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\newcommand{\iw}{\mathrm{i}\omega}
```

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\newcommand{\wmax}{\omega_{\mathrm{max}}}
```

```
\newcommand{\dd}{\mathrm{d}}
```

```
\newcommand{\tauk}{\bar{\tau}_k}
```

```
\newcommand{\wk}{\bar{\omega}_k}
```

```
\newcommand{\vk}{\bar{\nu}_k}
```

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\newcommand{\hatFmat}{\hat{\mathbf{F}}}
```

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\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)

品岡寛 (埼玉大学)



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

虚時間計算と関係にある超伝導転移温度の第一原理計算

T. Wang *et al.*, PRB 102, 134503 (2020), Nb: $T_C = O(10)$ K

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

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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
 - i. 虚時間グリーン関数の性質のまとめ
 - ii. 中間表現基底
 - iii. スパースサンプリング法
- Part II
 - i. 開発環境のセットアップ

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 ($A(\tau) = e^{\tau H} A e^{-\tau H}$).
- $\langle \dots \rangle = \text{Tr}(e^{-\beta H} \dots)$, where $\beta = 1/T$ ($k_B = 1$).

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:

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

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

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

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

- $z = i\omega \rightarrow$ Matsubara Green's function
- $z = \omega + i0^+ \rightarrow$ Retarded Green's function (not used in this lecture)

How Green's function look like in τ ?

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

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

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

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 Green's function look like in Matsubara frequency space

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

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

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

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

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 \rightarrow 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 $\rightarrow \beta W = 10^5$.

We need a compact basis with exponential convergence.

Compact representations

- **Intermediate representation** (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

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

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

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 $s_1 \geq s_2 \geq \dots \geq s_L \geq 0$.

- 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:

$$G(\backslash \mathbf{i} \mathbf{v}) = \int_{-\infty}^{\infty} \backslash \mathbf{d} \mathbf{d} \omega \underbrace{\frac{1}{\backslash \mathbf{i} \mathbf{v} - \omega}}_{\equiv K(\backslash \mathbf{i} \mathbf{v}, \omega)} A(\omega)$$

$K(\backslash \mathbf{i} \mathbf{v}, \omega)$ is system independent and $A(\omega) = -\backslash \mathbf{i} \mathbf{i} (G^R(\omega) - G^A(\omega))$.

Analytic continuation kernel

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

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

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

$$G(\tau) = - \int_{-\infty}^{\infty} d\omega K^{\text{L}}(\tau, \omega) \rho(\omega)$$

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

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

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

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

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 $0 < \Lambda < \infty$ and a dimensionless parameter $\Lambda \equiv \Lambda \beta$

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

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

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

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

→ Intermediate representation basis functions

Singular values

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

Basis functions

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

Basis functions in Matsubara frequency

$$U_l(\mathbf{iv}) \equiv \int_0^\beta d\tau e^{i\mathbf{v}\tau} U_l(\tau).$$

Fourier transform can be done numerically.

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Expansion in IR

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

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

where ϵ_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

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

Convergence

If $|\rho_l|$ is bounded from above, $|G_l|$ converges as fast as S_l (system independent).

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

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

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Reconstruction of spectral function

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

A: Very difficult

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

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

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

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

Side story: Reconstructing spectral function

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

A: Very numerical unstable!

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

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

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

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

Noise is amplified by small singular values. → Reconstruction of spectral function is an ill-posed inverse problem. We need to use a regularized solver: MaxEnt, SpM, etc..

