虚時間グリーン関数に対するスパースモデリング入門(2)

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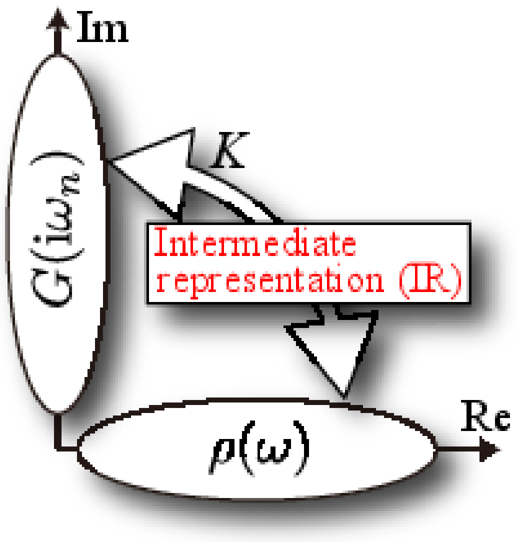


Part II: Exercise

前置き

- 共通の環境を使うため、Google Colabを使います。
- 簡単のためフェルミオンに限ります。
- Julia用のサンプルファイル

最初の目標

1. IR基底を構成してみる
2. 松原グリーン関数を計算してみよう

- 松原和を密なメッシュで計算してみる
- 松原和を素なメッシュで計算してみる

Exercise0: Compute IR basis

1. Open Notebook on Google Colab
2. Copy the notebook and run it!

Matsubara frequency summation

In many situations, one needs to evaluate

$$a = T \sum_n G(\mathrm{i}\omega_n),$$

where $G(\mathrm{i}\omega_n)$ is a Green's function object.

Fermi-Dirac distribution

$$\begin{cases} \rho(\omega) & = \delta(\omega - \omega_0), \\ G(\mathrm{i}\omega) & = \frac{1}{\mathrm{i}\omega - \omega_0}. \end{cases}$$

Electron occupation:

$$\begin{aligned} n \equiv \langle c^\dagger c \rangle &= -\langle T c(0^-) c^\dagger(0) \rangle \\ &= G(\tau = 0^-) = -\frac{1}{\beta} \sum_n e^{\mathrm{i}\omega_n 0^+} G(\mathrm{i}\omega_n) = \frac{1}{1 + e^{\beta\omega_0}}. \end{aligned}$$

Here, we used

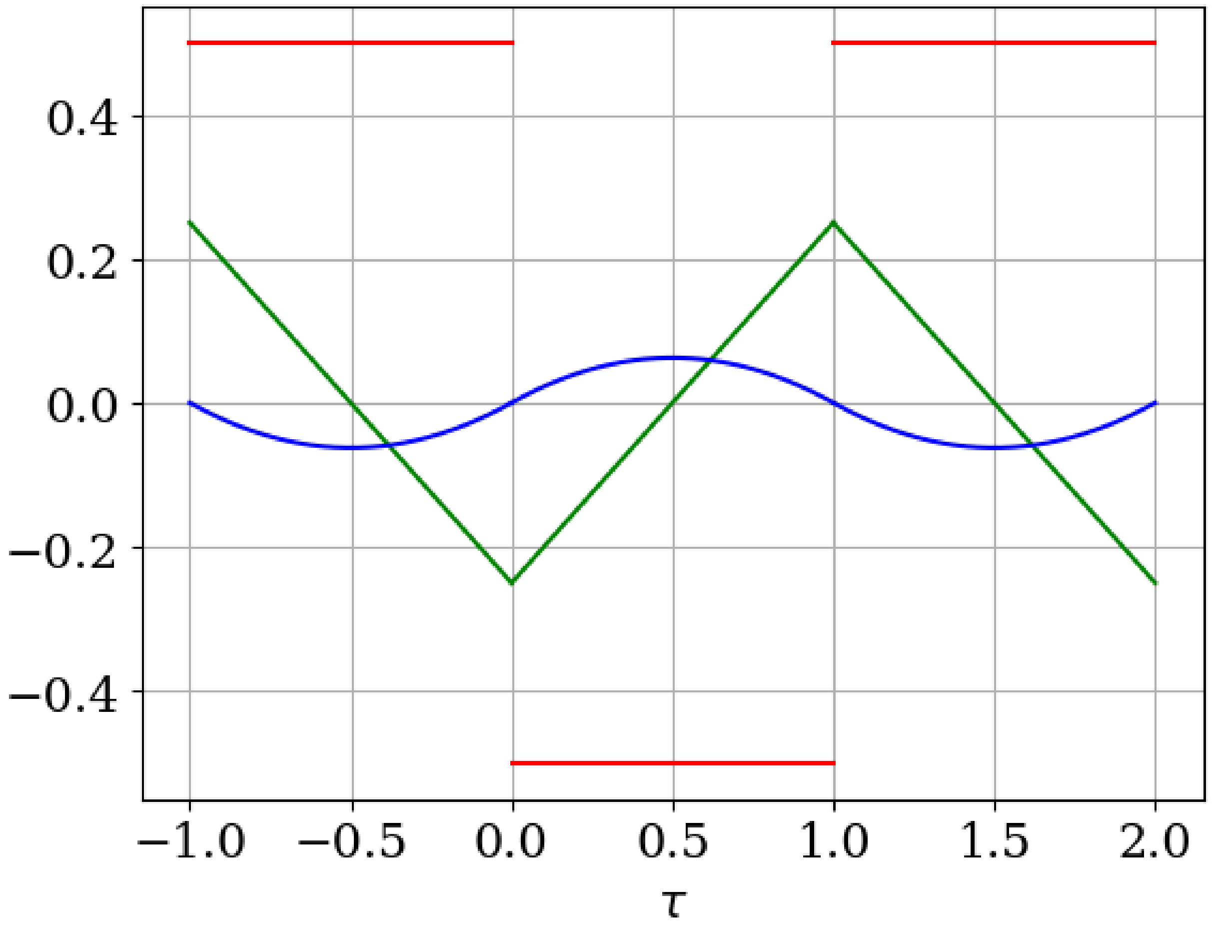
$$G(\tau) \equiv -\langle T_\tau c(\tau) c^\dagger(0) \rangle = -\frac{1}{\beta} \sum_n e^{-\mathrm{i}\omega\tau} G(\mathrm{i}\omega).$$

