\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(1)

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前提知識

- 虚時間形式グリーン関数の基礎
- Python or Juliaの基礎知識
  - 基本文法
  - 多次元配列
  - ...

何ができる？

虚時間・松原形式に基づく「数値」計算の高速・省メモリ化

超伝導転移温度の第一原理計算

T. Wang *et al.*, PRB 102, 134503 (2020), Nb

- メモリの使用量が40分の1に!
  [松原周波数 4096点$\longrightarrow$ 103点]
- 計算速度が20倍に!

他の応用例

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背後にある技術

- 虚時間グリーン関数のコンパクトな中間表現基底
    - $G(\tau) = \sum_{l=0}^{L-1} U_l(\tau) g_l + \epsilon$
    - $L \propto \log \beta W$ (β: inverse temperature, W: band width)
    - $\epsilon \propto \exp(-aL)$ (ϵ: truncation error, $a > 0$)
- 虚時間・虚周波数におけるスパースメッシュ: # of points $\simeq L$.
- SparseIR.jl (Julia), sparse-ir (Python)

参考資料

- 固体物理 2021年6月 温度グリーン関数の情報圧縮に基づく高速量子多体計算法
- ↑の英語訳・加筆 + 新ライブラリsparse-irに更新
  H. Shinaoka *et al.*, SciPost Phys. Lect. Notes 63 (2022)
- sparse-ir tutorials (大量のサンプルコード)
  https://spm-lab.github.io/sparse-ir-tutorial/index.html

概要

- Part I
  1. 虚時間グリーン関数の性質のまとめ
  2. 中間表現基底
  3. スパースサンプリング法

Imaginary-time Green's functions

Also known as Matsubara Green's functions:

$$G(\tau) = -\langle T_\tau A(\tau) B(0) \rangle,$$

where

- $A(\tau)$, $B(\tau)$ are operators in the Heisenberg picture ($A(\tau) = e^{\tau H} A e^{-\tau H}$).
- $\langle \cdots \rangle = \mathrm{Tr}(e^{-\beta H} \cdots)$, where $\beta = 1/T$ ($k_\mathrm{B} = 1$).

We use the Hamiltonian formalism throughout this lecture.

Imaginary-time Green's functions

$$G(\tau) = -\langle T_\tau A(\tau) B(0) \rangle$$

- A and B are fermionic operators $\rightarrow G(\tau) = -G(\tau + \beta)$
- A and B are bosonic operators $\rightarrow G(\tau) = G(\tau + \beta)$

In general, $G(\tau)$ has a discontinuity at $\tau = n\beta$ ($n \in \mathbb{N}$).

Imaginary-frequency (Matsubara) Green's functions

Matsubara Green's function:

$$G(\mathrm{i}\omega) = \int_0^\beta \mathrm{d}\tau e^{\mathrm{i}\omega\tau} G(\tau).$$

From $G(\tau + \beta) = \mp G(\tau)$,

- $\omega = (2n + 1)T\pi$ (fermion)
- $\omega = 2nT\pi$ (boson)

($n \in \mathbb{N}$)

These discrete imaginary frequencies are denoted as Matsubara frequencies.

Spectral/Lehmann representation

$$G(z) = \int_{-\infty}^{+\infty} \mathrm{d}\omega' \, \frac{\rho(\omega')}{z - \omega'},$$

where $\rho(\omega)$ is a spectral function.

- $z = \mathrm{i}\omega \to$ Matsubara Green's function
- $z = \omega + \mathrm{i}0^{+} \to$ Retarded Green's function (not used in this lecture)

How Greeen's function look like in τ?

Example (single pole): $\rho(\omega) = \delta(\omega - \omega_0)$, $\omega_0 > 0$

$$G(\mathrm{i}\omega) = \frac{1}{\mathrm{i}\omega - \omega_0}$$

$$G(\tau) = -\frac{e^{-\tau\omega_0}}{1 + e^{-\beta\omega_0}}\ (0 < \tau < \beta)$$

At $\tau \approx 0$, $G(\tau) \propto e^{-\tau\omega_0}$.

For $\beta\omega_0 \gg 1$, coexisting two time scales : $1/\omega_0 \ll \beta$

How Greeen's function look like in Matsubara frequency space

Example (single pole): $\rho(\omega) = \delta(\omega - \omega_0)$, $\omega_0 > 0$

$$G(\mathrm{i}\omega) = \frac{1}{\mathrm{i}\omega - \omega_0}$$

$$G(\tau) = -\frac{e^{-\tau\omega_0}}{1 + e^{-\beta\omega_0}} \; (0 < \tau < \beta)$$

At high frequencies $|\omega| \gg |\omega_0|$, $G(\mathrm{i}\omega) \approx 1/(\mathrm{i}\omega)$.

