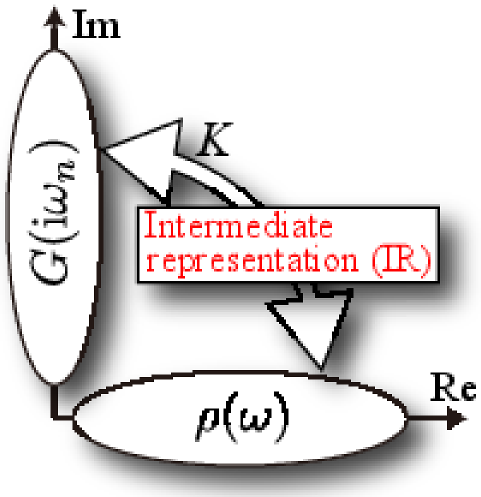
虚時間グリーン関数に対するスパースモデリング入門(1)

品岡寛 (埼玉大学)



自己紹介 https://shinaoka.github.io

- 経歴
  - 博士 (工学) 2009年3月@東大物工
  - ポスドク 2009年3月～2015年9月 (東大、産総研、チューリッヒ連邦工科大)
  - 研究室主催@埼玉大 2015年10月～
- 専門
  - 量子多体理論、第一原理計算、幾何学的フラストレート磁性･･･
  - 計算物理バックエンドの開発に興味
    ALPS量子モンテカルロコード、スパースモデリング･･･
- 海外との連携
  ウィーン工科大学、ミシガン大、フリブール大、ミュンヘン大、King's College London･･･

宣伝

- 学術変革領域B「量子古典融合アルゴリズムが拓く計算物質科学」(代表: 品岡)
  - 2023〜2025年度
  - 計画研究班代表: 品岡、大久保、水上
  - スパースモデリング、テンソルネットワーク、動的平均場理論、密度汎関数理論、変分波動関数理論、量子情報・・・
- JST創発「2粒子レベルの量子埋め込み理論に基づく新規第一原理計算手法の開発と実証」2024年度から基本7年
  - RA (博士課程学生支援あり)

近日、ポスドク、博士後期課程学生の公募が出る予定！→詳しくはポスターで

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
    - ...

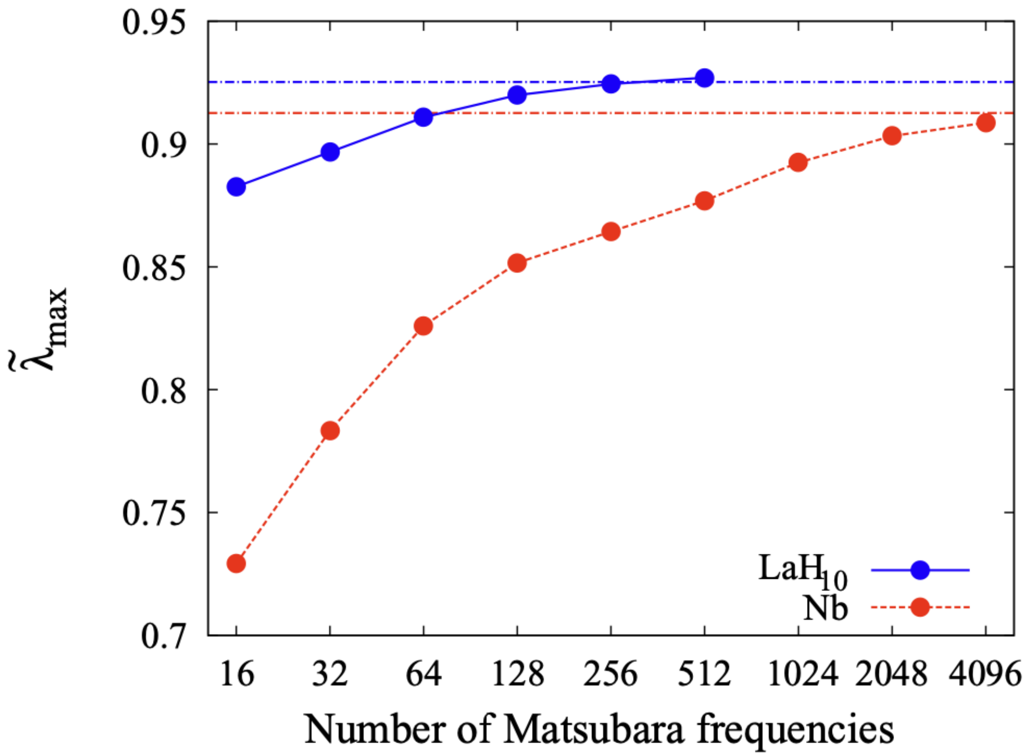
何ができる？

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→ 103点]
- 計算速度が20倍に!



