Subroutine Introduction —— 32 subroutines in total

1. SuNF : main subroutine
2. blockc : define and allocate variables
3. block_obs : define and allocate observables
4. salph : define and assign value for the intermediate variables alpha 用于更新和测量
5. sli : define functions related to lattice structure
6. setH : set up hopping matrix
7. sthop : set up exponential hopping matrix
8. upgradeU : update auxiliary field of Hubbard interaction
9. upgradeJ : update auxiliary field of hopping square (J) interaction
10. mmuur : ITEM * UR (ITEM ≡ interaction trotter exponential matrix)
11. mmthr : HTEM * UR (HTEM ≡ hopping trotter exponential matrix)
12. mmuul : ITEM * UL
13. mmthl : HTEM * UL
14. mmuurml : UR ÷ ITEM
15. mmthrml : UR ÷ HTEM
16. mmuulml : UL ÷ ITEM
17. mmthlml : UL ÷ HTEM
18. ortho : SVD orthogalization of UR matrix
19. dyn
20. propr
21. obsert
22. proprml
23. prtau

$\left.\begin{array}{l}\text{19. dyn}\\ \text{20. propr}\\ \text{21. obsert}\\ \text{22. proprml}\\ \text{23. prtau}\end{array}\right\}$ time-dependent measurement

24. calcgr : calculate equal-time single-particle Greens' function
25. obser : evaluate equal-time observables using equal-time Greens' function
26. preq : output equal-time observables

27. sproj：计算试探波函数PROJ和TWF，以及DEGEN和EN-FREE

28. sethproj：无相互作用哈密顿量中放入微扰

29. outconfc：输出辅助场构型

30. inconfc：初始化辅助场

31. nranf：由随机数种子随机取1/2/3

32. npbc：在SLI中的period boundary condition

Parameter introduction

Through "paramC-sets" file we input the parameters in the programme.

BETA : inverse of tempreture $\beta = \frac{1}{T} = \delta\tau \cdot L_{trot}$

Ltrot : the number of trotter slice in total imaginary time

Ltrot_quench : the number of trotter slice in quench imaginary time

NWRAP : the frequency of imaginary-time sweep to do stabilization

若NWRAP=10，则每10个τ点做一次数值稳定（UDV）

RT1 : nearest-neighbor hopping

RHUB1 : Hubbard interaction of initial $\hat{H}$ in quench process

RHUB2 : Hubbard interaction of final $\hat{H}$ in quench process

RJ : hopping square interaction 次近邻相互作用参数 chiral ising相互作用项

在mc中，bins可以理解为结果的可能差别。对于QMC就是系综。这里是测量nbin次，每次都是不同系综。

NBIN : the number of MC bins

NSWEEP : the number of time-space sweep in a MC bin

做n次sweep测量1次可观测量，一次sweep把时空上每个点的辅助场都过一遍

LTAU : 1 → perform time-dependent Greens' function computation

0 → do not perform ...

NTDM : the number of imaginary-time point to do time-dependent Greens' function computation

NLX, NLY : linear system size x、y方向元胞个数

Itwist : 微扰种类（1，2）

TwistX : twist of momentum on the lattice 在H里加的较小的微扰，破坏可能的能级简并

N_sun : the number of fermion flavors ✓ 电子的自旋取向自由度

NE : the number of electrons × SU(N)

Other variables

$LQ = NLX \cdot NLY$ 元胞数

$NDIM = 2 \cdot LQ$ 格点数

Norb 每个元胞的原子个数

MPI 并行分布 $\begin{cases} \text{ISIZE 核数(节点数)} \\ \text{IRANK} = 0 \end{cases}$

DEGEN : 空态最低能量与占据态最高能量之差, DEGEN → 0 反映 Dirac点处简并 (gapless)

