Hubbard Model(Fermion) 的 QMC

首先我们考虑 Hubbard Model 的巨正则哈密顿量：

$$H = -t\sum_{<i,j>,\sigma} c_{i,\sigma}^{\dagger}c_{j,\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow} - \mu\sum_{i,\sigma} n_{i,\sigma}$$

对应的 Hubbard Model 的巨配分函数为：

$$Z = \mathcal{T}r\ \mathrm{e}^{-\beta H}$$

考虑到哈密顿量各项之间并不对易,我们要利用 Suzuki-Trotter 分解。Suzuki-Trotter 分解利用到的事实就是：

$$\mathrm{e}^{\Delta\tau(A+B)} = \mathrm{e}^{\Delta\tau A}\mathrm{e}^{\Delta\tau B} + O(\Delta\tau^2[A,B])$$

Suzuki-Trotter 分解即为：

$$\mathrm{e}^{-\beta(K+V)} = (\mathrm{e}^{-\Delta\tau(K+V)})^M = (\mathrm{e}^{-\Delta\tau K}\mathrm{e}^{-\Delta\tau V})^M + O(\Delta\tau^2)$$

这与路径积分相似，将虚时 $(0,\beta)$ 分成 M 段。对于哈密顿量中的相互作用项，我们将使用 Hubbard-Stratonovich 变换。其变换形式如下：

$$\mathrm{e}^{-\Delta\tau U n_\uparrow n_\downarrow} = \frac{1}{2}\mathrm{e}^{-\frac{\Delta\tau U}{2}n}\sum_{s=\pm1}\mathrm{e}^{-sm\lambda} = \frac{1}{2}\sum_{s=\pm1}\prod_{\sigma=\uparrow\downarrow}\mathrm{e}^{-\left(\sigma s\lambda + \frac{\Delta\tau U}{2}\right)n_\sigma}$$

其中 $n = n_\uparrow + n_\downarrow$，$m = n_\uparrow - n_\downarrow$,$\lambda$ 的值满足下列方程

$$\cosh\lambda = \mathrm{e}^{\Delta\tau U/2}$$

这个 HS 变换很容易验证，因为对于费米子系统上述算符的希尔伯特空间是四维的，我们只需要验证左边的算符与右边的算符作用在希尔伯特空间的基矢上得到相同的结果。

①$|n_\uparrow = 0, n_\downarrow = 0\rangle$

$$lhs = 1$$

$$rhs = \frac{1}{2}(1+1) = 1$$

②$|n_\uparrow=0,n_\downarrow=1\rangle$

$$\begin{aligned} lhs &= 1 \\ rhs &= \frac{1}{2}\mathrm{e}^{-\frac{\Delta\tau U}{2}}\left(\mathrm{e}^{\lambda}+\mathrm{e}^{-\lambda}\right)=\mathrm{e}^{-\frac{\Delta\tau U}{2}}\cosh\lambda=1 \end{aligned}$$

③$|n_\uparrow=1,n_\downarrow=0\rangle$

$$\begin{aligned} lhs &= 1 \\ rhs &= \frac{1}{2}\mathrm{e}^{-\frac{\Delta\tau U}{2}}\left(\mathrm{e}^{-\lambda}+\mathrm{e}^{\lambda}\right)=\mathrm{e}^{-\frac{\Delta\tau U}{2}}\cosh\lambda=1 \end{aligned}$$

④$|n_\uparrow=1,n_\downarrow=1\rangle$

$$\begin{aligned} lhs &= \mathrm{e}^{-\Delta\tau U} \\ rhs &= \frac{1}{2}\mathrm{e}^{-\Delta\tau U}\left(1+1\right)=\mathrm{e}^{-\Delta\tau U} \end{aligned}$$

经过 Hubbard-Stratonovich 变换之后我们可以把配分函数写成如下形式：

$$Z=\left(\frac{1}{2}\right)^{L^dM}\operatorname*{Tr}_{\{s\}}\mathcal{T}r\prod_{\sigma=\uparrow,\downarrow}\prod_{l=M}^{1}\mathrm{e}^{-\Delta\tau\sum_{i,j}c^\dagger_{i,\sigma}K_{ij}c_{j,\sigma}}\mathrm{e}^{-\Delta\tau\sum_{i,j}c^\dagger_{i,\sigma}V^\sigma_{ij}(l)c_{j,\sigma}}$$

