1 DQMC review

In DQMC algorithm, we decomposite two-body term with

$$e^{-\Delta\tau U A^2} = \sum_l \gamma(l) e^{\sqrt{-\Delta\tau U}\eta(l)A} \tag{1}$$

The partition funtion can be written as

$$\mathcal{Z} = Tr_F \sum_C \prod_\tau^{L_{trot}} e^{-\Delta\tau K} \prod_i^{N_s ite} \gamma_{\tau,i} e^{\sqrt{-\Delta\tau U}\eta_{\tau,i}A_i} \tag{2}$$

trace out the fermionic trace, (the const γ_i should pull out of Tr_F)

$$\begin{aligned}
\mathcal{Z} &= \sum_C \left[\prod^{L_{trot}} \prod_i^{N_{site}} \gamma_{\tau,i}\right] det(\mathcal{I} + \prod^{L_{trot}} e^{-\Delta\tau K} \prod_i^{N_{site}} e^{\sqrt{-\Delta\tau U}\eta_{\tau,i}A_i}) \\
&= \sum_C \left[\prod^{L_{trot}} \prod_i^{N_{site}} \gamma_{\tau,i}\right] det(\mathcal{I} + \prod^{L_{trot}} B_\tau(C)) \\
&= \sum_C W(C)D(C)
\end{aligned} \tag{3}$$

where $W(C) = \prod^{L_{trot}} \prod_i^{N_{site}} \gamma_{\tau,i}$, $D(C) = det(\mathcal{I} + \prod^{L_{trot}} B_\tau(C))$ and $D(C) = Tr_F \prod^{L_{trot}} e^{-\Delta\tau K} \prod_i^{N_{site}} e^{\sqrt{-\Delta\tau U}\eta_{\tau,i}A_i}$

The finite temperature observables

$$\langle O \rangle = \frac{1}{\mathcal{Z}} Tr_F e^{-\beta H} O \tag{4}$$

we can also decomposite two-body term in numerator

$$\begin{aligned}
\langle O \rangle &= \frac{1}{\mathcal{Z}} Tr_F \sum_C \prod_\tau^{L_{trot}} e^{-\Delta\tau K} \prod_i^{N_{site}} \gamma_{\tau,i} e^{\sqrt{-\Delta\tau U}\eta_{\tau,i}A_i} O \\
&= \sum_C W(C) Tr_F \prod_\tau^{L_{trot}} e^{-\Delta\tau K} \prod_i^{N_{site}} e^{\sqrt{-\Delta\tau U}\eta_{\tau,i}A_i} O / \sum_{C'} W(C')D(C') \\
&= \sum_C \left[W(C)D(C) \frac{Tr_F \prod_\tau^{L_{trot}} B_\tau(C) O}{D(C)} / \sum_{C'} W(C')D(C') \right] \\
&= \sum_C S(C) \langle O \rangle_C / \sum_{C'} S(C')
\end{aligned} \tag{5}$$

where $S(C) = W(C)D(C)$ and $\langle O \rangle_C = Tr_F \prod_\tau^{L_{trot}} B_\tau(C) O / Tr_F \prod_\tau^{L_{trot}} B_\tau(C)$.

2 Sign Problem

We can rewrite the observables as

$$\begin{aligned}\langle O\rangle &= \sum_C S(C)\langle O\rangle_C / \sum_{C'} S(C') \\ &= \frac{\sum_C |S(C)|\frac{S(C)}{|S(C)|}\langle O\rangle_C / \sum_{C''}|S(C'')|}{\sum_{C'}|S(C)|\frac{S(C)}{|S(C)|}/\sum_{C'''}|S(C''')|}\end{aligned} \tag{6}$$

where $S(C) = W(C)D(C)$ and the partition function $Z = \sum_C S(C)$. We can calculate the denominator and numerator in Eq.(6) by Monte Carlo algorithm. If the denominator goes to zero, the Sign Problem occurs.

3 divide the sampling

The steps in this section may be confused, we first explain the main idea of this procedure.

- First, we introduce an artificial cutoff λ in the observables, $\langle O\rangle^{\lambda}$, the observables recover the exact one when $\lambda \to -\infty$, $\langle O\rangle = \langle O\rangle^{-\infty}$.
- Second, we find a relation between exact one and cutoff one $\langle O\rangle^{-\infty} = \Omega + \langle O\rangle^{\lambda}/(\omega+1)$
- Third, rescaling the observables, $\langle O\rangle \leftarrow \langle O\rangle^{\lambda}$, and repeat the second untill the results are solvable.