EN_FREE : 自由能

$MMULT = UR \cdot UL = ULR$

$INV = ULR^{-1}$

RATIOUP : 两个行列式比值

dtau : $\Delta\tau$

ISIZE : 并行运算的节点个数

Files

unit =50 , info

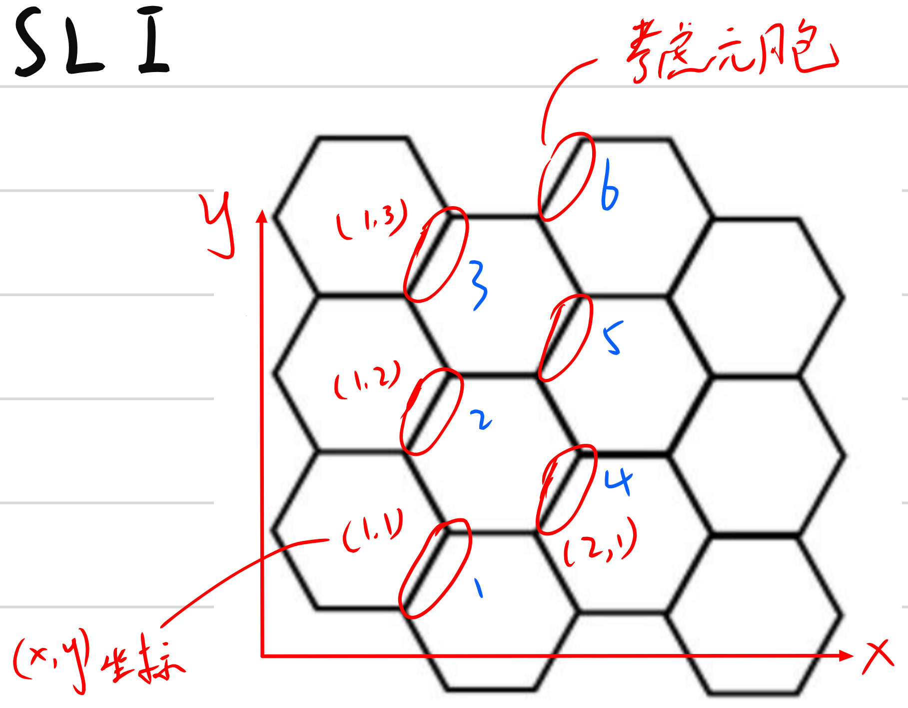
unit=20 , paramC-sets

unit=30 , confin

unit = 10 , seeds

unit = 35 , confout

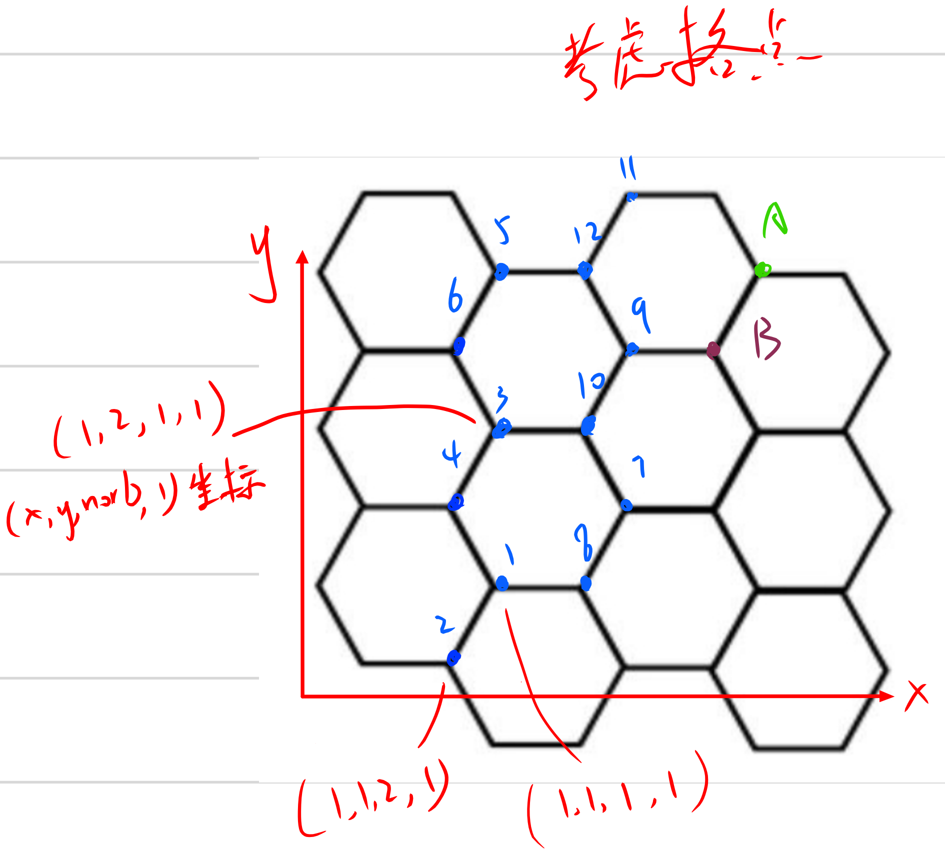
SLI



list(元胞序号, 第几个坐标参量)
用于导出坐标参量值

invlist(x, y)
用于导出坐标对应序号

★这里"序号"可理解为元胞/格点的索引



nlist(格点序号, 第几个坐标参量)
用于导出坐标参量值

invnlist(x, y, norb, 1)
用于导出坐标对应序号
(norb=1 表示A子格点)

L_bonds(元胞序号, 0/1/2/3)

导出A子格点序号　导出B子格点序号　导出x+1处元胞的B子格点序号　导出y+1处元胞的B子格点序号

附有 period boundary condition

※ 单位矩阵 $ZKRON_{NDIM \times NDIM}$

※ 函数 Iscalar(vec1, vec2) 二阶向量点乘

NPBCX(NR)　NR>nlx 则导出 NR-nlx, NR<1 则导出 NR+nlx, 否则导出NR

NPBCY(NR) 同上

SALPH

4分量辅助场 $l=\pm1,\pm2$

ETAL 即 $\eta(\pm1)=\pm\sqrt{2(3-\sqrt{6})}$, $\eta(\pm2)=\pm\sqrt{2(3+\sqrt{6})}$

GAML 即 $\gamma(\pm1)=1+\sqrt{6}/3$, $\gamma(\pm2)=1-\sqrt{6}/3$

① for J term

ALPHA 即 $\alpha=\sqrt{\frac{1}{4N\_SUN}RJ\cdot\Delta\tau}$

XSIGP2(l) $=e^{\alpha\cdot\eta(l)}$

XSIGM2(l) $=e^{-\alpha\cdot\eta(l)}$

存储 l 的 4 种情况

DELLP2(l=-2/-1/1/2, 1/2/3) $=e^{\alpha[\eta(l')-\eta(l)]}-1$

DELLM2(l=-2/-1/1/2, 1/2/3) $=e^{-\alpha[\eta(l')-\eta(l)]}-1$

DGAML(l=-2/-1/1/2, 1/2/3) $=\frac{\gamma(l')}{\gamma(l)}$

存储从任意 l 到另外3个 l' 的 12 种情况

③ for flipping

NFLIPL(l, 1/2/3) 用于导出另外3个 l'

④ pair-hopping

$$UR\_K=\begin{bmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\end{bmatrix},\quad URT\_K\equiv UR\_K^{\dagger}$$

用于 chiral Ising 相互作用项表象变换

⑤ for Hubbard

若 $U\ge0$, 则 alpha_U 记为 $\alpha_U=i\sqrt{\frac{1}{N\_SUN}U\cdot\Delta\tau}$ (N_SUN=2)