其中

$$K_{ij}=\begin{cases}-t & \text{if i and j are nearest neighbours}\\ 0 & \text{otherwise}\end{cases}$$

$$V^\sigma_{ij}(l)=\left[\frac{1}{\Delta\tau}\sigma s_i(l)\lambda+\left(\frac{U}{2}-\mu\right)\right]\delta_{ij}$$

利用 A的命题三，我们将费米子算符的 trace 求出。则配分函数为：

$$Z=\left(\frac{1}{2}\right)^{L^dM}\operatorname*{Tr}_{\{s\}}\prod_{\sigma=\uparrow,\downarrow}\det\left[1+B^\sigma_M\cdots B^\sigma_2B^\sigma_1\right]$$

其中：

$$B^\sigma_l=\mathrm{e}^{-\Delta\tau K}\mathrm{e}^{-\Delta\tau V^\sigma(l)}$$

由于 V 矩阵是对角的，我们可以直接计算出 B 矩阵以及 B^{-1} 矩阵：

$$\begin{aligned} [B^\sigma_l]_{ij} &= [\mathrm{e}^{-\Delta\tau K}]_{ij}[\mathrm{e}^{-\Delta\tau V^\sigma(l)}]_{jj} \\ &= [\mathrm{e}^{-\Delta K}]_{ij}\mathrm{e}^{-\Delta\tau\left[\frac{\sigma s_j(l)\lambda}{\Delta\tau}+\left(\frac{U}{2}-\mu\right)\right]} \end{aligned}$$

$$\begin{aligned} \left\{[B^\sigma_l]^{-1}\right\}_{ij} &= [\mathrm{e}^{\Delta\tau V^\sigma(l)}]_{ii}[\mathrm{e}^{\Delta K}]_{ij} \\ &= \mathrm{e}^{\Delta\tau\left[\frac{\sigma s_i(l)\lambda}{\Delta\tau}+\left(\frac{U}{2}-\mu\right)\right]}[\mathrm{e}^{\Delta K}]_{ij} \end{aligned}$$

定义

$$O^\sigma(\{s\}) = 1 + B_M^\sigma \cdots B_2^\sigma B_1^\sigma$$

则

$$\begin{aligned} Z &= \left(\frac{1}{2}\right)^{L^d M} \operatorname*{Tr}_{\{s\}} \det O^\uparrow(\{s\}) \cdot \det O^\downarrow(\{s\}) \\ &= \operatorname*{Tr}_{\{s\}} \rho(\{s\}) \end{aligned}$$

最后一个等号可以认为是辅助场的等效密度矩阵的定义。可以证明在 half-filling($\mu = \frac{U}{2}$) 时,$\rho(\{s\}) > 0$。首先，我们引入电子空穴变换，即

$$\begin{aligned} d_{i,\sigma} &= (-1)^i c_{i,\sigma}^\dagger \\ d_{i,\sigma}^\dagger &= (-1)^i c_{i,\sigma} \end{aligned}$$

则

$$\tilde{n}_{i,\sigma} = d_{i,\sigma}^\dagger d_{i,\sigma} = c_{i,\sigma} c_{i,\sigma}^\dagger = 1 - n_{i,\sigma}$$

从而

$$\begin{aligned} \det O^\uparrow(\{s\}) &= \mathcal{T}r \prod_{l=M}^{1} \mathrm{e}^{-\Delta\tau \sum_{i,j} c_i^\dagger K_{ij} c_j} \mathrm{e}^{-\lambda \sum_i c_i^\dagger s_i(l) c_i} \\ &= \mathcal{T}r \prod_{l=M}^{1} \mathrm{e}^{-\Delta\tau \sum_{i,j} d_i^\dagger K_{ij} d_j} \mathrm{e}^{-\lambda \sum_i s_i(l)(1 - d_i^\dagger d_i)} \\ &= \mathcal{T}r \prod_{l=M}^{1} \mathrm{e}^{-\Delta\tau \sum_{i,j} d_i^\dagger K_{ij} d_j} \mathrm{e}^{\lambda \sum_i s_i(l) d_i^\dagger d_i} \mathrm{e}^{-\lambda \sum_i s_i(l)} \\ &= \mathrm{e}^{-\lambda \sum_{i,l} s_i(l)} \det O^\downarrow(\{s\}) \end{aligned}$$

故 $\det O^\uparrow(\{s\}) \cdot \det O^\downarrow(\{s\}) > 0$。

现在我们来考虑一些物理量的期待值:

考虑算符 $O_\sigma = \mathbf{c}_\sigma^\dagger A \mathbf{c}_\sigma$

$$\langle O_\sigma(l) \rangle = \frac{\mathrm{Tr}[\langle O_\sigma(l) \rangle_{\{s\}} \rho(\{s\})]}{\mathrm{Tr}[\rho(\{s\})]}$$

$$\begin{aligned} \langle O_\sigma(l) \rangle_{\{s\}} &= \frac{\partial}{\partial\eta} \ln \mathrm{Tr} \left[D_M^\sigma \cdots D_{l+1}^\sigma \mathrm{e}^{\eta O_\sigma} D_l^\sigma \cdots D_1^\sigma \right] \Big|_{\eta=0} \\ &= \frac{\partial}{\partial\eta} \ln \det \left[1 + B_M^\sigma \cdots B_{l+1}^\sigma \mathrm{e}^{\eta O_\sigma} B_l^\sigma \cdots B_1^\sigma \right] \Big|_{\eta=0} \\ &= \frac{\partial}{\partial\eta} \mathrm{Tr} \ln \left[1 + B_M^\sigma \cdots B_{l+1}^\sigma \mathrm{e}^{\eta O_\sigma} B_l^\sigma \cdots B_1^\sigma \right] \Big|_{\eta=0} \\ &= \mathrm{Tr} \left[B_l^\sigma \cdots B_1^\sigma \left(1 + B_M^\sigma \cdots B_1^\sigma\right)^{-1} B_M^\sigma \cdots B_{l+1}^\sigma O_\sigma \right] \\ &= \mathrm{Tr} \left[\left(1 - \left(1 + B_l^\sigma \cdots B_1^\sigma B_M^\sigma \cdots B_{l+1}^\sigma\right)^{-1} \right) O_\sigma \right] \end{aligned}$$

上式用到了 $B\left(1+AB\right)^{-1}A=1-\left(1+BA\right)^{-1}$ 如果 A,B 是是可交换的，那么这是显然的，事实上，对于 A,B 不对易的情况这也是对的：

$$
\begin{aligned}
&B\left(1+AB\right)^{-1}A\\
=&\left[A^{-1}\left(1+AB\right)B^{-1}\right]^{-1}\\
=&\left(A^{-1}B^{-1}+1\right)^{-1}\\
=&\left(A^{-1}B^{-1}+1\right)^{-1}\left(A^{-1}B^{-1}+1-A^{-1}B^{-1}\right)\\
=&1-\left[BA\left(A^{-1}B^{-1}+1\right)\right]^{-1}\\
=&1-\left(1+BA\right)^{-1}
\end{aligned}
$$

上上式中 $D_l^\sigma=\mathrm{e}^{-\Delta\tau\sum_{i,j}c_{i,\sigma}^\dagger K_{ij}c_{j,\sigma}}\mathrm{e}^{-\Delta\tau\sum_{i,j}c_{i,\sigma}^\dagger V_{ij}^\sigma(l)c_{j,\sigma}}$。很容易可以验证

$$
\left\langle c_{i,\sigma}(l)c_{j,\sigma}^\dagger(l)\right\rangle_{\{s\}}=\left[\left(1+B_l^\sigma\cdots B_1^\sigma B_M^\sigma\cdots B_{l+1}^\sigma\right)^{-1}\right]_{ij}
$$

接下来我们考虑 $\left\langle c_{i,\sigma}(l_1)c_{j,\sigma}^\dagger(l_2)\right\rangle_{\{s\}}$，其中 $l_1>l_2$

$$
\begin{aligned}
\left\langle c_{i,\sigma}(l_1)c_{j,\sigma}^\dagger(l_2)\right\rangle_{\{s\}}&=\frac{\mathrm{Tr}[D_M^\sigma\cdots D_{l_1+1}^\sigma c_{i,\sigma}D_{l_1}^\sigma\cdots D_{l_2+1}^\sigma c_{j,\sigma}^\dagger D_{l_2}^\sigma\cdots D_1^\sigma]}{\mathrm{Tr}[D_M^\sigma\cdots D_1^\sigma]}\\
&=\frac{\mathrm{Tr}[D_M^\sigma\cdots D_{l_2+1}^\sigma(D_{l_1}^\sigma\cdots D_{l_2+1}^\sigma)^{-1}c_{i,\sigma}D_{l_1}^\sigma\cdots D_{l_2+1}^\sigma c_{j,\sigma}^\dagger D_{l_2}^\sigma\cdots D_1^\sigma]}{\mathrm{Tr}[D_M^\sigma\cdots D_1^\sigma]}
\end{aligned}
$$