Note on treatment of discontinuity

Section B.3 of Emanuel Gull's Ph. D thesis:

$$\frac{1}{\mathrm{i}\omega} \leftrightarrow -\frac{1}{2}$$
$$\left(\frac{1}{\mathrm{i}\omega}\right)^2 \leftrightarrow \frac{1}{4}(-\beta + 2\tau)$$
$$\left(\frac{1}{\mathrm{i}\omega}\right)^3 \leftrightarrow \frac{1}{4}(\beta\tau - \tau^2)$$

for $0 < \tau < \beta$. The proof is straightforward for the $\leftarrow$ direction.



Conventional approach for Matsubara summation

$$\tilde{G}(\mathrm{i}\omega) \equiv G(\mathrm{i}\omega) - \frac{1}{\mathrm{i}\omega} \propto O((1/\mathrm{i}\omega)^2)$$

$\because \tilde{G}(\tau)$ is continuous at $\tau = 0$,

$$\begin{aligned} n &= G(\tau = 0^-) \\ &= \tilde{G}(\tau = 0) + G_\mathrm{tail}(\tau = 0^-) \\ &= \tilde{G}(\tau = 0) - G_\mathrm{tail}(\tau = \beta + 0^-) \\ &= \frac{1}{\beta} \sum_{n=-N}^{N-1} \tilde{G}(\mathrm{i}\omega_n) + \frac{1}{2}, \end{aligned}$$

where $G_\mathrm{tail}(\mathrm{i}\omega) = 1/\mathrm{i}\omega$. The truncation error in the first term converges only as $O(1/N)$ 😢.

Exercise1: Naive Matsubara summation

1. Open Notebook on Google Colab
2. Copy the notebook and run it!

Matsubara summation using sparse sampling

IR basis + sparse sampling

$$\begin{cases} G(\tau) & = \sum_l G_l U_l(\tau), \\ G(\mathrm{i}\omega) & = \sum_l G_l U_l(\mathrm{i}\omega), \end{cases}$$

$$n = G(\tau = 0^-) = -\sum_{l=0}^{\infty} U_l(\tau = \beta) G_l$$

The convergence n is exponential $\because$ exponential convergence of G_l.

We can determine G_l from $G(\mathrm{i}\bar{\omega}_k)$ on the sampling frequencies!

$$G(\mathrm{i}\bar{\omega}_k) \to G_l \to n$$

Exercise2: Matsubara summation by sparse sampling

1. Open Notebook on Google Colab
2. Copy the notebook and run it!

Check!

- How does the error in N decay as cutoff for singular values ϵ is decreased?
- (Advanced) More complicated spectral model (e.g., many poles)