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 $\Sigma(\backslash \mathbf{i} \mathbf{w})$:

$$G(\backslash \mathbf{i} \mathbf{w}) = (G_0^{-1}(\backslash \mathbf{i} \mathbf{w}) + \Sigma(\backslash \mathbf{i} \mathbf{w}))^{-1}$$

We do not want to solve the equation on a huge dense mesh 😓

Solve the equation on a sparse mesh of size L and transform the result to IR of size L



Heuristic choice of sampling points

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

$\beta = 10$, $\backslash \text{wmax} = 10$, $L = 30$:

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Heuristic choice of sampling points

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

$\beta = 10$, $\backslash \text{wmax} = 10$, $L = 30$:

center

Transform from time/frequency to IR

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

$$\begin{aligned} G_l &= \operatorname{argmin}_{G_l} \sum_k \left| G(\backslash \mathbf{tauk}) - \sum_{l=0}^{N_{\text{smp}}-1} U_l(\backslash \mathbf{tauk}) G_l \right|^2 \\ &= (\backslash \mathbf{Fmat}^+ \mathbf{G})_l, \end{aligned} \tag{1}$$

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

Condition number

- Numerical stability determined by the condition number of $\backslash \mathbf{Fmat}$
- Lose *only* a few digits out of ≈ 16 significant digits of 64bit float

Numerical demonstration

Two-pole model: $\beta = 100$, $\backslash \mathbf{w}_{\max} = 1$: Almost 16 significant digits!

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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:

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

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

Non-interacting band dispersion:

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

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

Self-consistent equations

$$G(i\nu, \mathbf{k}) = \frac{1}{i\nu - \epsilon(\mathbf{k}) + \mu - \Sigma(\backslash \mathbf{i}\mathbf{v}, \mathbf{k})} \quad (1)$$

$$\downarrow \quad (1)$$

$$\downarrow (\backslash \mathbf{i}\mathbf{v} \rightarrow \tau, \mathbf{k} \rightarrow \mathbf{r}) \quad (1)$$

$$\downarrow \quad (1)$$

$$\Sigma(\tau, \mathbf{r}) = U^2 G^2(\tau, \mathbf{r}) G(\beta - \tau, \mathbf{r}) \quad (1)$$

$$\downarrow \quad (1)$$

$$\downarrow (\tau \rightarrow \backslash \mathbf{i}\mathbf{v}, \mathbf{r} \rightarrow \mathbf{k}) \quad (1)$$

$$\downarrow \quad (1)$$

$$\text{Go back to (1)} \quad (1)$$

Self-consistent equations (sparse sampling)

$$G(\backslash \textcolor{red}{i} \mathbf{v} \mathbf{k}, \mathbf{k}) = \frac{1}{\backslash \textcolor{red}{i} \mathbf{v} \mathbf{k} - \epsilon(\mathbf{k}) + \mu - \Sigma(\backslash \textcolor{red}{i} \mathbf{v} \mathbf{k}, \mathbf{k})} \quad (1)$$

$$\downarrow \quad (1)$$

$$\downarrow (\backslash \textcolor{red}{i} \mathbf{v} \mathbf{k} \rightarrow \textcolor{red}{I} \mathbf{R} \rightarrow \backslash \textcolor{red}{t} \mathbf{a} \mathbf{u} \mathbf{k}, \mathbf{k} \rightarrow \mathbf{r}) \quad (1)$$

$$\downarrow \quad (1)$$

$$\Sigma(\backslash \textcolor{red}{t} \mathbf{a} \mathbf{u} \mathbf{k}, \mathbf{r}) = U^2 G^2(\backslash \textcolor{red}{t} \mathbf{a} \mathbf{u} \mathbf{k}, \mathbf{r}) G(\beta - \backslash \textcolor{red}{t} \mathbf{a} \mathbf{u} \mathbf{k}, \mathbf{r}) \quad (1)$$

$$\downarrow \quad (1)$$

$$\downarrow (\backslash \textcolor{red}{t} \mathbf{a} \mathbf{u} \mathbf{k} \rightarrow \textcolor{red}{I} \mathbf{R} \rightarrow \backslash \textcolor{red}{i} \mathbf{v} \mathbf{k}, \mathbf{r} \rightarrow \mathbf{k}) \quad (1)$$

$$\downarrow \quad (1)$$

$$\text{Go back to (1)} \quad (1)$$

The whole calculaiton can be performed on sparse meshes.