考察

$$
c_i(\tau)=\mathrm{e}^{\tau\mathbf{c}^\dagger A\mathbf{c}}c_i\mathrm{e}^{-\tau\mathbf{c}^\dagger A\mathbf{c}}
$$

$$
\frac{\partial c_i}{\partial\tau}=\mathrm{e}^{\tau\mathbf{c}^\dagger A\mathbf{c}}[\mathbf{c}^\dagger A\mathbf{c},c_i]\mathrm{e}^{-\tau\mathbf{c}^\dagger A\mathbf{c}}=-\sum_j A_{ij}c_j(\tau)
$$

故

$$
c_i(\tau)=\sum_j\left[\mathrm{e}^{-A\tau}\right]_{ij}c_j
$$

故

$$
(D_{l_1}^\sigma\cdots D_{l_2+1}^\sigma)^{-1}c_{i,\sigma}D_{l_1}^\sigma\cdots D_{l_2+1}^\sigma=\sum_k[B_{l_1}^\sigma\cdots B_{l_2+1}^\sigma]_{ik}c_{k,\sigma}
$$

从而

$$
\begin{aligned}
\left\langle c_{i,\sigma}(l_1)c_{j,\sigma}^\dagger(l_2)\right\rangle_{\{s\}}&=\sum_k[B_{l_1}^\sigma\cdots B_{l_2+1}^\sigma]_{ik}\left\langle c_{k,\sigma}(l_1)c_{j,\sigma}^\dagger(l_2)\right\rangle_{\{s\}}\\
&=\left[B_{l_1}^\sigma\cdots B_{l_2+1}^\sigma\left(1+B_l^\sigma\cdots B_1^\sigma B_M^\sigma\cdots B_{l+1}^\sigma\right)^{-1}\right]_{ij}
\end{aligned}
$$

现在考察翻转自旋的概率。假如我们试图翻转 l 时间片段 i 格点上的 Ising 自旋即 $s_i(l) \to -s_i(l)$ ，这引起的变化为

$$V_{ii}^{\sigma}(l) = \frac{1}{\Delta\tau}\sigma\lambda s_i(l) \to \tilde{V}_{ii}^{\sigma}(l) = -\frac{1}{\Delta\tau}\sigma\lambda s_i(l)$$

这将会导致 $B_l^{\sigma} \to \tilde{B}_l^{\sigma} = B_l^{\sigma}\Delta_l^{\sigma}(i)$, 其中 $\Delta_l^{\sigma}(i)$ 的各个矩阵元为

$$[\Delta_l^{\sigma}(i)]_{jk} = \begin{cases} 0 & \text{if j}\neq\text{k} \\ 1 & \text{if j=k}\neq\text{i} \\ \mathrm{e}^{2\sigma\lambda s_i(l)} & \text{if j=k=i} \end{cases}$$

新旧构型的概率比为

$$r = \frac{\det O^{\uparrow}(\{s\}') \cdot \det O^{\downarrow}(\{s\}')}{\det O^{\uparrow}(\{s\}) \cdot \det O^{\downarrow}(\{s\})} = R_{\uparrow}R_{\downarrow}$$

其中:

$$\begin{aligned} R_{\sigma} &= \frac{\det O^{\sigma}(\{s\}')}{\det O^{\sigma}(\{s\})} \\ &= \frac{\det[1 + B_M^{\sigma} \cdots B_{l+1}^{\sigma} B_l^{\sigma} \Delta_l^{\sigma}(i) B_{l-1}^{\sigma} \cdots B_1^{\sigma}]}{\det[1 + B_M^{\sigma} \cdots B_1^{\sigma}]} \\ &= \frac{\det[1 + A^{\sigma}(l)\Delta_l^{\sigma}(i)]}{\det[1 + A^{\sigma}(l)]} \\ &= \det\left[\left[1 + \left([g^{\sigma}(l)]^{-1} - 1\right)\Delta_l^{\sigma}(i)\right] g^{\sigma}(l)\right] \\ &= \det[[g^{\sigma}(l)]^{-1}\left[g^{\sigma}(l) + (1 - g^{\sigma}(l))\,\Delta_l^{\sigma}(i)\right] g^{\sigma}(l)] \\ &= \det[1 + (1 - g^{\sigma}(l))(\Delta_l^{\sigma}(i) - 1)] \\ &= 1 + (1 - [g^{\sigma}(l)]_{ii})(\mathrm{e}^{2\sigma\lambda s_i(l)} - 1) \end{aligned}$$