若 $U\le0$, 则 $\alpha_U=\sqrt{-\frac{1}{2}U\cdot\Delta\tau}$

XSIGM_U(l) $=e^{\alpha_U\cdot\eta(l)}$

DELTA_U(l=-2/-1/1/2, 1/2/3) $=e^{\alpha_U[\eta(l')-\eta(l)]}-1$

DETA_U(l=-2/-1/1/2, 1/2/3) $=e^{-\frac{1}{2}\alpha_U[\eta(l')-\eta(l)]}$

SetH

把 RT1 记作 t

用固定的随机数种子，生成 0~1 随机数 random = ranf(3958195)

$$HLP2(i\_o,\ i\_n) = -t + TwistX \cdot (random - 0.5)$$

$$HLP2(i\_n,\ i\_o) = HLP2(i\_o,\ i\_n)^*$$

某元胞A子格点序号

与该格点最近邻的B子格点序号

$HLP2_{ndim \times ndim}$

SetH proj

把 RT1 记作 t

用固定的随机数种子，生成 0~1 随机数 random = ranf(3958195)

$$HLP2(i\_o,\ i\_n) = -t$$

$$HLP2(i\_n,\ i\_o) = -t^*$$

与该格点最近邻的B子格点序号

某元胞A子格点序号

恒有 $i\_o \neq i\_n$

故 $HLP2(n,n) \equiv 0$

这里 n 为任意整数 $\in [0, ndim)$

若 $Itwist = 1$，则 $HLP2(i\_o,\ i\_n) = -t + TwistX \cdot (random - 0.5)$

$$HLP2(i\_n,\ i\_o) = HLP2(i\_o,\ i\_n)^*$$

若 $Itwist = 2$，则 $HLP2(n,n) = TwistX \cdot (-1)^{norb}$

norb → 1 或 2

A 或 B 子格点

☆ 这里得到的 HLP2 是没有相互作用的、加了微扰的多体 $\hat{H}$

（动能项系数矩阵）

S proj

把 SetHproj 导出的 HLP2 记为 TMP，　　Diag(TMP, PROJ, WC)

$$TMP_{ndim\times ndim}\,|n\rangle_{ndim\times 1} = n\,|n\rangle_{ndim\times 1}$$

这里不同于 PQMC 算法讲义，讲义上还有自旋维数 $x=(i,\sigma)$

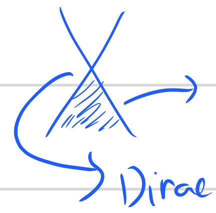
各个 $|n\rangle$ 组成 PROJ 试探波函数　　PROJ $[\;\vdots\;\vdots\;\vdots\;\vdots\;]$ 每一列都是一个本征向量

WC 是本征值表 (ndim维向量)

EN_FREE = 前NE个本征值相加 · N_SUN ～系统自由能

DEGEN = WC(NE+1) − WC(NE) ～ 可以用来表征简并度，但不是简并度。对于半填充系统，这表示空态最低能量与占据态最高能量之差；若为0，则简并，无能隙；若不为0，则不简并，有能隙。

※对于我们的系统，低能区域能谱为



→ 占据态/基态，在 Dirac点 线性色散 ⇓ Dirac费米子

Dirac点处应当有DEGEN→0 (L→∞)

★ L取3的倍数使得动量能取到Dirac点

St Hop

从 SetH 导出 HLP2

Diag(HLP2, HLP1, WC)

$$URT\_tot(i,j) \mathrel{+}= HLP1(i,m)\cdot e^{-\Delta\tau\cdot WC(m)}\cdot HLP1(j,m)^{\dagger}$$

$$URTM1\_tot(i,j) \mathrel{+}= HLP1(i,m)\cdot e^{\Delta\tau\cdot WC(m)}\cdot HLP1(j,m)^{\dagger}$$

1~ndim

要把动能项系数矩阵放到指数上，但没法直接把非对角的矩阵放上去，需要先对角化

这里理解为 $URT\_tot_{ij}\,HLP1_{jm} = HLP1_{im}\,e^{-\Delta\tau\cdot WC(m)}$

那么 URT_tot 即 $e^{-\Delta\tau\cdot h_t}$ → 动能项系数矩阵

INconfc

从confin文件读取Iseed，

若Iseed=0，则从seeds文件中读取ISEED() 作为随机数种子，

对格个节点，随机决定 { NSIGL_K(元胞序号，1/2/3，虚时位置) = ±1
NSIGL_U(格点序号，虚时位置) = ±1 }

若 Iseed≠0，则从 confin文件中读取 NSIGL_K 和 NSIGL_U
（或记为ITMPK 和 ITMPU）

假设是单核，那只用到一行seed，然后剩下 nbin·Ltrot·Lq·Nfam 次调用 RANF，靠的是它按照内置算法自动更新种子（故是伪随机）

如果初始用的seed不同，那后面自动更新种子也不同，伪随机产生的辅助场也就不同。

如果是多核，则按核数N读取N行seed，每个节点的初始seed不同。

MMTHR

输入 A

输出 URT_tot · A 即 $e^{-\Delta\tau\cdot h_t}\cdot A$

（调用了 mmult(A1, URT_tot, A) 将 URT_tot 和 A 相乘）

MMUUR

输入 A

输出 $e^{\alpha_U\cdot\eta(NSIGL\_U)}\cdot A$ 即 $e^{\alpha_U\cdot\eta(\pm 1)}\cdot A$

