

```
\newcommand{\iw}{\mathrm{i}\omega}
\newcommand{\wmax}{\omega_{\mathrm{max}}}
\newcommand{\dd}{\mathrm{d}}
\newcommand{\tauk}{\bar{\tau}_k}
\newcommand{\wk}{\bar{\omega}_k}
\newcommand{\vk}{\bar{\nu}_k}
\newcommand{\hatFmat}{\hat{\mathbf{F}}}
\newcommand{\Fmat}{\mathbf{F}}
```

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. 松原グリーン関数を計算してみよう
2. 松原和を密なメッシュで計算してみる
3. 松原和を素なメッシュで計算してみる

Matsubara frequency summation

In many situations, one needs to evaluate

$$a = T \sum_n G(\backslash \textcolor{red}{i}\mathbf{w}_n),$$

where $G(\backslash \textcolor{red}{i}\mathbf{w}_n)$ is a Green's function object.

Fermi-Dirac distribution

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

Electron occupation:

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

Here, we used

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

Note on treatment of discontinuity

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

$$\frac{1}{\sqrt{i\omega}} \leftrightarrow -\frac{1}{2} \quad (1)$$

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

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

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

Conventional approach for Matsubara summation

$$\tilde{G}(\backslash \textcolor{red}{i}\textcolor{red}{w}) \equiv G(\backslash \textcolor{red}{i}\textcolor{red}{w}) - \frac{1}{\backslash \textcolor{red}{i}\textcolor{red}{w}} \propto O((1/\backslash \textcolor{red}{i}\textcolor{red}{w})^2)$$

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

$$n = G(\tau = 0^-) \quad (1)$$

$$= \tilde{G}(\tau = 0) + G_{\text{tail}}(\tau = 0^-) \quad (1)$$

$$= \tilde{G}(\tau = 0) - G_{\text{tail}}(\tau = \beta + 0) \quad (1)$$

$$= \frac{1}{\beta} \sum_{n=-N}^{N-1} \tilde{G}(\backslash \textcolor{red}{i}\textcolor{red}{w}_n) + \frac{1}{2}, \quad (1)$$

where $G_{\text{tail}}(\backslash \textcolor{red}{i}\textcolor{red}{w}) = 1/\backslash \textcolor{red}{i}\textcolor{red}{w}$. 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

$$\begin{cases} G(\tau) &= \sum_l G_l U_l(\tau), \\ G(\backslash \mathbf{i} \mathbf{w}) &= \sum_l G_l U_l(\backslash \mathbf{i} \mathbf{w}), \end{cases}$$

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

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

We can determine G_l from $G(\backslash \mathbf{i} \mathbf{w} \mathbf{k})$ on the sampling frequencies!

$$G(\backslash \mathbf{i} \mathbf{w} \mathbf{k}) \rightarrow G_l \rightarrow n$$

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)