This three procedure form a renormalization process. At the end, we reverse these steps, so we start from a solvable results, and recursively find the origin exact results.

We write the observables

$$\begin{aligned}\langle O\rangle &= \frac{\sum_C S(C)\langle O\rangle_C}{\sum_{C'} S(C')} \\ &= \frac{\sum_C ReS(C)\frac{S(C)}{ReS(C)}\langle O\rangle_C}{\sum_{C'} ReS(C')}\end{aligned} \tag{7}$$

The second line is true because the partition function is real, and Re means real part. Before we reweight the denominator and numerator, we first divide the sampling space. For example, we can divide the denominator

$$\sum_{C'} ReS(C') = \sum_{C'} \Theta(\lambda - ReS(C'))ReS(C') + \sum_{C'} \Theta(ReS(C') - \lambda)ReS(C') \tag{8}$$

For notation convenience, we define

$$\begin{aligned}\sum_C^{>\lambda} &= \sum_C \Theta(ReS(C)-\lambda)\\ \sum_C^{\mu<<\nu} &= \sum_C \Theta(ReS(C)-\mu)\Theta(\nu-ReS(C))\end{aligned} \tag{9}$$

The first one means the summation of these HS configurations which have $ReS(C) > \lambda$ and the latter one means the summation of these HS configurations whose $ReS(C)$ lying in a shell, $\mu < ReS(C) < \nu$.

Next, we devide the numerator and denominator,

$$\begin{aligned}\langle O\rangle &= \frac{\sum_C ReS(C)\frac{S(C)}{ReS(C)}\langle O\rangle_C}{\sum_{C'} ReS(C')}\\ &= \frac{\sum_{C_1}^{-\infty<<\lambda_1} ReS(C_1)\frac{S(C_1)}{ReS(C_1)}\langle O\rangle_{C_1} + \sum_{C_2}^{>\lambda_1} ReS(C_2)\frac{S(C_2)}{ReS(C_2)}\langle O\rangle_{C_2}}{\sum_{C_3}^{-\infty<<\lambda_1} ReS(C_3) + \sum_{C_4}^{>\lambda_1} ReS(C_4)}\end{aligned} \tag{10}$$

dividing $\sum_C^{>\lambda_1} ReS(C)$ in the numerator and denominator simultaneously, the denominator will be

$$\begin{aligned}&\frac{\sum_{C_1}^{-\infty<<\lambda_1} ReS(C_1) + \sum_{C_2}^{>\lambda_1} ReS(C_2)}{\sum_{C_3}^{>\lambda_1} ReS(C_3)}\\ &= \frac{\sum_{C_1}^{-\infty<<\lambda_1} ReS(C_1)}{\sum_{C_2}^{>\lambda_1} ReS(C_2)} + 1\\ &= \omega(-\infty, \lambda) + 1\end{aligned} \tag{11}$$

Here we define $\omega(\mu, \nu) = \frac{\sum_{C_1}^{\mu<<\nu} ReS(C_1)}{\sum_{C_2}^{>\nu} ReS(C_2)}$ And now, we look at the numerator, the first term

$$\begin{aligned}&\frac{\sum_{C_1}^{-\infty<<\lambda_1} ReS(C_1)\frac{S(C_1)}{ReS(C_1)}\langle O\rangle_{C_1}}{\sum_{C_2}^{>\lambda} ReS(C_2)}\\ &= \frac{\sum_{C_1}^{-\infty<<\lambda_1} ReS(C_1)\frac{S(C_1)}{ReS(C_1)}\langle O\rangle_{C_1} / \sum_{C_3}^{-\infty<<\lambda_1} ReS(C_3)}{\sum_{C_2}^{>\lambda} ReS(C_2) / \sum_{C_4}^{-\infty<<\lambda_1} ReS(C_4)}\\ &= \langle O\rangle^{-\infty<<\lambda_1}\omega(-\infty, \lambda_1)\end{aligned} \tag{12}$$

the second term

$$\frac{\sum_{C_1}^{>\lambda_1} ReS(C_1)\frac{S(C_1)}{ReS(C_1)}\langle O\rangle_{C_1}}{\sum_{C_2}^{>\lambda} ReS(C_2)} = \langle O\rangle^{>\lambda_1} \tag{13}$$