For $\beta\omega_0 \gg 1$, coexisting two energy scales: $\omega_0 \ll T = 1/\beta$

Difficulties in numerical simulations

If band width W and temperature T differ by orders of magnitudes as $\beta W \gg 1$:

- Slow power-law decay at high frequencies $\to$ Large truncation errors
- Uniform dense mesh in τ requires a huge number of points $\propto \beta W$.

Example:

- Band width 10 eV, superconducting temperature 1 K ≈ 0.1 meV $\to \beta W = 10^5$.

We need a compact basis with exponetial convergence.

Compact representations

- **Intermediate represenation** (sparse-ir)
  - *Ab initio* calculations (Eliashberg theory, *GW*, Lichtenstein formula)
  - Diagrammatic calculations (FLEX)
- Discrete Lehmann representation (implemented in sparse-ir as well)
- Minmax method (from Kresse's group)

Mathematical background: singular value decomposition (SVD)

Any complex-valued matrix A of size $M \times N$ can be decomposed as

$$A = U\Sigma V^\dagger,$$

where

$$U = (u_1, u_2, \cdots, u_L) : M \times L,$$

$$V = (v_1, v_2, \cdots, v_L) : N \times L,$$

where $u_i^\dagger u_j = \delta_{ij}, v_i^\dagger v_j = \delta_{ij}, L = \min(M, N)$. Σ is a diagonal matrix with non-negative diagonal elements $s_1 \geq s_2 \geq \cdots \geq s_L \geq 0$.

- Unique up to a phase if the singular values s_i are non-degenerate.
- If A is a real matrix, U and V are also real orthogonal matrices.

Intermediate representation

Shinaoka *et al.* Phys. Rev. B 96, 035147 (2017)

Analytic continuation kernel

Fermion & boson:

$$G(\backslash\mathrm{iv}) = \int_{-\infty}^{\infty} \backslash\mathrm{dd}\omega \underbrace{\frac{1}{\backslash\mathrm{iv} - \omega}}_{\equiv K(\backslash\mathrm{iv},\omega)} A(\omega) \quad (1)$$

$K(\backslash\mathrm{iv}, \omega)$ is system independent and $A(\omega) = -\backslash\mathrm{ii}(G^R(\omega) - G^A(\omega))$.

Analytic continuation kernel

$$G(\tau) = -\int_{-\infty}^{\infty} \dd\omega K(\tau, \omega) A(\omega), \tag{1}$$

$$K(\tau, \omega) \equiv -\frac{1}{\beta} \sum_{\iv} e^{-\iv\tau} K(\iv, \omega) = \begin{cases} \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}} & (\mathrm{fermion}) \\ \frac{e^{-\tau\omega}}{1-e^{-\beta\omega}} & (\mathrm{boson}) \end{cases}, \tag{1}$$

where $0 < \tau < \beta$.

For bosons, $|K(\tau, \omega)| \rightarrow +\infty$ at $\omega \rightarrow 0$. We want to use the same kernel for fermion & boson. How?

Logistic kernel

$$G(\tau) = -\int_{-\infty}^{\infty} \textcolor{red}{\backslash\mathrm{dd}}\omega K^{\mathrm{L}}(\tau,\omega)\rho(\omega), \quad (1)$$

where $K^{\mathrm{L}}(\tau,\omega)$ is the "logistic kernel" defined as

$$K^{\mathrm{L}}(\tau,\omega) = \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}},$$

and $\rho(\omega)$ is the modified spectral function

$$\rho(\omega) \equiv \begin{cases} A(\omega) & (\mathrm{fermion}), \\ \frac{A(\omega)}{\tanh(\beta\omega/2)} & (\mathrm{boson}). \end{cases} \quad (1)$$

This trick has been widely used in the lattice QCD community for a long time. This was introduced into condensed matter physics in J. Kaye *et al.* (2022).

Singular value expansion

We introduce an ultraviolet $0 < \wmax < \infty$ and a dimensionless parameter $\Lambda \equiv \wmax\beta$

Because $K^\mathrm{L} \in C^\infty$ and $\in L^2$:

$$K^\mathrm{L}(\tau, \omega) = \sum_{l=0}^{\infty} U_l(\tau) S_l V_l(\omega),$$

for $-\wmax \leq \omega \leq \wmax$ and $0 \leq \tau \leq \beta$.

Singular functions: $\int_{-\wmax}^{\wmax} \dd\omega V_l(\omega) V_{l'}(\omega) = \delta_{ll'}$ and $\int_0^\beta \dd\tau U_l(\tau) U_{l'}(\tau) = \delta_{ll'}$.

