At this point, you should sum up:

<u>The input reads:</u>

$$H = \sum_{s=1}^{N} \sum_{x,y} c^{+}_{x,s} M_{x,y} c_{y,s} - \sum_{k=1}^{M} U_k \left[\sum_{x,y,s} \left\{ c^{+}_{x,s} T^{(k)}_{x,y} c_{y,s} - d_k \right\} \right]^2$$

The $T^{(k)}$ matrices are sparse matrices such that

$\Rightarrow T^{(k)}_{x,y} \neq 0$ if $x, y \in [z_1, \dots, z_n]$ where n is the dimension of $T^{(k)}$ $\Rightarrow$ Let $P_{i,z} = \delta_{z,z_i}$

$i \in \{1, \dots, n\}$, $z = \{1 - \dots N_{dim}\}$ $\Rightarrow$

$T^{(k)} = P^{(k)T} O^{(k)} P^{(k)}$ such that: $T^{(k)}_{x,y} =$

$$\sum_{i,j} P_{i,x} O_{i,j} P_{j,y} = \sum_{i,j} \delta_{x,z_i} O_{i,j} \delta_{j,z_j} \Rightarrow$$

$\Rightarrow$ For the input you need $O_{i,j} = n \times n$ matrix and

$z_i : i = 1, \dots, n$, U_k and d_k

With this you will have:

$$\mathrm{Tr}\ \exp\{-\beta \hat{H}\} = \sum_{\{l\}} \left[\prod_{k=1}^{M} \prod_{\tau=1}^{L_\tau} \gamma(l_k(\tau))\right] \cdot \mathrm{Tr} \prod_{\tau=1}^{L_\tau} \cdot$$

$$\prod_{k=1}^{M} \exp\left[\sqrt{\Delta\tau V_k}\, \eta(l_k(\tau)) \sum_s \left(c_s^{\dagger} T^{(k)} c_s - \alpha_k\right)\right] \cdot \exp\left\{-\Delta\tau \sum_s c_s^{\dagger} M c_s\right]$$

$$= \sum_{\{l\}} \left[\prod_{k=1}^{M} \prod_{\tau=1}^{L_\tau} \gamma(l_k(\tau)) \exp\left\{-N\alpha_k \sqrt{\Delta\tau V_k}\, \eta(l_k(\tau))\right]\right]$$

$$\cdot \left[\det\left(1 + B_{L_\tau} \cdots B_1\right)\right]^N = \sum_{\{l\}} e^{-S_0(l)} \left[\det\left[1 + B_{L_\tau} \cdots B_1\right]\right]^N$$

$$\text{with} \quad B_\tau = \prod_{k=1}^{M} \exp\left[\sqrt{\Delta\tau V_k}\, \eta(l_k(\tau))\ T^{(k)}\right] \exp\left\{-\Delta\tau M\right]$$

To fomulate things nicely you have define:

$$B(k\tau, 0) = \prod_{\tilde{k}=1}^{k} \exp\left[\sqrt{\Delta\tau V_{\tilde{k}}}\, \eta(l_{\tilde{k}}(\tau))\ T^{(\tilde{k})}\right] \exp\left\{-\Delta\tau M\right] \cdot$$

$$\cdot B_{\tau-1} \cdots B_1$$

$$B(L_\tau, k\tau) = B_{L_\tau} \cdots B_{\tau+1} \prod_{\tilde{k}=L_\tau}^{k+1} \cdot \exp\left[\sqrt{\Delta\tau V_{\tilde{k}}}\, \eta(l_{\tilde{k}}(\tau))\ T^{(\tilde{k})}\right]$$

as well as the Greens function:

$$G(k\tau) = \left[1 + B(k\tau, 0)\, B(L_\tau, k\tau)\right]^{-1}$$

The input for the upgrade procedure is given by:

$G(1\tau)$ the output by $G(M\tau)$ with update of course

First things to change are wrapul, wrapur.

$$\exp\left[\sqrt{\Delta\tau v_k}\, \eta(l_k(\tau))\, T^{(k)}\right] A = \quad T = P^T O P$$

$$[T]^n = [P^T O \; P]^n = P^T O P [P^T O P]^{n-1}$$

Now PP^T is a $n \times n$ matrix. $(PP^T)_{i,j} =$

$$\sum_x P_{i,x} P^T_{x,j} = \sum_x P_{i,x} P_{j,x} = \sum_x \delta_{x,z_i} \delta_{x,z_j} = \delta_{i,j} \sum_x \delta_{x,z_i}$$