Here, we define $\langle O\rangle^{>\lambda}$ and $\langle O\rangle^{\nu<<\mu}$. The observables now can be written

$$\boxed{\langle O\rangle = \frac{\langle O\rangle^{-\infty<<\lambda_1}\omega(-\infty,\lambda_1)+\langle O\rangle^{>\lambda_1}}{\omega(-\infty,\lambda)+1}} \tag{14}$$

Now comes to the critical part, by choosing a proper λ_1, the denominator $\omega(-\infty,\lambda)+1$ **will not** goes to zero when Sign Problem occurs, and the Sign Problem will be absorbed in the $\langle O\rangle^{>\lambda_1}$ and $\omega(-\infty,\lambda)$. For example, we can choose a negative λ_1 with large absolute value, and the term of $\langle O\rangle^{-\infty<<\lambda_1}$ can be compute by

$$\begin{aligned}\langle O\rangle^{-\infty<<\lambda_1} &= \frac{\sum_{C_1}^{-\infty<<\lambda_1} ReS(C_1)\frac{S(C_1)}{ReS(C_1)}\langle O\rangle_{C_1}}{\sum_{C_2}^{-\infty<<\lambda_1} ReS(C_2)}\\ &= \frac{\sum_{C_1}^{-\infty<<\lambda_1} |ReS(C_1)|\frac{ReS(C_1)}{|ReS(C_1)|}\frac{S(C_1)}{ReS(C_1)}\langle O\rangle_{C_1}/\sum_{C_3}^{-\infty<<\lambda 1}|ReS(C_3)|}{\sum_{C_2}^{-\infty<<\lambda_1} |ReS(C_2)|\frac{ReS(C_2)}{|ReS(C_2)|}/\sum_{C_4}^{-\infty<<\lambda 1}|ReS(C_4)|}\end{aligned} \tag{15}$$

after reweight, this value is well behaved, because the $ReS(C)$ lie in a shell, the average sign equals to 1.

The $\langle O\rangle^{>\lambda_1}$ has the form

$$\langle O\rangle^{>\lambda_1} = \frac{\sum_{C_1}^{>\lambda_1} ReS(C_1)\frac{S(C_1)}{ReS(C_1)}\langle O\rangle_{C_1}}{\sum_{C_2}^{>\lambda_1} ReS(C_2)} \tag{16}$$

this is **not** well behaved since the denominator may be close to zero if the shell is narrow. this happend also in $\omega(-\infty,\lambda_1)$

$$\omega(\mu,\nu) = \frac{\sum_{C_1}^{\mu<<\nu} ReS(C_1)}{\sum_{C_2}^{>\nu} ReS(C_2)} \tag{17}$$

Then we divide the sampling recursively, we have this equation similiar with Eq.(14)

$$\begin{aligned}\langle O\rangle^{>\lambda_1} &= \frac{\sum_{C_1}^{>\lambda_1} ReS(C_1)\frac{S(C_1)}{ReS(C_1)}\langle O\rangle_{C_1}}{\sum_{C_2}^{>\lambda_1} ReS(C_2)}\\ &= \frac{\sum_{C_1}^{\lambda_1<<\lambda_2} ReS(C_1)\frac{S(C_1)}{ReS(C_1)}\langle O\rangle_{C_1}+\sum_{C_2}^{>\lambda_2} ReS(C_2)\frac{S(C_2)}{ReS(C_2)}\langle O\rangle_{C_2}}{\sum_{C_3}^{\lambda_1<<\lambda_2} ReS(C_3)+\sum_{C_4}^{>\lambda_2} ReS(C_4)}\\ &= \frac{\omega(\lambda_1,\lambda_2)\langle O\rangle^{\lambda_1<<\lambda_2}+\langle O\rangle^{>\lambda_2}}{\omega(\lambda_1,\lambda_2)+1}\end{aligned} \tag{18}$$