$\rightarrow$ **Indermediate-represetation** basis functions

Singular values: $\omega_{\mathrm{max}} = 1$

- Exponential decay
- Number of relevant S_l grows as $O(\log \Lambda)$ (only numerical evidence)

Basis functions: $\omega_{\mathrm{max}} = 1$ and $\beta = 100$

- Even/odd functions for even/odd l
- l roots
- Converge to Legendre polynomials at $\Lambda \to 0$

Basis functions in Matsubara frequency

$$U_l(\backslash\mathrm{iv}) \equiv \int_0^\beta \backslash\mathrm{dd}\tau e^{\backslash\mathrm{iv}\tau} U_l(\tau).$$

Fourier transform can be done numerically.

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Expansion in IR

$$G(\tau) = \sum_{l=0}^{L-1} G_l U_l(\tau) + \epsilon_L,$$

$$\hat{G}(\mathrm{i}\nu) = \sum_{l=0}^{L-1} G_l \hat{U}_l(\mathrm{i}\nu) + \hat{\epsilon}_L,$$

where $\epsilon_L,\ \hat{\epsilon}_L \approx S_L$. The expansion coefficients G_l can be determined from the spectral function as

$$G_l = -S_l \rho_l,$$

where

$$\rho_l = \int_{-\omega_\mathrm{max}}^{\omega_\mathrm{max}} \mathrm{d}\omega \rho(\omega) V_l(\omega).$$

Convergence

$|G_l|$ converges as fast as S_l.

Example:

$\rho(\omega) = \frac{1}{2}(\delta(\omega - 1) + \delta(\omega + 1))$

$$
\begin{aligned}
\rho_l &= \int_{-\omega_\mathrm{max}}^{\omega_\mathrm{max}} \mathrm{d}\omega \rho(\omega) V_l(\omega) \\
&= \frac{1}{2}(V_l(1) + V_l(-1)).
\end{aligned}
$$

$\beta = 100$, \wmax $= 1$.

Sparse sampling

Li, Wallerberger, Chikano, Yeh, Gull, and Shinaoka, Phys. Rev. B 101, 035144 (2000)

Sparse time and frequency meshes

Solving Dyson equation for given $\Sigma(\backslash\mathrm{iw})$:

$$G(\backslash\mathrm{iw}) = (G_0^{-1}(\backslash\mathrm{iw}) + \Sigma(\backslash\mathrm{iw}))^{-1} \tag{1}$$

$$G_l = \sum_{n=-\infty}^{+\infty} U_l^*(\backslash\mathrm{iw}_n) G(\backslash\mathrm{iw}_n) \tag{1}$$

Q. Need to compute $G(\backslash\mathrm{iw})$ on ALL Mastubara frequencies to determine L IR coefficients G_l?

A. No, we need to know $G(\backslash\mathrm{iw})$ on *appropriately chosen* $(\approx L)$ sampling frequencies.

Dense mesh in τ?

Second-order self-energy (Hubbard U):

$$\Sigma(\tau) \propto UG^2(\tau)G(\beta - \tau)$$

$$G_l = \int_0^\beta d\tau U_l(\tau) G(\tau) \tag{1}$$

Q: Need to compute $G(\tau)$ on a dense mesh of τ?

A: No, we need to know $G(\tau)$ on *appropriately chosen* $(\approx L)$ sampling points?

Sampling points

Simple rule: extrema (or somewhere in between two adjacent roots) of U_L

$\beta = 10$, \wmax $= 10$, $L = 30$:

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Sampling points

Simple rule: extrema (or somewhere in between two adjacent roots) of U_L

$\beta = 10, \textbackslash\mathrm{wmax} = 10, L = 30$:

center

Transform from time/frequency to IR

- Well conditioned fitting problem
- Implemented in sparse-ir as stable linear transform

$$
\begin{aligned}
G_l &= \underset{G_l}{\mathrm{argmin}} \sum_k \left| G(\backslash\mathrm{tauk}) - \sum_{l=0}^{N_{\mathrm{smpl}}-1} U_l(\backslash\mathrm{tauk}) G_l \right|^2 \\
&= (\backslash\mathrm{Fmat}^+ \boldsymbol{G})_l,
\end{aligned} \tag{1}
$$

where we define $(\backslash\mathrm{Fmat})_{kl} = U_l(\backslash\mathrm{tauk})$ and $\backslash\mathrm{Fmat}^+$ is its pseudo inverse.

Condition number

- Small condition number of $\color{red}{\backslash\mathrm{Fmat}}$
- If condition number is 10^p, you may loos p digits in transformation (three out of 16 digits)

Numerical demonstration

Two-pole model: $\beta = 100$, \wmax $= 1$: Almost 16 significant digits!