他の応用例

PHYSICAL REVIEW LETTERS **125**, 117204 (2020)

Formation Mechanism of the Helical Q Structure in Gd-Based Skyrmion Materials

Takuya Nomoto,[1,*] Takashi Koretsune,[2] and Ryotaro Arita[1,3]
[1]Department of Applied Physics, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo, 113-8656, Japan
[2]Department of Physics, Tohoku University, Miyagi 980-8578, Japan
[3]RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan

磁性体

Efficient *ab initio* Migdal-Eliashberg calculation considering the retardation effect in phonon-mediated superconductors

Tianchun Wang,[1,*] Takuya Nomoto,[1] Yusuke Nomura,[2] Hiroshi Shinaoka,[3] Junya Otsuki,[4] Takashi Koretsune,[5] and Ryotaro Arita[1,2]
[1]Department of Applied Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
[2]RIKEN Center for Emergent Matter Science, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan
[3]Department of Physics, Saitama University, Sakura, Saitama 338-8570, Japan
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超伝導体

High Energy Physics – Lattice

[Submitted on 26 Oct 2021 (v1), last revised 30 Oct 2021 (this version, v2)]

QCD viscosity by combining the gradient flow and sparse modeling methods

Etsuko Itou, Yuki Nagai

高エネルギー物理

PHYSICAL REVIEW B **103**, 205148 (2021)

Efficient fluctuation-exchange approach to low-temperature spin fluctuations and superconductivity: From the Hubbard model to $Na_xCoO_2 \cdot yH_2O$

Niklas Witt,[1,2,*] Erik G. C. P. van Loon,[1,2] Takuya Nomoto,[3] Ryotaro Arita,[3,4] and Tim O. Wehling[1,2]
[1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany
[2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany
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(Received 9 December 2020; revised 23 March 2021; accepted 30 April 2021; published 26 May 2021)

PHYSICAL REVIEW RESEARCH **2**, 043144 (2020)

Magnetic exchange coupling in cuprate-analog d^9 nickelates

Yusuke Nomura,[1,*] Takuya Nomoto,[2] Motoaki Hirayama,[1] and Ryotaro Arita[1,2]
[1]RIKEN Center for Emergent Matter Science, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan
[2]Department of Applied Physics, University of Tokyo,7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656

PHYSICAL REVIEW B **102**, 085105 (2020)

***Ab initio* self-energy embedding for the photoemission spectra of NiO and MnO**

Sergei Iskakov,[1] Chia-Nan Yeh,[1] Emanuel Gull,[1] and Dominika Zgid[2,1]
[1]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA
[2]Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, USA

PHYSICAL REVIEW B **106**, 085121 (2022)

Relativistic self-consistent *GW*: Exact two-component formalism with one-electron approximation for solids

Chia-Nan Yeh,[1] Avijit Shee,[2] Qiming Sun,[3] Emanuel Gull,[1] and Dominika Zgid[1,2]
[1]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA
[2]Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109, USA
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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
  IR基底の基礎、フーリエ変換、２次摂動、FLEX、DMFTなどなど
  Python, Julia (Jupyter notebook) + Fortran

虚時間以外を圧縮したい！: Quantics tensor trains

- 一般の時空依存性 (実時間、波数依存性など)の圧縮
- 指数的に異なるエネルギー・長さスケール間の低エンタングルメント構造を仮定
- Julia実装 (ITensors.jlベース)

Multi-scale space-time ansatz for correlation functions of quantum systems based on quantics representations

Hiroshi Shinaoka,[1,2] Markus Wallerberger,[3] Yuta Murakami,[4]
Kosuke Nogaki,[5] Rihito Sakurai,[1] Philipp Werner,[6] and Anna Kauch[3]

[1] *Department of Physics, Saitama University, Saitama 338-8570, Japan*
[2] *JST, PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan*
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[5] *Department of Physics, Kyoto University, Kyoto 606-8502, Japan*
[6] *Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland*

arXiv:2210.12984 (to appear in PRX)

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.

- $z = \mathrm{i}\omega \rightarrow$ Matsubara Green's function
- $z = \omega + \mathrm{i}0^+ \rightarrow$ 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 $\rightarrow$ 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 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:

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

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

Analytic continuation kernel

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

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

where $0 < \tau < \beta$.