Similiar to this, the $\omega(-\infty, \lambda_1)$ can be written as

$$
\begin{aligned}
\omega(-\infty, \lambda_1) &= \frac{\sum_{C_1}^{-\infty<<\lambda_1} ReS(C_1)}{\sum_{C_2}^{>\lambda_1} ReS(C_2)} \\
&= \frac{\sum_{C_1}^{-\infty<<\lambda_1} ReS(C_1)}{\sum_{C_2}^{\lambda_1<<\lambda_2} ReS(C_2) + \sum_{C_3}^{>\lambda_2} ReS(C_3)} \\
&= \frac{\sum_{C_1}^{-\infty<<\lambda_1} ReS(C_1)/\sum_{C_2}^{\lambda_1<<\lambda_2} ReS(C_2)}{1+\sum_{C_3}^{>\lambda_2} ReS(C_3)/\sum_{C_4}^{\lambda_1<<\lambda_2} ReS(C_4)} \\
&= \frac{\omega'(-\infty, \lambda_1, \lambda_2)}{1+1/\omega(\lambda_1, \lambda_2)} \\
&= \frac{\omega'(-\infty, \lambda_1, \lambda_2)\omega(\lambda_1, \lambda_2)}{\omega(\lambda_1, \lambda_2)+1}
\end{aligned} \tag{19}
$$

Here we define the

$$
\begin{aligned}
\omega'(\mu, \nu, \xi) &= \frac{\sum_{C_1}^{\mu<<\nu} ReS(C_1)}{\sum_{C_2}^{\nu<<\xi} ReS(C_2)} \\
&= \frac{\sum_{C_1}^{\mu<<\xi} |ReS(C_1)| \frac{ReS(C_1)}{|ReS(C_1)|} \Theta(\nu - ReS(C_1))/\sum_{C_2}^{\mu<<\xi} |ReS(C_2)|}{\sum_{C_3}^{\mu<<\xi} |ReS(C_3)| \frac{ReS(C_3)}{|ReS(C_3)|} \Theta(ReS(C_3) - \nu)/\sum_{C_4}^{\mu<<\xi} |ReS(C_4)|}
\end{aligned} \tag{20}
$$

This is also well behaved since μ and ξ are close.

We can **recursively repeat this procedure**, and every observables in the narrow shell $\langle O \rangle^{\lambda_n<<\lambda_{n+1}}$ is well behaved, untill we reach a boundary, that is $\lambda_M = 0$. When we reach this boundary, the higher observables is

$$
\begin{aligned}
\langle O \rangle^{>\lambda_M} &= \langle O \rangle^{>0} \\
&= \frac{\sum_{C_1} \Theta(ReS(C_1)) ReS(C_1) \frac{S(C_1)}{ReS(C_1)} \langle O \rangle_{C_1}}{\sum_{C_2} \Theta(ReS(C_2)) ReS(C_2)} \\
&= \frac{\sum_{C_1}^{>0} |ReS(C_1)| \frac{ReS(C_1)}{|ReS(C_1)|} \frac{S(C_1)}{ReS(C_1)} \langle O \rangle_{C_1}/\sum_{C_3}^{>0} |ReS(C_3)|}{\sum_{C_2}^{>0} |ReS(C_2)| \frac{ReS(C_2)}{|ReS(C_2)|}/\sum_{C_4}^{>0} |ReS(4)|}
\end{aligned} \tag{21}
$$

In fact, the reweight in the third line can be ignored, because the sign always positive. The $\omega(\lambda_{M-1}, \lambda_M)$ can be written as

$$
\begin{aligned}
&\omega(\lambda_{M-1}, \lambda_M) = \omega(\lambda_{M-1}, 0) \\
&= \frac{\sum_{C_1}^{\lambda_{M-1}<<0} ReS(C_1)}{\sum_{C_2}^{>0} ReS(C_2)} \\
&= \frac{\sum_{C_1}^{\lambda_{M-1}<<\infty} |ReS(C_1)| \frac{ReS(C_1)}{|ReS(C_1)|} \Theta(-ReS(C_1))/\sum_{C_2}^{\lambda_{M-1}<<\infty} |ReS(C_2)|}{\sum_{C_3}^{\lambda_{M-1}<<\infty} |ReS(C_3)| \frac{ReS(C_3)}{|ReS(C_3)|} \Theta(ReS(C_1))/\sum_{C_4}^{\lambda_{M-1}<<\infty} |ReS(C_4)|}
\end{aligned} \tag{22}
$$

This value is well behaved because of the Θ funtion, unless the $\sum_{C_4}^{\lambda_{M-1}<<\infty} |ReS(C_4)|$ is much larger than $\sum_{C_2}^{>0} ReS(C_2)$. However, we can choosing the value of λ_{M-1} to avoid.