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Stable and efficient numerical transform

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QA sessions

How to implement diagrammatic equations

Second-order perturbation theory

- Solving Dyson equation in frequency space
- Evaluating the self-energy in frequency space

Implementation of second-order perturbation theory

Online tutorial

Hubbard model on a square lattice:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}),$$

where $t = 1$ and $\mu = U/2$ (half filling). $c^\dagger_{i\sigma}$ $(c_{i\sigma})$ a creation (annihilation) operator for an electron with spin σ at site i.

Non-interacting band dispersion:

$$\epsilon(\boldsymbol{k}) = -2(\cos k_x + \cos k_y),$$

where $\boldsymbol{k} = (k_x, k_y)$.

Self-consistent equations

$$
\begin{aligned}
G(\mathrm{i}\nu, \boldsymbol{k}) &= \frac{1}{\mathrm{i}\nu - \epsilon(\boldsymbol{k}) + \mu - \Sigma(\textcolor{red}{\backslash\mathrm{iv}}, \boldsymbol{k})} && (1)\\
&\downarrow && (1)\\
&\downarrow (\textcolor{red}{\backslash\mathrm{iv} \rightarrow \tau}, \boldsymbol{k} \rightarrow \boldsymbol{r}) && (1)\\
&\downarrow && (1)\\
\Sigma(\tau, \boldsymbol{r}) &= U^2 G^2(\tau, \boldsymbol{r}) G(\beta - \tau, \boldsymbol{r}) && (1)\\
&\downarrow && (1)\\
&\downarrow (\textcolor{red}{\tau \rightarrow \backslash\mathrm{iv}}, \boldsymbol{r} \rightarrow \boldsymbol{k}) && (1)\\
&\downarrow && (1)\\
&\text{Go back to } (1) && (1)
\end{aligned}
$$

Self-consistent equations (sparse sampling)

$$
\begin{aligned}
G(\ivk, \boldsymbol{k}) &= \frac{1}{\ivk - \epsilon(\boldsymbol{k}) + \mu - \Sigma(\ivk, \boldsymbol{k})} && (1)\\
&\downarrow && (1)\\
&\downarrow (\ivk \rightarrow \mathrm{IR} \rightarrow \tauk,\ \boldsymbol{k} \rightarrow \boldsymbol{r}) && (1)\\
&\downarrow && (1)\\
\Sigma(\tauk, \boldsymbol{r}) &= U^2 G^2(\tauk, \boldsymbol{r}) G(\beta - \tauk, \boldsymbol{r}) && (1)\\
&\downarrow && (1)\\
&\downarrow (\tauk \rightarrow \mathrm{IR} \rightarrow \ivk, \boldsymbol{r} \rightarrow \boldsymbol{k}) && (1)\\
&\downarrow && (1)\\
&\text{Go back to } (1) && (1)
\end{aligned}
$$

The whole calculaiton can be performed on sparse meshes.

Reconstruction of spectral function

Please read our article in the sparse-ir tutorial!

Q: Can you reconstruct a spectral function from numerical data of $G(\tau)$?

A: Very difficult

$$G(\tau) = G_{\mathrm{exact}}(\tau) + \delta(\tau),$$

where $\delta(\tau)$ is noise.

$$\rho_l = -(S_l)^{-1}((G_l)_{\mathrm{exact}} + \delta_l),$$

where $(G_l)_{\mathrm{exact}} = \int_0^\beta \textbackslash\mathrm{dd}\tau U_l(\tau) G_{\mathrm{exact}}(\tau)$ and $\delta_l = \int_0^\beta \textbackslash\mathrm{dd}\tau U_l(\tau)\delta(\tau)$.

Reconstruction of spectral function

Q: Can you reconstruct a spectral function from numerical data of $G(\tau)$?

A: Very numerical unstable!

$$G(\tau) = G_{\mathrm{exact}}(\tau) + \delta(\tau),$$

where $\delta(\tau)$ is noise.

$$\rho_l = -(S_l)^{-1}((G_l)_{\mathrm{exact}} + \delta_l),$$

where $(G_l)_{\mathrm{exact}} = \int_0^\beta \textcolor{red}{\backslash\mathrm{dd}}\tau U_l(\tau) G_{\mathrm{exact}}(\tau)$ and $\delta_l = \int_0^\beta \textcolor{red}{\backslash\mathrm{dd}}\tau U_l(\tau)\delta(\tau)$.

Noise is amplified by small singular values. $\rightarrow$ ill-posed inverse problem. Needed a regularized solver: MaxEnt, SpM, Nevanlinna *etc*.

"Nevanlinna.jl: A Julia implementation of Nevanlinna analytic continuation", K. Nogaki, J. Fei, E. Gull, HS, arXiv:2302.10476v1