\newcommand{\ii}{{\mathrm{i}}}
\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)

品岡寛 (埼玉大学)

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Part II: Exercise

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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。

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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

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Matsubara frequency summation

In many situations, one needs to evaluate

$$a = T\sum_n G(\backslash\mathbf{iw}_n),$$

where $G(\backslash\mathbf{iw}_n)$ is a Green's function object.

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Fermi-Dirac distribution

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

Electron occupation:

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

Here, we used

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

Note on treatment of discontinuity

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

$$\frac{1}{\backslash\mathrm{iw}} \leftrightarrow -\frac{1}{2} \tag{1}$$

$$\left(\frac{1}{\backslash\mathrm{iw}}\right)^2 \leftrightarrow \frac{1}{4}(-\beta + 2\tau) \tag{1}$$

$$\left(\frac{1}{\backslash\mathrm{iw}}\right)^3 \leftrightarrow \frac{1}{4}(\beta\tau - \tau^2) \tag{1}$$

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

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Conventional approach for Matsubara summation

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

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

$$n = G(\tau = 0^-) \quad (1)$$
$$= \tilde{G}(\tau = 0) + G_{\mathrm{tail}}(\tau = 0^-) \quad (1)$$
$$= \tilde{G}(\tau = 0) - G_{\mathrm{tail}}(\tau = \beta + 0^-) \quad (1)$$
$$= \frac{1}{\beta} \sum_{n=-N}^{N-1} \tilde{G}(\backslash\mathrm{iw}_n) + \frac{1}{2}, \quad (1)$$

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

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Exercise1: Naive Matsubara summation

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

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Matsubara summation using sparse sampling

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IR basis + sparse sampling

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

$$n = G(\tau = 0^-) = -\sum_{l=0}^{\infty} U_l(\tau = \beta) G_l \quad (1)$$

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

We can determine G_l from $G(\backslash\mathrm{iwk})$ on the sampling frequencies!

$$G(\backslash\mathrm{iwk}) \to G_l \to n$$

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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)

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