其中 $A^{\sigma}(l)$ 和 $g^{\sigma}(l)$ 的定义为:

$$\begin{aligned} A^{\sigma}(l) &= B_{l-1}^{\sigma} \cdots B_1^{\sigma} B_M^{\sigma} \cdots B_l^{\sigma} \\ g^{\sigma}(l) &= [1 + A^{\sigma}(l)]^{-1} \end{aligned}$$

继续考虑 g 矩阵的更新:

$$\begin{aligned} [\tilde{g}^{\sigma}(l)]^{-1} &= 1 + \tilde{A}^{\sigma}(l) \\ &= 1 + A^{\sigma}(l)\Delta_l^{\sigma}(i) + A^{\sigma}(l) - A^{\sigma}(l) \\ &= 1 + A^{\sigma}(l) + A^{\sigma}(l)\left(\Delta_l^{\sigma}(i) - 1\right) \\ &= [g^{\sigma}(l)]^{-1} + \left[(g^{\sigma}(l))^{-1} - 1\right]\left(\Delta_l^{\sigma}(i) - 1\right) \end{aligned}$$

故：

$$\tilde{g}^\sigma(l) = \left[1 + (1 - g^\sigma(l))\,(\Delta_l^\sigma(i) - 1)\right]^{-1} g^\sigma(l)$$

我们定义矩阵

$$\Gamma_l^\sigma(l) \equiv \Delta_l^\sigma(i) - 1$$

注意这个矩阵只有一个矩阵元 $[\Gamma_l^\sigma(i)]_{ii} = \mathrm{e}^{2\sigma\lambda s_i(l)} - 1$ 不为零，其余矩阵元都为零。我们定义 $\gamma_i^\sigma(l) \equiv [\Gamma_l^\sigma(i)]_{ii}$ 则：

$$\tilde{g}^\sigma(l) = \left[1 + (1 - g^\sigma(l))\,\Gamma_l^\sigma(l)\right]^{-1} g^\sigma(l)$$

这样 g 矩阵的更新就可以通过一次矩阵求逆和一次矩阵乘法实现 (矩阵求逆和矩阵乘法的时间复杂度大致是 $O(n^3)$ 其中 n 为矩阵的维度), 但是考虑到 Γ 矩阵的稀疏性, 事实上我们是可以用手求出上式中矩阵的逆的，并且通过逆矩阵的稀疏性我们也可以手求出两个矩阵的乘法的。现在定义

$$M = 1 + (1 - g^\sigma(l))\,\Gamma_l^\sigma(i)$$

由于 Γ 矩阵只有一个元素不为零，所以 M 矩阵只有对角元以及第 i 列不为零，根据逆矩阵的基本求法

$$[A^{-1}]_{ij} = \frac{(-1)^{j+i} A_{ji}}{|A|}$$

我们只需要求出 M 矩阵的行列式,以及非零的代数余子式就可以了。M 的行列式很简单: $|M| = 1 + (1 - g_{ii}^\sigma(l))\gamma_l^\sigma(i)$ M 非零的代数余子式可以分为三种:1. $(-1)^{j+j} M_{jj} = 1 + (1 - g_{ii}^\sigma(l))\gamma_l^\sigma(i) = |M| \quad \mathrm{for} j \neq i$ 2. $(-1)^{i+j} M_{ij} = -(\delta_{ji} - g_{ji}^\sigma(l))\gamma_l^\sigma(i) \quad \mathrm{for} j \neq i$ 3. $(-1)^{i+i} M_{ii} = 1$ 综上：

$$\begin{aligned}
(-1)^{j+k} M_{jk} =& |M|\delta_{jk} - |M|\delta_{ji}\delta_{ki} \\
& - \delta_{ji}(\delta_{ki} - g_{ki}^\sigma(l))\gamma_l^\sigma(i) \\
& + \delta_{ji}\delta_{ki}(1 - g_{ii}^\sigma(l))\gamma_l^\sigma(i) \\
& + \delta_{ji}\delta_{ki} \\
=& |M|\delta_{jk} - \delta_{ji}(\delta_{ki} - g_{ki}^\sigma(l))\gamma_l^\sigma(i)
\end{aligned}$$