UPGRADEU

在某格点 $\vec{i}$ 和虚时间 τ 下，

由 iseed0 随机

$$DEL44 = DELTA\_U(l_{\vec i,\tau}' = \pm 1,\ 1/2/3) = e^{\alpha_U\cdot[\eta(l'_{\vec i,\tau})-\eta(l_{\vec i,\tau})]}-1$$

$$VHLP1(\text{电子}) = \left\{e^{\alpha_U\cdot[\eta(l'_{\vec i,\tau})-\eta(l_{\vec i,\tau})]}-1\right\}\cdot UR(\vec i,\ \text{电子})$$

$$UHLP1(\text{电子}) = UL(\text{电子},\ \vec i)$$

$$G44up \mathrel{+}= \left\{e^{\alpha_U\cdot[\eta(l'_{\vec i,\tau})-\eta(l_{\vec i,\tau})]}-1\right\}\cdot UR(\vec i, nl)\cdot ULRINV(nl,\text{电子})\cdot UL(\text{电子},\vec i)$$

$$= \Delta^{(\vec i)}\cdot\left[B(\tau,0)P\cdot\left(P^\dagger B(2\theta,0)P\right)^{-1}\cdot P^\dagger B(2\theta,\tau)\right]_{\vec i,\vec i}$$

$$= \Delta^{(\vec i)}\left[B^>\left(B^<B^>\right)^{-1}B^>\right]_{\vec i,\vec i}$$

$$RATIO_{up} = (1+G44up)\cdot e^{-\frac{1}{2}\alpha_U[\eta(l'_{\vec i,\tau})-\eta(l_{\vec i,\tau})]}$$

$$RATIO_{tot} = RATIO_{up}\ \hat{}\ N\_SUN = RATIO_{up}^2$$

$$RATIO\_RE\_ABS = |RATIO\_RE| = \left|\frac{\gamma(l'_{\vec i,\tau})}{\gamma(l_{\vec i,\tau})}RATIO_{tot}\right|$$

upgrade the inverse

若 RATIO_RE_ABS > RANF(ISEED0) 则 ACCM += 1 weight = 模(RATIO tot)

UI (·ℓ σ) += ULRINV(·ℓ σ, nl) · UL(nl, $\vec{i}$)

DENOM = 1 / (1+ G44 up) = $\frac{1}{1+\Delta B^{>}(B^{<}B^{>})^{-1}B^{>}}$

$$VI = \Delta B^{>}(B^{<}B^{>})^{-1} \frac{1}{1+\Delta B^{>}(B^{<}B^{>})^{-1}B^{>}}$$

ULRINV = ULRINV − ULRINV · UL · VI

$$= (B^{<}B^{>})^{-1}\left[1 - \frac{B^{>}\Delta B^{>}(B^{<}B^{>})^{-1}}{1+\Delta B^{>}(B^{<}B^{>})^{-1}B^{>}}\right]$$

$$(B^{\langle}_{\vec{s}'}B^{\rangle}_{\vec{s}'})^{-1} = \left(B^{\langle}_{\vec{s}}(1+\Delta^{(\vec{i})})B^{\rangle}_{\vec{s}}\right)^{-1} = \left(B^{\langle}_{\vec{s}}B^{\rangle}_{\vec{s}} + \sum_q \vec{u}^{(q)} \otimes \vec{v}^{(q)}\right)^{-1}$$

upgrade UR

$$UR = \left(1+\left(e^{\alpha_v\cdot[\eta(l'_{\vec{i},\tau})-\eta(l_{\vec{i},\tau})]}-1\right)\right) UR$$

$$= (1+\Delta)B^{>}$$

$$B_{\vec{l}'}(\bullet,0) = \overbrace{B_{\vec{l}}(\bullet,\tau)\left[\prod_{r'=1}^{r-1} e^{h_I^{r'}(\vec{l}_n)}\right]}^{\tilde{B}_{\vec{l}}(\bullet,\tau)} U^{(\vec{i})}\left(1+\Delta^{(\vec{i})}\right) \underbrace{U^{(\vec{i}),\dagger}\left[\prod_{r'\geq r} e^{h_I^{r'}(\vec{l}_n)}\right] B_{\vec{l}}(\tau,0)}_{\tilde{B}_{\vec{l}}(\tau,0)}$$

由 iseed0

随机

NSIGL_U($\vec{i}$, τ) = NFLIPL($l_{\vec{i},\tau}$, 1/2/3)

CALC gr

由费米子对易关系 $c_x c_y^\dagger + c_y^\dagger c_x = \delta_{x,y}$

等时格林函数 $O = c_x c_y^\dagger = \delta_{x,y} - c_y^\dagger c_x = \delta_{x,y} - c_{x_1}^\dagger \delta_{x_1,y} \delta_{x,x_2} c_{x_2}$

$= \delta_{x,y} - \vec{c}^\dagger A^{(y,x)} \vec{c}$

其中矩阵 $A^{(y,x)}$ 的元为 $A^{(y,x)}_{x_1,x_2} = \delta_{x_1,x} \delta_{x_2,y}$

由

$$\langle c_x c_y^\dagger \rangle_{\vec{s}} = \delta_{x,y} - \frac{\partial}{\partial \eta} \ln \langle \Psi_T | U_{\vec{s}}(2\Theta, \Theta) e^{\eta \vec{c}^\dagger A^{(y,x)} \vec{c}} U_{\vec{s}}(\Theta, 0) | \Psi_T \rangle |_{\eta=0} =$$

$$\delta_{x,y} - \frac{\partial}{\partial \eta} \ln \det \left(P^\dagger B_{\vec{s}}(2\Theta, \Theta) e^{\eta A^{(y,x)}} B_{\vec{s}}(\Theta, 0) P \right) |_{\eta=0} =$$