$= \delta_{i,j} \Rightarrow PP^T = 1_{n \times n}$. With this you have:

$$\exp\left[\overbrace{\sqrt{\Delta\tau v_k}\, \eta(l_k(\tau))}^{=\alpha}\, T^{(k)}\right] A = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} T^n A =$$

$$\left[1 + \sum_{n=1}^{\infty} \frac{\alpha^n}{n!} (P^T O P)^n\right] A = \left[1 + P^T \left(e^{\alpha O} - 1\right) P\right] A =$$

$$\left[1 + P^T \left(e^{\alpha O} - 1\right) P\right] A = A + P^T\left(e^{\alpha O} - 1\right) P A$$

$$\Rightarrow \left[\exp\left[\overbrace{\sqrt{\Delta\tau v_k}\,\eta(\ell_k(\tau))}^{=\alpha}\, T^{(k)}\right] A\right]_{x,y} = A_{x,y} +$$

$$P^T_{x,i}\left(e^{\alpha O}-1\right)_{i,j} P_{j,x_1} A_{x_1,y} = A_{x,y} + \sum_{i,j=1}^{n} \delta_{x,z_i}\left(e^{+\alpha O}-1\right)_{i,j}\, \delta_{x_1,z_j}$$

$$\cdot A_{x_1,y} = A_{x,y} + \sum_{i,j=1}^{n} \delta_{x,z_i}\left(e^{\alpha O}-1\right)_{i,j}\, A_{z_j,y}$$

$$\left[\exp\left[\overbrace{\sqrt{\Delta\tau v_k}\,\eta(\ell_k(\tau))}^{=\alpha}\, T^{(k)}\right] A\right]_{x,y} = A_{x,y} + \sum_{i,j=1}^{n} \delta_{x,z_i}\left(e^{\alpha O}-1\right)_{i,j} A_{z_j,y}$$

$$= \begin{cases} A_{x,y} & \text{if } x \notin \{z_1, \dots, z_n\} \\ A_{z_i,y} + \sum_{i,j}\left(e^{\alpha O}-1\right)_{i,j} A_{z_j,y} = \sum_{j=1}^{n}\left(e^{\alpha O}\right)_{i,j} A_{z_j,y} & \text{if } x = z_i \end{cases}$$

So you will store $\exp[\alpha O] = \exp\left[\sqrt{\Delta\tau v_k}\,\eta(\ell_k(\tau))\, O\right]$

$$= U \exp\left[\sqrt{\Delta\tau v_k}\,\eta(\ell_k(\tau))\,\lambda\right] U^{+}$$ Good.

Wrapur is equivalent. $\quad A\, e^{\alpha T^{(k)}} =$

$$\left[A\left[1+P^T\left(e^{\alpha O}-1\right)P\right]\right]_{x,y} = \left[A + A P^T\left(e^{\alpha O}-1\right)P\right]_{x,y}$$

$$= A_{x,y} + A_{x,x_1} P^T_{x_1,i}\left(e^{\alpha O}-1\right)_{i,j} P_{j,y} =$$

$$= A_{x,y} + A_{x,z_i}\left(e^{\alpha O}-1\right)_{i,j} \delta_{y,z_j}$$

$$= \begin{cases} A_{x,y} & \text{if } y \notin \{z_1 \cdots z_n\} \\ \cancel{A_{x,z_j}} - \cancel{A_{x,z_j}} + \sum_{i=1}^{n} A_{x,z_i}\left(e^{\alpha O}\right)_{i,j} & \text{if } y = z_j \end{cases}$$

Upgrading.