所以

$$[M^{-1}]_{jk} = \delta_{jk} - \frac{\delta_{ki}(\delta_{ji} - g_{ji}^\sigma(l))\gamma_l^\sigma(i)}{|M|}$$

所以

$$[\tilde{g}^\sigma(l)]_{jk} = g_{jk}^\sigma(i) - \frac{(\delta_{ji} - g_{ji}^\sigma(l))\gamma_l^\sigma(i) g_{ik}^\sigma(l)}{|M|}$$

A 需要用到的一些命题的证明

首先我们给出一些符号约定。对于一个有 N_s 个单粒子态的系统我们把产生湮灭算符写成矢量的形式：

$$\mathbf{c}=\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_{N_s} \end{pmatrix}, \qquad \mathbf{c}^\dagger=\begin{pmatrix} c_1^\dagger & c_2^\dagger & \cdots & c_{N_s}^\dagger \end{pmatrix}$$

下文中出现的 P 矩阵，是 $N_s\times N_p$ 维的矩阵。

命题一：

$$\mathrm{e}^{\mathbf{c}^\dagger T\mathbf{c}}\prod_{n=1}^{N_p}\left(\mathbf{c}^\dagger P\right)_n|0\rangle=\prod_{n=1}^{N_p}\left(\mathbf{c}^\dagger\mathrm{e}^T P\right)_n|0\rangle$$

其中 T 是厄米矩阵。

证：厄米矩阵总是可以写成如下的形式：$T=U\Lambda U^\dagger$，其中 Λ 是对角矩阵，U 是酉矩阵。我们假设 $\boldsymbol{\gamma}^\dagger=\mathbf{c}^\dagger U$，我们可以很容易验证 γ_n 满足费米子算符的反对易关系，$\{\gamma_m,\gamma_n\}=\{\gamma_m^\dagger,\gamma_n^\dagger\}=0$,$\{\gamma_m,\gamma_n^\dagger\}=\delta_{mn}$。

$$\begin{aligned}
&\mathrm{e}^{\mathbf{c}^\dagger T\mathbf{c}}\prod_{n=1}^{N_p}\left(\mathbf{c}^\dagger P\right)_n|0\rangle=\mathrm{e}^{\boldsymbol{\gamma}^\dagger\Lambda\boldsymbol{\gamma}}\prod_{n=1}^{N_p}\left(\boldsymbol{\gamma}^\dagger U^\dagger P\right)_n|0\rangle\\
=&\sum_{y_1,y_2,\cdots,y_{N_p}}\mathrm{e}^{\sum_i\gamma_i^\dagger\lambda_i\gamma_i}\gamma_{y_1}^\dagger\gamma_{y_2}^\dagger\cdots\gamma_{y_{N_p}}^\dagger|0\rangle\left(U^\dagger P\right)_{y_1 1}\left(U^\dagger P\right)_{y_2 2}\cdots\left(U^\dagger P\right)_{y_{N_p}N_p}\\
=&\sum_{y_1,y_2,\cdots,y_{N_p}}\gamma_{y_1}^\dagger\mathrm{e}^{\lambda_{y_1}}\gamma_{y_2}^\dagger\mathrm{e}^{\lambda_{y_2}}\cdots\gamma_{y_{N_p}}^\dagger\mathrm{e}^{\lambda_{y_{N_p}}}|0\rangle\left(U^\dagger P\right)_{y_1 1}\left(U^\dagger P\right)_{y_2 2}\cdots\left(U^\dagger P\right)_{y_{N_p}N_p}\\
=&\prod_{n=1}^{N_p}\left(\boldsymbol{\gamma}^\dagger\mathrm{e}^\Lambda U^\dagger P\right)_n|0\rangle=\prod_{n=1}^{N_p}\left(\mathbf{c}^\dagger U\mathrm{e}^\Lambda U^\dagger P\right)_n|0\rangle=\prod_{n=1}^{N_p}\left(\mathbf{c}^\dagger\mathrm{e}^T P\right)_n|0\rangle
\end{aligned}$$

命题二：令

$$|\Psi\rangle=\prod_{n=1}^{N_p}\left(\mathbf{c}^\dagger P\right)_n|0\rangle$$

$$\left|\tilde{\Psi}\right\rangle=\prod_{n=1}^{N_p}\left(\mathbf{c}^\dagger\tilde{P}\right)_n|0\rangle$$