$$\delta_{x,y} - \frac{\partial}{\partial \eta} \mathrm{Tr} \ln \left(P^\dagger B_{\vec{s}}(2\Theta, \Theta) e^{\eta A^{(y,x)}} B_{\vec{s}}(\Theta, 0) P \right) |_{\eta=0} =$$

$$\delta_{x,y} - \mathrm{Tr} \left[\left(P^\dagger B_{\vec{s}}(2\Theta, 0) P \right)^{-1} P^\dagger B_{\vec{s}}(2\Theta, \Theta) A^{(y,x)} B_{\vec{s}}(\Theta, 0) P \right]$$

$$\left(1 - B_{\vec{s}}(\Theta, 0) P \left(P^\dagger B_{\vec{s}}(2\Theta, 0) P \right)^{-1} P^\dagger B_{\vec{s}}(2\Theta, \Theta) \right)_{x,y} \equiv (G_{\vec{s}}(\Theta))_{x,y}$$

建立格林函数与传播子的关系式:

$$G = 1 - B^{\rangle} \left(B^{\langle} B^{\rangle} \right)^{-1} B^{\langle}$$

$TEMP_{ndim \times ne} = UR \cdot ULRINV = B^{>} (B^{<} B^{>})^{-1}$

$GRup_{ndim \times ndim} = I - TEMP \cdot UL = I - B^{>} (B^{<} B^{>})^{-1} B^{<}$

$GRupc = I - GRup$

那么 $GRup(i,j)$ 其实就代表 $\langle c_i c_j^\dagger \rangle$，也即 G_{ij}

同样地 $GRupc(i,j) = \langle c_j^\dagger c_i \rangle \equiv \bar{G}_{ij}$

$\{ c_x, c_y \} = 0$

$\{ c_x^\dagger, c_y^\dagger \} = 0$ (x,y 为任意值)

OBSER

对 A 子格点，$xI=-1$，$xJ=-1$ 　　　　i, j 为格点

对 B 子格点，$xI=1$，$xJ=1$

$GR\,do(i,j) = xI\cdot xJ\cdot GR\,upc(i,j)$

$GR\,doc(i,j) = xI\cdot xJ\cdot GR\,up(i,j)$

即 $\langle c_{i\downarrow} c_{j\downarrow}^\dagger\rangle = \begin{cases} (\langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle)^* & i,j \text{ same sublattice} \\ -(\langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle)^* & i,j \text{ different sublattice} \end{cases}$

Assaad 讲义中自旋分量要写进 dimension 里面（$\vec{x}=(\vec{i},\sigma)$，即维数是格点数 2 倍）；但在程序中，维数只是格点数，而用上述约束来区分不同自旋分量费米子的关联！

推导：Hamiltonian after HS transformation

$$H[\varphi] = -t\sum_{\langle ij\rangle}(c_{i\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{j\downarrow}) + \lambda\sum_i i\varphi(n_{i\uparrow}+n_{i\downarrow})$$

introduce $d_{i\downarrow} \equiv (-)^i c_{i\downarrow}^\dagger = \begin{cases} c_{i\downarrow}^\dagger & A \text{ sub} \\ -c_{i\downarrow}^\dagger & B \text{ sub} \end{cases}$ 　　①

$d_{i\downarrow}^\dagger \equiv (-)^i c_{i\downarrow}$

$$\begin{aligned} H[\varphi] &= -t\sum_{\langle ij\rangle} c_{i\uparrow}^\dagger c_{j\uparrow} - t\sum_{\langle ij\rangle}(-)^{i+j} d_{i\downarrow} d_{j\downarrow}^\dagger + \lambda\sum_i i\phi_i(c_{i\uparrow}^\dagger c_{i\uparrow} + d_{i\downarrow} d_{i\downarrow}^\dagger) \\ &= -t\sum_{\langle ij\rangle} c_{i\uparrow}^\dagger c_{j\uparrow} - t\sum_{\langle ij\rangle} d_{i\downarrow}^\dagger d_{j\downarrow} + \lambda\sum_i i\phi_i[c_i^\dagger c_i + (1-d_{i\downarrow}^\dagger d_{i\downarrow})] \\ &= -t\sum_{\langle ij\rangle} c_{i\uparrow}^\dagger c_{j\uparrow} - t\sum_{\langle ij\rangle} d_{i\downarrow}^\dagger d_{j\downarrow} + \lambda\sum_i i\phi_i(c_i^\dagger c_i - d_{i\downarrow}^\dagger d_{i\downarrow}) + \text{const} \\ &= \underbrace{\Big[-t\sum_{\langle ij\rangle} c_{i\uparrow}^\dagger c_{j\uparrow} + \lambda\sum_i i\phi_i c_{i\uparrow}^\dagger c_{i\uparrow}\Big]}_{} + \underbrace{\Big[-t\sum_{\langle ij\rangle} d_{i\downarrow}^\dagger d_{j\downarrow} - \lambda\sum_i i\phi_i d_{i\downarrow}^\dagger d_{i\downarrow}\Big]}_{} + \text{const}. \end{aligned}$$

∵ $H=H^\dagger$ 　∴ 互为 Hermitt 共轭

∴ $\langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle = \langle d_{i\downarrow}^\dagger d_{j\downarrow}\rangle^*$ 　　②

∴ $\langle c_{i\downarrow} c_{j\downarrow}^\dagger\rangle \overset{①}{=} \begin{cases} \langle d_{i\downarrow}^\dagger d_{j\downarrow}\rangle \overset{②}{=} \langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle^* & i,j \text{ same sub} \\ -\langle d_{i\downarrow}^\dagger d_{j\downarrow}\rangle \overset{②}{=} -\langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle^* & i,j \text{ diff sub} \end{cases}$