In $\quad G([k-1]\tau) = \left[1 + B([k-1]\tau,0)\, B(L_\tau, [k-1]\tau)\right]^{-1}$

$$B(k\tau, 0) = \prod_{\tilde{k}=1}^{k} \exp\left[\sqrt{\Delta\tau v_{\tilde{k}}}\, \eta(l_{\tilde{k}}(\tau))\; T^{(\tilde{k})}\right] \exp\left[-\Delta\tau M\right] \cdot$$

$$\cdot\, B_{\tau-1} \cdots\cdots B_1$$

$$B(L_\tau, k\tau) = B_{L_\tau} \cdots B_{\tau+1} \prod_{\tilde{k}=L_\tau}^{k+1} \exp\left[\sqrt{\Delta\tau v_{\tilde{k}}}\, \eta(l_{\tilde{k}}(\tau))\; T^{(\tilde{k})}\right]$$

Let: $\exp\left[\sqrt{\Delta\tau V_{\tilde{k}}}\,\eta(l_{\tilde{k}}(\tau))\;T^{(\tilde{k})}\right] = U \exp\left[\alpha\,\eta\,\lambda\right] U^{+}$

Let $g = \left[1 + \exp[\alpha\eta\lambda]\,U^{+}\,B([k-1]\tau, 0)\,B(L_{\tau}, [k-1]\tau)\,U e^{-\alpha\eta\lambda}\right]^{-1}$

$= \left[e^{\alpha\eta\lambda}\,U^{+}\,G^{-1}([k-1]\tau)\,U e^{-\alpha\eta\lambda}\right]^{-1} =$

$= e^{\alpha\eta\lambda}\,U^{+}\,G([k-1]\tau)\,U e^{-\alpha\eta\lambda}$

Now you can update g.

$g = [1 + B_1 B_2]^{-1} \rightarrow \left[1 + e^{-\alpha\eta\lambda} e^{\alpha\eta'\lambda} B_1 B_2\right]^{-1} =$

$= \left[1 + (1+\Delta)\,B_1 B_2\right]^{-1}$ with $\Delta = \left(e^{\alpha(\eta'-\eta)\lambda} - 1\right)$

Δ is a diagonal matrix with n non-zero matrix elements.

1) Ratio. $\dfrac{\det\left[1 + (1+\Delta)\,B_1 B_2\right]}{\det\left[1 + B_1 B_2\right]} =$

$= \det\left[\left[1 + (1+\Delta)\,B_1 B_2\right] \cdot g\right] =$ $\ulcorner g = [1 + B_1 B_2]^{-1} \Rightarrow B_1 B_2 =$

$(g^{-1} - 1)\lrcorner = \det\left[\left[1 + (1+\Delta)\,(g^{-1}-1)\right] g\right] = \det\left[g + (1+\Delta)(1-g)\right] =$

$$= \det\left[g + (1+\Delta) - (1+\Delta) g \right] = \det\left[\cancel{g} + (1+\Delta) - \cancel{g} - \Delta g \right] =$$

$$= \det\left[1 + \Delta - \Delta g \right] = \det\left[1 + \Delta (1-g) \right]$$

Now you have to compute this explicitly.

$$\Delta = \left(e^{\alpha(\eta' - \eta)\lambda} - 1 \right), \qquad \lambda = U^{+} T U$$

Now: $T = P^{T} O P = P^{T} u d u^{+} P$

$$\boxed{T^{(k)} = P^{(k)T} O^{(k)} P^{(k)}}$$

$$\boxed{P P^{T} = \mathbb{1}_{n\times n}}$$

$\Rightarrow$ Let $U^{+} = 1 + P^{T}(u^{+} - 1) P$

$$\Rightarrow U^{+} U = \left[1 + P^{T}(u^{+}-1) P \right] \left[1 + P^{T}(u-1) P \right] =$$

$$= 1 + P^{T}(u^{+}-1) P + P^{T}(u-1) P + P^{T}(u^{+}-1)(u-1) P =$$

$$= 1 + P^{T}\left[\cancel{u^{+}} \cancel{-1} + \cancel{u} \cancel{-1} + \cancel{1} + \cancel{1} - \cancel{u^{+}} - \cancel{u} \right] P = 1$$

$$\Rightarrow U^{+} T U = \left[1 + P^{T}(u^{+}-1) P \right] P^{T} O P \left[1 + P^{T}(u-1) P \right] =$$

$$= P^{T} \left[1 + (u^{+}-1) \right] O \left[1 + (u-1) \right] P =$$

$= P^{T} \boxed{\underbrace{u^{+} O u}_{\equiv d}} P = \lambda \Rightarrow$ You can now do the calculation explicitly.

