1 First order QuaPI

If we have the hybridization in frequecy domain $\Delta(i\omega_n)$ [$\omega_n=(2n+1)\pi/\beta$ for fermions, $\Delta(\tau+\beta)=-\Delta(\tau)$], then

$$\Delta(\tau)=\frac{1}{\beta}\sum_{n=-\infty}^{\infty}\Delta(i\omega_n)e^{-i\omega_n\tau},\quad \Delta(i\omega_n)=\int_0^\beta \mathrm{d}\tau\,\Delta(\tau)e^{i\omega_n\tau}. \tag{1}$$

Now let us apply QuaPI procedures. For $i\neq j$, we have

$$\begin{aligned}
\int_{\left(i-\frac{1}{2}\right)\delta\tau}^{\left(i+\frac{1}{2}\right)\delta\tau}\mathrm{d}\tau\int_{\left(j-\frac{1}{2}\right)\delta\tau}^{\left(j+\frac{1}{2}\right)\delta\tau}\mathrm{d}\tau' e^{-i\omega_n(\tau-\tau')} &= \frac{1}{i\omega_n}\int_{\left(i-\frac{1}{2}\right)\delta\tau}^{\left(i+\frac{1}{2}\right)\delta\tau}\mathrm{d}\tau\left[e^{-i\omega_n\left(\tau-j-\frac{1}{2}\right)}-e^{-i\omega_n\left(\tau-j+\frac{1}{2}\right)}\right]\\
&= \frac{1}{\omega_n^2}\left[e^{-i\omega_n\left(i+\frac{1}{2}-j-\frac{1}{2}\right)}-e^{-i\omega_n\left(i-\frac{1}{2}-j-\frac{1}{2}\right)}-e^{-i\omega_n\left(i+\frac{1}{2}-j+\frac{1}{2}\right)}+e^{-i\omega_n\left(i-\frac{1}{2}-j+\frac{1}{2}\right)}\right]\\
&= \frac{1}{\omega_n^2}[e^{-i\omega_n(i-j)\delta\tau}-e^{-i\omega_n(i-j-1)\delta\tau}-e^{-i\omega_n(i-j+1)\delta\tau}+e^{-i\omega_n(i-j)\delta\tau}]\\
&= \frac{2}{\omega_n^2}e^{-i\omega_n(i-j)\delta\tau}(1-\cos\omega_n\delta\tau)
\end{aligned}\tag{2}$$

for $i=j$, we have (for $\tau>\tau'$)

$$\begin{aligned}
\int_{\left(i-\frac{1}{2}\right)\delta\tau}^{\left(i+\frac{1}{2}\right)\delta\tau}\mathrm{d}\tau\int_{\left(i-\frac{1}{2}\right)\delta\tau}^{\tau}\mathrm{d}\tau' e^{-i\omega_n(\tau-\tau')} &= \frac{1}{i\omega_n}\int_{\left(i-\frac{1}{2}\right)\delta\tau}^{\left(i+\frac{1}{2}\right)\delta\tau}\mathrm{d}\tau\left[1-e^{-i\omega_n\left(\tau-i+\frac{1}{2}\right)}\right]\\
&= \frac{\delta\tau}{i\omega_n}-\frac{1}{\omega_n^2}\left[e^{-i\omega_n\left(i+\frac{1}{2}-i+\frac{1}{2}\right)}-e^{-i\omega_n\left(i-\frac{1}{2}-i+\frac{1}{2}\right)}\right]\\
&= \frac{\delta\tau}{i\omega_n}-\frac{1}{\omega_n^2}[e^{-i\omega_n\delta\tau}-1],\\
&= -\frac{1}{\omega_n^2}[e^{-i\omega_n\delta\tau}-(1-i\omega_n\delta\tau)]
\end{aligned}\tag{3}$$

and for $\tau<\tau'$

$$\begin{aligned}
\int_{\left(i-\frac{1}{2}\right)\delta\tau}^{\left(i+\frac{1}{2}\right)\delta\tau}\mathrm{d}\tau'\int_{\left(i-\frac{1}{2}\right)\delta\tau}^{\tau'}\mathrm{d}\tau e^{-i\omega_n(\tau-\tau')} &= \frac{i}{\omega_n}\int_{\left(i-\frac{1}{2}\right)\delta\tau}^{\left(i+\frac{1}{2}\right)\delta\tau}\mathrm{d}\tau'\left[1-e^{-i\omega_n\left(i-\frac{1}{2}-\tau'\right)}\right]\\
&= \frac{i\delta\tau}{\omega_n}-\frac{1}{\omega_n^2}\left[e^{-i\omega_n\left(i-\frac{1}{2}-i-\frac{1}{2}\right)}-e^{-i\omega_n\left(i-\frac{1}{2}-i+\frac{1}{2}\right)}\right]\\
&= \frac{i\delta\tau}{\omega_n}-\frac{1}{\omega_n^2}[e^{i\omega_n\delta\tau}-1]\\
&= -\frac{1}{\omega_n^2}[e^{i\omega_n\delta\tau}-(1+i\omega_n\delta\tau)].
\end{aligned}\tag{4}$$

Therefore the discretized Δ_{ij} should be

$$\begin{aligned}
\Delta_{ij} &= \frac{2}{\beta\omega_n^2}\sum_{n=-\infty}^{\infty}\Delta(i\omega_n)e^{-i\omega_n(i-j)\delta\tau}(1-\cos\omega_n\delta\tau),\quad i\neq j\\
&= -\frac{1}{\beta\omega_n^2}\sum_{n=-\infty}^{\infty}\Delta(i\omega_n)[e^{-i\omega_n\delta\tau}-(1-i\omega_n\delta\tau)+e^{i\omega_n\delta\tau}-(1+i\omega_n\delta\tau)]=\frac{2}{\beta\omega_n^2}\sum_{n=-\infty}^{\infty}\Delta(i\omega_n)[1-\cos\omega_n\delta\tau],\quad i=j
\end{aligned}\tag{5}$$