则

$$\left\langle\Psi\middle|\tilde{\Psi}\right\rangle=\det\left(P^\dagger\tilde{P}\right)$$

证：

$$
\begin{aligned}
\left\langle \Psi \middle| \tilde{\Psi} \right\rangle &= \langle 0| \prod_{n=N_p}^{1} \left(P^\dagger \mathbf{c}\right)_n \prod_{n'=1}^{N_p} \left(\mathbf{c}^\dagger \tilde{P}\right)_n |0\rangle \\
&= \sum_{\substack{x_1, x_2, \cdots, x_{N_p} \\ y_1, y_2, \cdots, y_{N_p}}} \langle 0| c_{x_{N_p}} \cdots c_{x_1} c^\dagger_{y_1} \cdots c^\dagger_{y_{N_p}} |0\rangle \\
&\times \left(P^\dagger\right)_{N_p x_{N_p}} \cdots \left(P^\dagger\right)_{1x_1} \tilde{P}_{y_1 1} \cdots \tilde{P}_{y_{N_p} N_p} \\
&= \sum_{x_1, x_2, \cdots, x_{N_p}, \pi} (-1)^\pi \left(P^\dagger\right)_{N_p x_{N_p}} \cdots \left(P^\dagger\right)_{1x_1} \tilde{P}_{x_{\pi(1)} 1} \cdots \tilde{P}_{x_{\pi(N_p)} N_p} \\
&= \sum_{x_1, x_2, \cdots, x_{N_p}, \pi} (-1)^{\pi^{-1}} \left(P^\dagger\right)_{N_p x_{N_p}} \cdots \left(P^\dagger\right)_{1x_1} \tilde{P}_{x_1 \pi^{-1}(1)} \cdots \tilde{P}_{x_{N_p} \pi^{-1}(N_p)} \\
&= \sum_\pi (-1)^\pi \left(P^\dagger \tilde{P}\right)_{1,\pi(1)} \left(P^\dagger \tilde{P}\right)_{2,\pi(2)} \cdots \left(P^\dagger \tilde{P}\right)_{N_p, \pi(N_p)} \\
&= \det(P^\dagger \tilde{P})
\end{aligned}
$$

命题三：

$$
\mathrm{Tr}\left[\mathrm{e}^{\mathbf{c}^\dagger T_1 \mathbf{c}} \mathrm{e}^{\mathbf{c}^\dagger T_2 \mathbf{c}} \cdots \mathrm{e}^{\mathbf{c}^\dagger T_n \mathbf{c}}\right] = \det\left[1 + \mathrm{e}^{T_1} \mathrm{e}^{T_2} \cdots \mathrm{e}^{T_n}\right]
$$

证：令 $U = \mathrm{e}^{\mathbf{c}^\dagger T_1 \mathbf{c}} \mathrm{e}^{\mathbf{c}^\dagger T_2 \mathbf{c}} \cdots \mathrm{e}^{\mathbf{c}^\dagger T_n \mathbf{c}}$, $B = \mathrm{e}^{T_1} \mathrm{e}^{T_2} \cdots \mathrm{e}^{T_n}$

$$
\begin{aligned}
&\det(1+B) \\
=&\sum_\pi (-1)^\pi \left(B_{1,\pi(1)} + \delta_{1,\pi(1)}\right) \left(B_{2,\pi(2)} + \delta_{2,\pi(2)}\right) \cdots \left(B_{N_s,\pi(N_s)} + \delta_{N_s,\pi(N_s)}\right) \\
=&\sum_\pi (-1)^\pi \delta_{1,\pi(1)} \delta_{2,\pi(2)} \cdots \delta_{N_s,\pi(N_s)} \\
&+ \sum_x \sum_\pi (-1)^\pi B_{x,\pi(x)} \delta_{1,\pi(1)} \delta_{2,\pi(2)} \cdots \overbrace{\delta_{x,\pi(x)}} \cdots \delta_{N_s,\pi(N_s)} \\
&+ \sum_{x<y} \sum_\pi (-1)^\pi B_{x,\pi(x)} B_{y,\pi(y)} \delta_{1,\pi(1)} \cdots \overbrace{\delta_{x,\pi(x)}} \cdots \overbrace{\delta_{y,\pi(y)}} \cdots \delta_{N_s,\pi(N_s)} \\
&+ \sum_{x<y<z} \sum_\pi (-1)^\pi B_{x,\pi(x)} B_{y,\pi(y)} B_{z,\pi(z)} \delta_{1,\pi(1)} \cdots \overbrace{\delta_{x,\pi(x)}} \cdots \overbrace{\delta_{y,\pi(y)}} \cdots \overbrace{\delta_{z,\pi(z)}} \cdots \delta_{N_s,\pi(N_s)} \\
&+ \cdots
\end{aligned}
$$