$$\Delta = \left(e^{\alpha(\eta'-\eta)\lambda} - 1\right) = \exp\left(\alpha(\eta'-\eta) P^T \alpha P\right) - 1$$

$$\sum_{n=1}^{\infty} \frac{[\alpha(\eta'-\eta)]^n}{n!} [P^T \alpha P]^n - 1 = \cancel{1} + P^T \underbrace{\left(e^{\alpha(\eta'-\eta)\alpha} - 1\right)}_{\equiv \sigma} P - \cancel{1}$$

$$= P^T \sigma P \Rightarrow \det[1 + \Delta(1-g)] = \det[1 + P^T \sigma P (1-g)] =$$

$$= \det[1 + P(1-g) P^T \sigma]$$ Here you have used that:

$\det(1 + AB) = \det(1 + BA) \Rightarrow$ This is very nice. At this point you can compute the ration. For the $SU(N)$ symmetric problem you have, it is given by:

$$\boxed{R = \left[\det\left[1 + P_k(1-g) P_k^T \sigma_k(\tau)\right]\right]^N \cdot \frac{\gamma[\ell_k'(\tau)]}{\gamma[\ell_k(\tau)]} \cdot \frac{\exp\{-N\alpha_k \sqrt{\Delta\tau U_k}\, \eta(\ell_k'(\tau))\}}{\exp\{-N\alpha_k \sqrt{\Delta\tau U_k}\, \eta(\ell_k(\tau))\}}}$$

$\Rightarrow$ At this point you will have to upgrade the Green function

$$g \to g' = [1 + (1+\Delta) B_1 B_2]^{-1}$$

$$g = [1 + B_1 B_2]^{-1} \Rightarrow g^{-1} - 1 = B_1 B_2 \Rightarrow g' =$$

$$[1 + (1+\Delta)(g^{-1}-1)]^{-1} = [1 + (1+\Delta)(1-g)\, g^{-1}]^{-1} =$$

$$= [[g + (1+\Delta)(1-g)]\, g^{-1}]^{-1} = g\, [g + (1+\Delta)(1-g)]^{-1} =$$

$$= g\, [\cancel{g} + 1 - \cancel{g} + \Delta(1-g)]^{-1} = g\, [1 + \Delta(1-g)]^{-1}$$ Now,

$$\Delta = P^T \sigma P \Rightarrow \Delta(1-g)_{xy} = [P^T \sigma P\, (1-g)]_{xy} =$$

$$P^T_{x,i}\, \sigma_i\, P_{i,x_1} (1-g)_{x_1,y} \underset{\substack{\uparrow \\ P_{i,x} = \delta_{x,z_i}}}{=} \sum_{i=1}^{n} \delta_{x,z_i}\, \sigma_i\, \delta_{x_1,z_i} (1-g)_{x_1,y} =$$

$$\sum_{i=1}^{n} \delta_{x,z_i}\, \sigma_i\, (1-g)_{z_i,y} = \sum_i u_i \otimes v_i$$

with $(u_i)_x = \delta_{x,z_i}\, \sigma_i$ and $(v_i)_y = (1-g)_{z_i,y}$. And you can now use Sherman Morison for the update.

Finish wraping up the Green function

$$g' = \left[1 + \exp[\alpha \eta' \lambda] \, U^{+} \, B([k-1]\tau, 0) \, B'(L_\tau, [k-1]\tau) \, U e^{-\alpha \eta' \lambda} \right]^{-1}$$

$$G(k\tau) = U g' U^{+} =$$

$$= \left[U \left[1 + e^{\alpha \eta' \lambda} U^{+} B([k-1]\tau, 0) \, B'(L_\tau, [k-1]\tau) \, U e^{-\alpha \eta' \lambda} \right] U^{+} \right]^{-1}$$

$$= \left[1 + B'[k\tau, 0] \, B[L_\tau, k\tau] \right]^{-1} = G(k\tau) \Rightarrow$$ You can now

loop back. So this completes the description of the algorithm. You should start the implementation and also think about a flag for the Ising case.