I_0为某元胞A子格点，I_1为某元胞B子格点

I_2为 $x+1$处元胞B子格点，I_3为 $y+1$处元胞B子格点

$$\text{density} \quad t = \frac{1}{2L_Q}\left[GR_{upc}(I_0, I_0) + GR_{doc}(I_0, I_0) + GR_{upc}(I_1, I_1) + GR_{doc}(I_1, I_1)\right]$$

$$= \frac{1}{2L_Q}\sum_i^{L_Q}\sum_j^{L_Q}\left(\langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle + \langle c_{j\downarrow}^\dagger c_{j\downarrow}\rangle + \langle c_{j\uparrow}^\dagger c_{j\downarrow}\rangle + \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle\right)$$

double_ocupy - - - - - - -

kinetiC - - - - - - -

这里的i还是格点序号

$$TMP\_D(i) = GR_{upc}(i, i) + GR_{doc}(i, i)$$

$$= \langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle + \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle$$

$$TMP\_S(i) = \langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle - \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle$$

!!! 这里的i和j变为元胞序号

$$\text{den} = \frac{1}{L_Q}\sum_{ij}^{2L_Q}\Big[\left(\langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle + \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle\right)\left(\langle c_{j\uparrow}^\dagger c_{j\uparrow}\rangle + \langle c_{j\downarrow}^\dagger c_{j\downarrow}\rangle\right) + \langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle\langle c_{i\uparrow} c_{j\uparrow}^\dagger\rangle + \langle c_{i\downarrow}^\dagger c_{j\downarrow}\rangle\langle c_{i\downarrow} c_{j\downarrow}^\dagger\rangle$$

$N = L_Q$

$$- \langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle - \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle - \langle c_{j\uparrow}^\dagger c_{j\uparrow}\rangle - \langle c_{j\downarrow} c_{j\downarrow}^\dagger\rangle + 1\Big]$$

$$\text{spin}_{(no1,no2)}(imj) = \frac{1}{N}\sum_{ij}^{N}\Big[\left(\langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle - \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle\right)\left(\langle c_{j\uparrow}^\dagger c_{j\uparrow}\rangle - \langle c_{j\downarrow}^\dagger c_{j\downarrow}\rangle\right) + \langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle\langle c_{i\uparrow} c_{j\uparrow}^\dagger\rangle + \langle c_{i\downarrow}^\dagger c_{j\downarrow}\rangle\langle c_{i\downarrow} c_{j\downarrow}^\dagger\rangle\Big]_{(no1,no2)}$$

$$= \frac{1}{N}\sum_{ij}^{N}\Big[\langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle\langle c_{j\uparrow}^\dagger c_{j\uparrow}\rangle + \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle\langle c_{j\downarrow}^\dagger c_{j\downarrow}\rangle - \langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle\langle c_{j\downarrow}^\dagger c_{j\downarrow}\rangle - \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle\langle c_{j\uparrow}^\dagger c_{j\uparrow}\rangle + \langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle\langle c_{i\uparrow} c_{j\uparrow}^\dagger\rangle + \langle c_{i\downarrow}^\dagger c_{j\downarrow}\rangle\langle c_{i\downarrow} c_{j\downarrow}^\dagger\rangle\Big]_{(no1,no2)}$$

记 i元胞位置−j元胞位置
对应位矢的元胞的序号为imj

推导：

物理上

$$AFMzz(no1, no2) = \frac{1}{N}\sum_{imj}^{N} e^{0}\, \text{spin}_{(no1,no2)}(imj)$$

物理上

$$= \frac{1}{N^2}\sum_{ij}^{N}\langle S_i^z S_j^z\rangle_{(no1,no2)}$$

S_i^z为i上的自旋

$$= \frac{1}{N^2}\sum_{ij}\left\langle\left(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}\right)\left(c_{j\uparrow}^\dagger c_{j\uparrow} - c_{j\downarrow}^\dagger c_{j\downarrow}\right)\right\rangle_{(no1,no2)}$$

$$= \frac{1}{N^2}\sum_{ij}\Big\{\langle c_{i\uparrow}^\dagger c_{i\uparrow} c_{j\uparrow}^\dagger c_{j\uparrow}\rangle + \langle c_{i\downarrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\downarrow}\rangle - \langle c_{i\uparrow}^\dagger c_{i\uparrow} c_{j\downarrow}^\dagger c_{j\downarrow}\rangle - \langle c_{i\downarrow}^\dagger c_{i\downarrow} c_{j\uparrow}^\dagger c_{j\uparrow}\rangle\Big\}_{(no1,no2)}$$

Wick theorem: $\langle c_{x_2}^\dagger c_{y_2} c_{x_1}^\dagger c_{y_1}\rangle_{\vec{s}} = \langle c_{x_2}^\dagger c_{y_1}\rangle_{\vec{s}}\langle c_{y_2} c_{x_1}^\dagger\rangle_{\vec{s}} + \langle c_{x_2}^\dagger c_{y_2}\rangle_{\vec{s}}\langle c_{x_1}^\dagger c_{y_1}\rangle_{\vec{s}}.$

Wick定理 $= \frac{1}{N^2}\sum\{\langle c_{i\uparrow}^\dagger c_{j\uparrow}\rangle\langle c_{i\uparrow} c_{j\uparrow}^\dagger\rangle + \langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle\langle c_{j\uparrow}^\dagger c_{j\uparrow}\rangle$

$+ \langle c_{i\downarrow}^\dagger c_{j\downarrow}\rangle\langle c_{i\downarrow} c_{j\downarrow}^\dagger\rangle + \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle\langle c_{j\downarrow}^\dagger c_{j\downarrow}\rangle$