其中 $\overbrace{\delta_{x,\pi(x)}}$ 代表这个连乘中没有这一项。考察前几个项：

$$
\sum_\pi (-1)^\pi \delta_{1,\pi(1)} \delta_{2,\pi(2)} \cdots \delta_{N_s,\pi(N_s)} = 1
$$

$$
\begin{aligned}
&\sum_{\pi}(-1)^{\pi}B_{x,\pi(x)}\delta_{1,\pi(1)}\delta_{2,\pi(2)}\cdots\overbrace{\delta_{x,\pi(x)}}\cdots\delta_{N_s,\pi(N_s)}\\
=&B_{x,x}\\
=&\det\left(P(x)^{\dagger}BP(x)\right)\\
=&\langle 0|\left(P(x)^{\dagger}\mathbf{c}\right)\left(\mathbf{c}^{\dagger}BP(x)\right)|0\rangle\\
=&\langle 0|\left(P(x)^{\dagger}\mathbf{c}\right)U\left(\mathbf{c}^{\dagger}P(x)\right)\right)|0\rangle\\
=&\langle 0|c_xUc_x^{\dagger}|0\rangle
\end{aligned}
$$

$$
\begin{aligned}
&\sum_{\pi}(-1)^{\pi}B_{x,\pi(x)}B_{y,\pi(y)}\delta_{1,\pi(1)}\cdots\overbrace{\delta_{x,\pi(x)}}\cdots\overbrace{\delta_{y,\pi(y)}}\cdots\delta_{N_s,\pi(N_s)}\\
=&B_{x,x}B_{y,y}-Bx,yBy,x\\
=&\det\left(P(x,y)^{\dagger}BP(x,y)\right)\\
=&\langle 0|\prod_{n=2}^{1}\left(P(x,y)^{\dagger}\mathbf{c}\right)_n\prod_{n'=1}^{2}\left(\mathbf{c}^{\dagger}BP(x,y)\right)_{n'}|0\rangle\\
=&\langle 0|\prod_{n=2}^{1}\left(P(x,y)^{\dagger}\mathbf{c}\right)_nU\prod_{n'=1}^{2}\left(\mathbf{c}^{\dagger}P(x,y)\right)\right)_{n'}|0\rangle\\
=&\langle 0|c_yc_xUc_x^{\dagger}c_y^{\dagger}|0\rangle
\end{aligned}
$$

上面推导利用了定理一和定理二。其中 $P(x)$ 代表 $N_s\times 1$ 的矩阵，其中只有第 x 行的矩阵元为 1，其余矩阵元为零。$P(x,y)$ 代表 $N_s\times 2$ 的矩阵，第一列中只有第 x 行的矩阵元为 1，其余矩阵元为零，第二列中只有第 y 行的矩阵元为 1，其余矩阵元为零。重复上述的讨论我们可以得到：

$$
\begin{aligned}
&\det(1+B)\\
=&1+\sum_{x}\langle 0|c_xUc_x^{\dagger}|0\rangle+\sum_{x<y}\langle 0|c_yc_xUc_x^{\dagger}c_y^{\dagger}|0\rangle\\
&+\sum_{x<y<z}\langle 0|c_zc_yc_xUc_x^{\dagger}c_y^{\dagger}c_z^{\dagger}|0\rangle+\cdots\\
=&\mathrm{Tr}[U]
\end{aligned}
$$

即

$$
\mathrm{Tr}\left[\mathrm{e}^{\mathbf{c}^{\dagger}T_1\mathbf{c}}\mathrm{e}^{\mathbf{c}^{\dagger}T_2\mathbf{c}}\cdots\mathrm{e}^{\mathbf{c}^{\dagger}T_n\mathbf{c}}\right]=\det\left[1+\mathrm{e}^{T_1}\mathrm{e}^{T_2}\cdots\mathrm{e}^{T_n}\right]
$$

命题三得证。