All in all, you can do things by induction.

$$\left(1+\sum_{n=1}^{N} u_n \otimes v_n\right)^{-1} = 1 - \sum_{n=1}^{N} X_n \otimes Y_n$$

For $N=1$ you have

$$\left(1+ u_n \otimes v_n\right)^{-1} = 1 - \frac{u_1 \otimes v_1}{1+v_1 \cdot u_1} = 1 - X_1 \otimes Y_1$$

with $X_1 = u_1 / _{1+v_1 \cdot u_1}$ $\quad Y_1 = v_1$

$\Rightarrow$ Assume that things work for N.

$$\Rightarrow \left(1+\sum_{n=1}^{N+1} u_n \otimes v_n\right)^{-1} = \left(A + u_{N+1} \otimes v_{N+1}\right)^{-1} =$$

$$= A^{-1} - \frac{A^{-1} u_{N+1} \otimes v_{N+1} A^{-1}}{1+ v_{N+1} A^{-1} u_{N+1}}$$

$\boxed{\text{Now:}}$ $(A + \bar{u} \otimes \bar{v})^{-1} = \left[A\left(1 + A^{-1} u \otimes v\right)\right]^{-1} = \left(1 + A^{-1} u \otimes v\right)^{-1} A^{-1} =$

$$= \left[1 - A^{-1} u \otimes v + A^{-1} u \otimes \underbrace{v A^{-1} u}_{\equiv \lambda} \otimes v - \cdots\right] A^{-1}$$

$$= \left[1 - A^{-1} u \otimes v \sum_{n=0}^{\infty} \lambda^n (-1)^n\right] A^{-1} = A^{-1} - \frac{A^{-1} u \otimes v A^{-1}}{1 + v \cdot A^{-1} u}$$

Now $A = \mathbb{1} + \sum_{n=1}^{N} u_n \otimes v_n \Rightarrow A^{-1} = \mathbb{1} - \sum_{n=1}^{N} X_n \otimes Y_n$

$$\Rightarrow \left(1 + \sum_{n=1}^{N+1} u_n \otimes v_n\right)^{-1} = \mathbb{1} - \sum_{n=1}^{N} X_n \otimes Y_n - \frac{A^{-1} u_{N+1} \otimes v_{N+1} A^{-1}}{1 + v_{N+1} A^{-1} u_{N+1}}$$

$$\Rightarrow X_{N+1} = \frac{A^{-1} u_{N+1}}{1 + v_{N+1} A^{-1} u_{N+1}} \quad , \quad Y_{N+1} = v_{N+1} A^{-1}.$$

You now want an explicit calculation.

$$1 + v_{N+1} A^{-1} u_{N+1} = 1 + v_{N+1} \left(1 - \sum_{n=1}^{N} X_n \otimes Y_n\right) u_{N+1} =$$

$$= 1 + (v_{N+1} \cdot u_{N+1}) - \sum_{n=1}^{N} (v_{N+1} \cdot X_N)(Y_n \cdot u_{N+1})$$

$$A^{-1} u_{N+1} = u_{N+1} - \sum_{n=1}^{N} X_n \cdot (Y_n \cdot u_{N+1})$$

$$v_{N+1} A^{-1} = v_{N+1} - \sum_{n=1}^{N} (v_{N+1} \cdot X_n) \cdot Y_n \, .$$

<u>Notes</u>: for wrapdo

Type = 2

$$(1 + U e^{\lambda S} U^{+} B)^{-1} =$$

$$(1 + e^{\lambda S} U^{+} B U)^{-1} = \quad [U^{+}(1 + U e^{\lambda S} U^{+} B) U]^{-1} =$$

$$= U^{+}(1 + U e^{\lambda S} U^{+} B)^{-1} U.$$

Type = 1.

$$(1 + B U e^{\lambda S} U^{+})^{-1} = [U e^{-\lambda S}(1 + e^{\lambda S} U^{+} B U) e^{\lambda S} U^{+}]^{-1} =$$

$$= U e^{-\lambda S} [1 + e^{\lambda S} U^{+} B U]^{-1} e^{\lambda S} U^{+}$$

$$\Rightarrow \quad U e^{-\lambda S} U^{+} (1 + U e^{\lambda S} U^{+} B)^{-1} U e^{\lambda S} U^{+} =$$

$$= [U e^{-\lambda S} U^{+} (1 + U e^{\lambda S} U^{+} B) U e^{\lambda S} U^{+}]^{-1}$$

$$= (1 + B U e^{\lambda S} U^{+})^{-1} \checkmark \quad \text{O.K.}$$