$- \langle c_{i\uparrow}^\dagger c_{j\downarrow}\rangle\langle c_{i\uparrow} c_{j\downarrow}^\dagger\rangle - \langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle\langle c_{j\downarrow}^\dagger c_{j\downarrow}\rangle$

$- \langle c_{i\downarrow}^\dagger c_{j\uparrow}\rangle\langle c_{i\downarrow} c_{j\uparrow}^\dagger\rangle - \langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle\langle c_{j\uparrow}^\dagger c_{j\uparrow}\rangle\}_{(no1,no2)}$

∵ Hubbard Hamiltonian 不含↑↓的耦合项，故可严格证明 $\langle c_{i\uparrow}^\dagger c_{j\downarrow}\rangle$ 这类关联函数为0

∴ $-\langle c_{i\uparrow}^\dagger c_{j\downarrow}\rangle\langle c_{i\uparrow} c_{j\downarrow}^\dagger\rangle - \langle c_{i\downarrow}^\dagger c_{j\uparrow}\rangle\langle c_{i\downarrow} c_{j\uparrow}^\dagger\rangle = 0$

∴ $spin_{(no1,no2)}(\vec{i}-\vec{j})$ 形式即为程序所示

☆ AFMzz11 即 AFMzz(1,1) A子格点与A子格点上的自旋关联

☆ 物理上，AFM structure factor $S(\vec{q}) \equiv \frac{1}{N^2}\sum_{ij} e^{i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)}\langle m_i^{(z)} m_j^{(z)}\rangle$

staggered magnetization $m_i^{(z)} \equiv \vec{c}_{i,A}^{\,\dagger}\sigma^z\vec{c}_{i,A} - \vec{c}_{i,B}^{\,\dagger}\sigma^z\vec{c}_{i,B}$, $\vec{c} = (c_\uparrow, c_\downarrow)$

$= S_{i,A}^z - S_{i,B}^z$

$\Rightarrow \langle m_i^{(z)} m_j^{(z)}\rangle = \langle (S_{i,A}^z - S_{i,B}^z)(S_{j,A}^z - S_{j,B}^z)\rangle$

$= \langle S_{i,A}^z S_{j,A}^z + S_{i,B}^z S_{j,B}^z - S_{i,A}^z S_{j,B}^z - S_{i,B}^z S_{j,A}^z\rangle$

☆ 程序中

序号imj的元胞的位矢 $(\vec{r}_i-\vec{r}_j)$

$S(\vec{q})_{(no1,no2)} = \frac{1}{N}\sum_{imj}^{N} e^{i\vec{q}\cdot\vec{r}(imj)}\, spin_{(no1,no2)}(imj)$

$= \frac{1}{N}\sum_{imj}^{N}\frac{1}{N}\sum_{ij}^{N} e^{i\vec{q}\cdot\vec{r}(imj)}\langle S_i^z S_j^z\rangle_{(no1,no2)}$

$\Rightarrow S(\vec{q}) = \frac{1}{N}\sum_{imj}^{N}\frac{1}{N}\sum_{ij}^{N} e^{i\vec{q}\cdot\vec{r}(imj)}\langle m_i^z m_j^z\rangle = \frac{1}{N}\sum_{imj}^{N}\frac{1}{N}\sum_{ij}^{N} e^{i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)}\langle m_i^z m_j^z\rangle$

imj, i, j 都為2維矢量

$= \frac{1}{N^2}\sum_{ij}^{N} e^{i\vec{q}\cdot(\vec{r}_i-\vec{r}_j)}\langle m_i^z m_j^z\rangle$

$\therefore$ the square of order parameter of AFM: $m^2 = S(0)$

$$= \frac{1}{N^2} \sum_{ij} e^0 \langle m_i^{(z)} m_j^{(z)} \rangle$$

$$= \text{AFMzz11} + \text{AFMzz22} - \text{AFMzz12} - \text{AFMzz21}$$

$$(= \text{AFMzz})$$

$$\text{AFMzzdeltaq} = S(\vec{K}_h) = \frac{1}{N^2} \sum_{ij} e^{i \vec{K}_h \cdot (\vec{r}_i - \vec{r}_j)} \langle m_i^{(z)} m_j^{(z)} \rangle$$

$$= \text{AFMzzdeltaq11} + \text{AFMzzdeltaq22} - \text{AFMzzdeltaq12} - \text{AFMzzdeltaq21}$$

$$\vec{K}_h = \vec{b}_1 \frac{1}{L_x} + \vec{b}_2 \frac{1}{L_y} = \begin{pmatrix} 2\pi/L \\ 2\pi/\sqrt{3}L \end{pmatrix} = \vec{a} \frac{2\pi}{L}, \quad \vec{a} \equiv \vec{x} + \vec{y}/\sqrt{3}$$

MMUUL

輸入 A

輸出 $A \cdot e^{\alpha_U \cdot \eta(\text{NSIGL\_U})}$ 即 $A \cdot e^{\alpha_U \cdot \eta(t_1)}$

MMUURM1

輸入 A

輸出 $A / e^{\alpha_U \cdot \eta(\text{NSIGL\_U})}$ 即 $A / e^{\alpha_U \cdot \eta(t_1)}$

$l_{i,t}$

MMTHL

輸入 A

輸出 $A \cdot \text{URT\_tot}$ 即 $A \cdot e^{-\Delta\tau \cdot h_t}$

(调用了 mmult(A1, A, URT_tot) 将 A 与 URT_tot 相乘)

MMTHRM1 (UR)

