

$$\text{span} \{ |V_0\rangle, H|V_0\rangle, \dots, H^L|V_0\rangle \}$$

做Schmidt正交化, 到正交空间

$$|V_0\rangle, |V_1\rangle, \dots, |V_L\rangle$$

原本为 $|V_0\rangle, |V_1\rangle, \dots, |V_\infty\rangle$ 在 $|V_L\rangle$ 处截断, 后验截断误差, 在Basis $|V_0\rangle, \dots, |V_\infty\rangle$ 下.

$$H \mapsto U_L^\dagger H U_L = \begin{pmatrix} \text{---} & & 0 \\ & \text{---} & \\ 0 & & \text{---} \end{pmatrix} \text{三对角矩阵.}$$

在对角化 (QR) 三对角矩阵即可.

对 $\forall H$ 对称矩阵均可表示. 而 $G = \frac{1}{z - H}$

由于 $(z - H)$ 对称, 可表示为 $\begin{pmatrix} z - a_0 & & 0 \\ & \text{---} & \\ 0 & & \text{---} \end{pmatrix}$

三对矩阵写作

$$\begin{pmatrix} z-a_0 & B \\ C & z-H_1 \end{pmatrix}_{2 \times 2}$$

$$G = \left[\frac{1}{z-H} \right]_{00}$$

H_0 按自大向小排: a_0 :

用 Lanczos 得到基态 $|\psi_0\rangle$ S_g 激发谱.

$$S_g = -\frac{1}{\epsilon} \lim_{\eta \rightarrow 0} \text{Im} G_g^R(\omega + i\eta) \text{ 自旋 Green's Function.}$$

定义 $|\phi\rangle = S_g |\psi_0\rangle$ 为 $|\psi_0\rangle$ 为输入

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} A - BD^{-1}C & B \\ C & D \end{pmatrix}^{-1} \rightarrow G_{00} = \frac{1}{z-a_0 - \frac{b_1^2}{z-H_1}}$$

一直往下做:

$$G = \frac{1}{z-a_0 - \frac{b_1^2}{z-a_1 - \frac{b_2^2}{z-a_2 - \dots \text{cutoff}}}}$$

$$\text{Matrix } G: \langle 0 | S_g H S_g | 0 \rangle = E_1 = \omega + E_0$$

理论上:

$$G = \left(\frac{1}{\omega + E_0} \right), \quad G(\omega) = \langle 0 | S_g \frac{1}{z-H} S_g | 0 \rangle$$

用 $|\phi\rangle$ 表示

矩阵 $z = \omega + E_0$.

因此, 计算 $G(\omega)$ 步骤为

① 得到 H 基态 $|0\rangle$: E_0

② 得到 $S_g |0\rangle = |\phi\rangle$ 为

③ 以 $|\phi\rangle$ 为 $|\psi_0\rangle$ 以 $\begin{pmatrix} z-a_0 & b_1 \\ -b_1 & z-a_1 \end{pmatrix}$ 为 Matrix: G^{-1}

④ 再进行 Lanczos, 得到

从 G^{-1} 到 G :

$$\text{⑤ } G = \left(\frac{1}{z-a_0 - \frac{b_1^2}{z-a_1 - \frac{b_2^2}{\dots}}} \right)$$

$$\begin{pmatrix} z-a_0 & b_1 \\ -b_1 & z-a_1 \\ & & \ddots & \ddots \\ & & & z-a_{n-1} \end{pmatrix}$$