Rechnungen

stobbe.julian

October 2022

1 Matsubara/Imarignary time, FFTs

1.1 Definition FFTs

$$X_k = \mathcal{FFT}[X_n] = \sum_{n=0}^{N-1} X_n e^{-2\pi i k n/N} \tag{1}$$

$$X_n = i\mathcal{FFT}[X_k] = \frac{1}{N}\sum_{k=0}^{N-1} X_k e^{2\pi i k n/N} \tag{2}$$

1.2 τ to ω_n

Transformations of data from imaginary time to Matsubara frequencies. We start with a function over Matsubara frequencies $F(i\nu_n)$ and an associated high frequency tail $T(i\nu_n)$.

$$\begin{aligned}
F_\tau(\tau) &= \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\nu_n\tau} F(i\nu_n) \\
&= \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\nu_n\tau} \overbrace{(F(i\nu_n) - T(i\nu_n))}^{\widetilde{F}(i\nu_n)} + \overbrace{\frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\nu_n\tau} T(i\nu_n)}^{=T(\tau)} \\
&\approx \frac{1}{\beta}\sum_{n=N_{\min}}^{N_{\max}} e^{-i\nu_n\tau} \widetilde{F}(i\nu_n) + T(\tau)
\end{aligned}$$

From here we assume a equidistant τ spacing $\tau_k = \beta\frac{k}{N_\tau}$. Furthermore, we write $\widetilde{F}_n = \widetilde{F}(i\nu_n)$ to emphasis that $\widetilde{F}(i\nu_n)$ is also evaluated on a equidistant grid.

$$F_k = \frac{1}{\beta}\sum_{n=N_{\min}}^{N_{\max}} e^{-i\frac{(2n+1)\pi}{\beta}\frac{k}{N_\tau}\beta} \widetilde{F}_n + T(\tau)$$

$$
\begin{aligned}
&= \frac{1}{\beta} \sum_{n=0}^{(N_{\max}-N_{\min})-1} e^{-i\pi(2(n+N_{\min})+1)\frac{k}{N_\tau}} \widetilde{F}_n + T_k \\
&= \frac{1}{\beta} e^{-2\pi i (N_{\min}+1/2)\frac{k}{N_\tau}} \sum_{n=0}^{N_\nu -1} e^{-2\pi i \frac{n\cdot k}{N_\tau}} \widetilde{F}_n + T_k \\
&= \underbrace{\frac{1}{\beta} e^{-2\pi i (N_{\min}+1/2)\frac{k}{N_\tau}}}_{P_k^{n\to k}} \mathcal{FFT}_k \left[\widetilde{F}_n\right] + T_k \\
&= P_k^{n\to k} \cdot \mathcal{FFT}_k \left[\widetilde{F}_n\right] + T_k
\end{aligned} \tag{3}
$$

Where we defined $N_\nu = N_{\max} - N_{\min}$, $\mathcal{FFT}_k[\cdot]$ indicates the k=th component of the fast Fourier transformation and $P_k^{n\to k} = \frac{1}{\beta} e^{-2\pi i (N_{\min}+1/2)\frac{k}{N_\tau}}$ is the phase factor for the k-th index of the result (i.e., requires an element wise multiplication after a call to the fft routine).

1.2.1 Examples for T_n and T_k

calculation for some examples

T_n	T_k
1.0	$-\mathrm{sign}(\tau)\frac{1}{2}$

Table 1: Fourier transforms for some Matsubara tails

1.3 ω_n to τ

Here, we assume an evenly spaces τ-grid (i.e., Riemann sum integrals).

look into solutions with nfft

$$
\begin{aligned}
F(i\nu_n) &= \int_0^\beta e^{i\nu_n\tau} F(\tau)\, \mathrm{d}\tau && (4)\\
&= \int_0^\beta e^{i\nu_n\tau} \left(F(\tau) - T(\tau)\right) \mathrm{d}\tau + \int_0^\beta e^{i\nu_n\tau} T(\tau)\, \mathrm{d}\tau && (5)\\
&= \int_0^\beta e^{i\nu_n\tau} \left(\widetilde{F}(\tau)\right) \mathrm{d}\tau + T(i\nu_n) && (6)
\end{aligned}
$$

We now again change notation, to indicate evaluation of the functions on a grid, i.e. $\widetilde{F}_k = \widetilde{F}(\tau_k) = \widetilde{F}(\frac{k}{N_\tau}\beta)$. Note, that we assume equidistant τ_k spacing for this case.

$$
F_n \approx \sum_{k=0}^{N-1} \frac{\beta}{N_\tau} e^{i\nu_n \beta \frac{k}{N_\beta}} \widetilde{F}_k + T_n \tag{7}
$$

$$
= \sum_{k=0}^{N-1} \frac{\beta}{N_\tau} e^{i\frac{(2n+1)\pi}{\beta}\beta\frac{k}{N_\beta}} \widetilde{F}_k + T_n = \frac{1}{N_\tau} \sum_{k=0}^{N-1} e^{2\pi i n\frac{k}{N_\beta}} \underbrace{\beta e^{\pi i\frac{k}{N_\beta}} \widetilde{F}_k}_{P_k^{k\to n}\widetilde{F}_k} + T_n
$$

$$
F_n = i\mathcal{F}\mathcal{F}\mathcal{T}_n \left[P_k^{k\to n} \widetilde{F}_k \right] + T_n \tag{8}
$$

Here, we first multiply the τ input array F_k element wise by the k-dependent phase factor $P_k^{k\to n} = \beta e^{\pi i\frac{k}{N_\beta}} F_k$ (note, that the $1/N_\beta$ factor is absorbed into the definition of the inverse Fourier transformation), before submitting the result to the inverse fast Fourier transform routine.