輸入 A

輸出 $\text{URTM1\_tot} \cdot A$ 即 $e^{\Delta\tau \cdot h_t} \cdot A$

ORTHO

① UDV (UR, U, D, V, NCON)
输入UR，输出U

② 输入UL，先转置为 UL^T
再 UDV (UL, U, D, V, NCON)
输出 U^T

PREQ

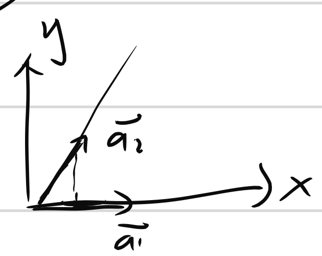
① SWEEP一次，先测量2次，观测量取均值

② 每个节点的观测量求和取均值

③ $AFM_{zz}21$ structurefactor(spin, filek, 0, 0, 2, 1)

$AFM_{zz}21$ deltaq structurefactor(spin, filek, $\frac{1}{L_x}$, $\frac{1}{L_y}$, 2, 1)

④ structurefactor(gr, filek, px, py, no1, no2)



正空间基矢 $\begin{cases} a1\_p = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ a2\_p = \begin{pmatrix} 1/2 \\ \sqrt{3}/2 \end{pmatrix} \end{cases}$

倒空间基矢 $\begin{cases} b1\_p = \begin{pmatrix} 2\pi \\ -\frac{2\pi}{\sqrt{3}} \end{pmatrix} \\ b2\_p = \begin{pmatrix} 0 \\ \frac{2\pi \cdot 2}{\sqrt{3}} \end{pmatrix} \end{cases}$

满足 $\vec{a}_i \cdot \vec{b}_j = \delta_{ij} \cdot 2\pi$

$$\vec{K}_n = xk\_p = \begin{pmatrix} p_x \cdot b1\_p(1) + p_y \cdot b2\_p(1) \\ p_x \cdot b1\_p(2) + p_y \cdot b2\_p(2) \end{pmatrix} = p_x \begin{pmatrix} b1\_p(1) \\ b1\_p(2) \end{pmatrix} + p_y \begin{pmatrix} b2\_p(1) \\ b2\_p(2) \end{pmatrix}$$

$$= h_1 \vec{b}_1 + h_2 \vec{b}_2$$

第q个元胞的位置矢量 $\vec{R}_q = aimj\cdot p = \begin{pmatrix} l_x \cdot a1\_p(1) + l_y \cdot a2\_p(1) \\ l_x \cdot a1\_p(2) + l_y \cdot a2\_p(2) \end{pmatrix}$

$$= l_x \begin{pmatrix} a1\_p(1) \\ a1\_p(2) \end{pmatrix} + l_y \begin{pmatrix} a2\_p(1) \\ a2\_p(2) \end{pmatrix}$$

$$= x_q \vec{a}_1 + y_q \vec{a}_2$$

第q个元胞横坐标

对于 AFM_{zzij} deltaq，$\vec{K}_n = \begin{pmatrix} \frac{2\pi}{L} \\ \frac{2\pi}{\sqrt{3}L} \end{pmatrix} = \vec{a}\,\frac{2\pi}{L}$，$\vec{a} \equiv \vec{x} + \frac{\vec{y}}{\sqrt{3}}$

correlation length ratio $R \equiv 1 - \frac{S(0 + \vec{a}\frac{2\pi}{L})}{S(0)} = 1 - \frac{AFM_{zz}\,deltaq}{AFM_{zz}}$

整个过程

① 建立晶格、数与矩阵

SLI, SALPH (α_v), SetHproj, Sproj, SetH, St hop, inconfc

② 把无相互作用的基态波函数 PROJ(1~ndim, 1~ne) 赋予初始 UR

之前定义 PROJ 是 ndim × ndim，故 ne ≤ ndim；然后 $UR_{ndim \times ne}$

τ 从 1~ Ltrot，$U = U(\tau)$，在每个 τ 上作 $UR = e^{\alpha_v \cdot \eta(\tau)} \cdot e^{-\Delta\tau \cdot h_t} \cdot UR$

（相当于 $B(2\theta, 0) P = \prod_{\tau=1}^{L_{trot}} e^{h_I(\vec{l})} e^{-\Delta\tau h_t} P$ ）

（规定 $\vec{l} = \{ l_{i,n} \}$ ）

此时 $UR(\tau = L_{trot})$，再将 $PROJ(1\sim ndim, 1\sim ne)^\dagger$ 赋予初始 UL

$ULR = UL \cdot UR$ 即 $P^\dagger B(2\theta, 0) P = B^< B^>$，$ULRINV = ULR^{-1} = (B^< B^>)^{-1}$

③ 开始 Sweep

将 $PROJ(1\sim ndim, 1\sim ne)^\dagger$ 赋予初始 UL

(1) τ 从 Ltrot 到 1，$U = U(\tau)$，正交化 UL 并存进 UST

若 $U > 0$，则 UPGRADEU；若 $\tau = \frac{L_{trot}}{2}$，则测量观测量

UL 为 $P^\dagger \to P^\dagger B(2\theta, 2\theta - \Delta\tau)$，UR 为 $B(2\theta, 0) P \to B(2\theta - \Delta\tau, 0) P$

$\to P^\dagger B(2\theta, \theta) \to P^\dagger B(2\theta, 0)$　　　$\to B(\theta, 0) P \to P$

(2) 将 PROJ(1~ndim, 1~ne) 赋予初始 UR

正交化 UL

(3) τ 从 1 到 Ltrot　　　若 $\tau = \frac{L_{trot}}{2}$，则测量观测量

$P \to B(\Delta\tau, 0) P$　　　$P^\dagger (2\theta, 0) \to P^\dagger (2\theta, \Delta\tau)$

$\to \to B(2\theta, 0) P$　　　$\to \to P^\dagger$

(4) PREQ 算出序参量并输出文件