Now, we have

$$\boxed{\langle O\rangle^{\lambda_M=0} = \frac{\sum_{C_1}^{>0} |ReS(C_1)| \frac{ReS(C_1)}{|ReS(C_1)|} \frac{S(C_1)}{ReS(C_1)} \langle O\rangle_{C_1} / \sum_{C_3}^{>0} |ReS(C_3)|}{\sum_{C_2}^{>0} |ReS(C_2)| \frac{ReS(C_2)}{|ReS(C_2)|} / \sum_{C_4}^{>0} |ReS(4)|}} \tag{23}$$

$$\boxed{\omega(\lambda_{M-1}, \lambda_M = 0) = \frac{\sum_{C_1}^{\lambda_{M-1}<<\infty} ReS(C_1)\Theta(-ReS(C_1))}{\sum_{C_3}^{\lambda_{M-1}<<\infty} ReS(C_3)\Theta(ReS(C_1))}} \tag{24}$$

And we have the recursive relation

$$\boxed{\omega(\lambda_{N-1}, \lambda_N) = \frac{\omega'(\lambda_{N-1}, \lambda_N, \lambda_{N+1})\omega(\lambda_N, \lambda_{N+1})}{\omega(\lambda_N, \lambda_{N+1}) + 1}} \tag{25}$$

and

$$\boxed{\langle O\rangle^{>\lambda_{N-1}} = \frac{\omega(\lambda_{N-1}, \lambda_N)\langle O\rangle^{\lambda_{N-1}<<\lambda_N} + \langle O\rangle^{>\lambda_N}}{\omega(\lambda_{N-1}, \lambda_N) + 1}} \tag{26}$$

where

$$\boxed{\omega'(\lambda_{N-1}, \lambda_N, \lambda_{N+1}) = \frac{\sum_{C_1}^{\lambda_{N-1}<<\lambda_{N+1}} ReS(C_1)\Theta(\lambda_N - ReS(C_1))}{\sum_{C_3}^{\lambda_{N-1}<<\lambda_{N+1}} ReS(C_3)\Theta(ReS(C_3) - \lambda_N)}} \tag{27}$$

and

$$\boxed{\langle O\rangle^{\lambda_{N-1}<<\lambda_N} = \frac{\sum_{C_1}^{\lambda_{N-1}<<\lambda_N} ReS(C_1) \frac{S(C_1)}{ReS(C_1)} \langle O\rangle_{C_1}}{\sum_{C_2}^{\lambda_{N-1}<<\lambda_N} ReS(C_2)}} \tag{28}$$

We can start from $\lambda_M = 0$, λ_{M-1}, λ_{M-2}, and repeat the recursion, which is the inverse of the origin recursion, to get the $\langle O\rangle = \langle O\rangle^{>-\infty}$ finally.

4 flow equation

In continumm limit

$$\begin{aligned} S^{>\lambda_1} &= (1 + \omega(\lambda_2) * d\lambda) S^{>\lambda_2} \\ dS^{\lambda_2} &= \omega(\lambda_2) * d\lambda \\ S^{\lambda_2} &= S^{>0} e^{\int_0^{\lambda_2} \omega(\lambda) d\lambda} \end{aligned} \tag{29}$$

observables

$$\begin{aligned} \langle O\rangle^{>\lambda_1} - \langle O\rangle^{>\lambda_2} &= \frac{\omega(\lambda_1, \lambda_2)}{1 + \omega(\lambda_1, \lambda_2)} (\langle O\rangle^{\lambda_1<<\lambda_2} - \langle O\rangle^{>\lambda_2}) \\ d\langle O\rangle^{\lambda_2} &= \omega(\lambda_2) d\lambda (\langle O\rangle^{\lambda_1<<\lambda_2} - \langle O\rangle^{>\lambda_2}) \\ \langle O\rangle^{\lambda_2} &= \langle O\rangle^{>0} e^{-\int_0^{\lambda_2} \omega(\lambda) d\lambda} + \langle O\rangle^{-\infty<<\lambda_2} \end{aligned} \tag{30}$$