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

Logistic kernel

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

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

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

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 $0 < \omega_{\mathrm{max}} < \infty$ and a dimensionless parameter $\Lambda \equiv \omega_{\mathrm{max}}\beta$

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

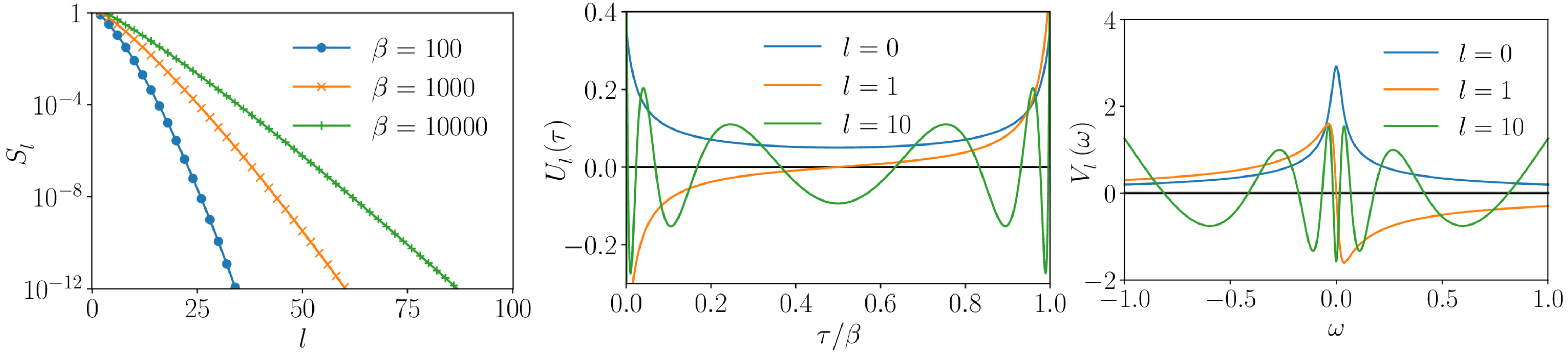
$$K^{\mathrm{L}}(\tau, \omega) = \sum_{l=0}^{\infty} U_l(\tau) S_l V_l(\omega),$$

for $-\omega_{\mathrm{max}} \leq \omega \leq \omega_{\mathrm{max}}$ and $0 \leq \tau \leq \beta$.

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

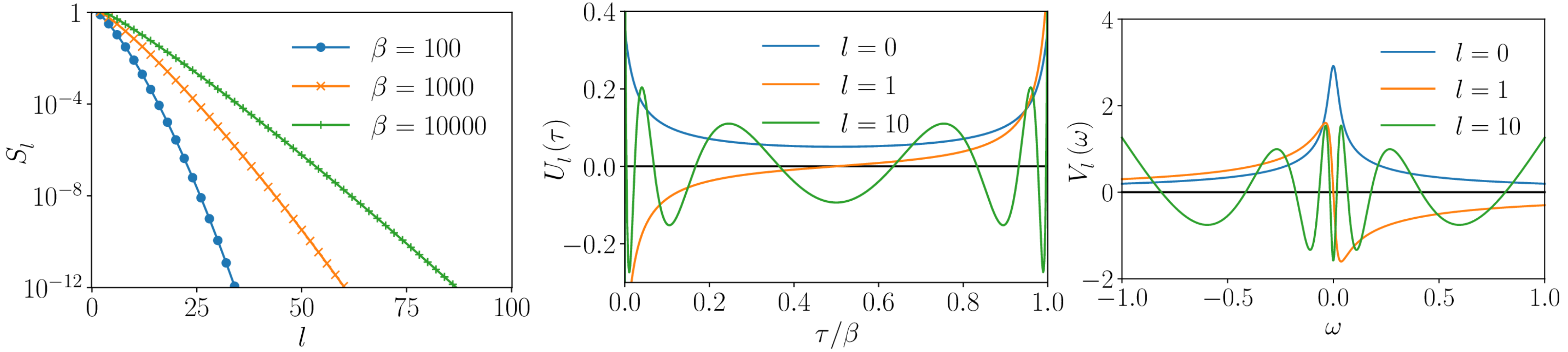
$\rightarrow$ **Indermediate-represetation** basis functions

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



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

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

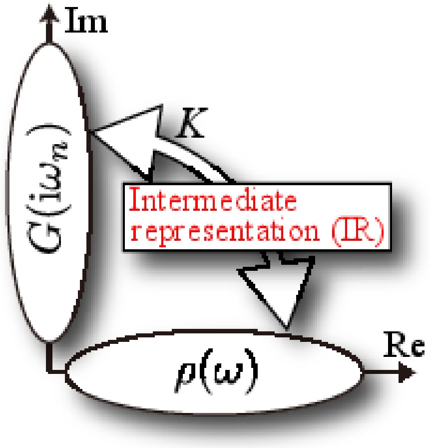


- Even/odd functions for even/odd l
- l roots
- Converge to Legendre polynomials at $\Lambda \to 0$

Basis functions in Matsubara frequency

$$U_l(\mathrm{i}\nu) \equiv \int_0^\beta \mathrm{d}\tau e^{\mathrm{i}\nu\tau} U_l(\tau).$$

Fourier transform can be done numerically.



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

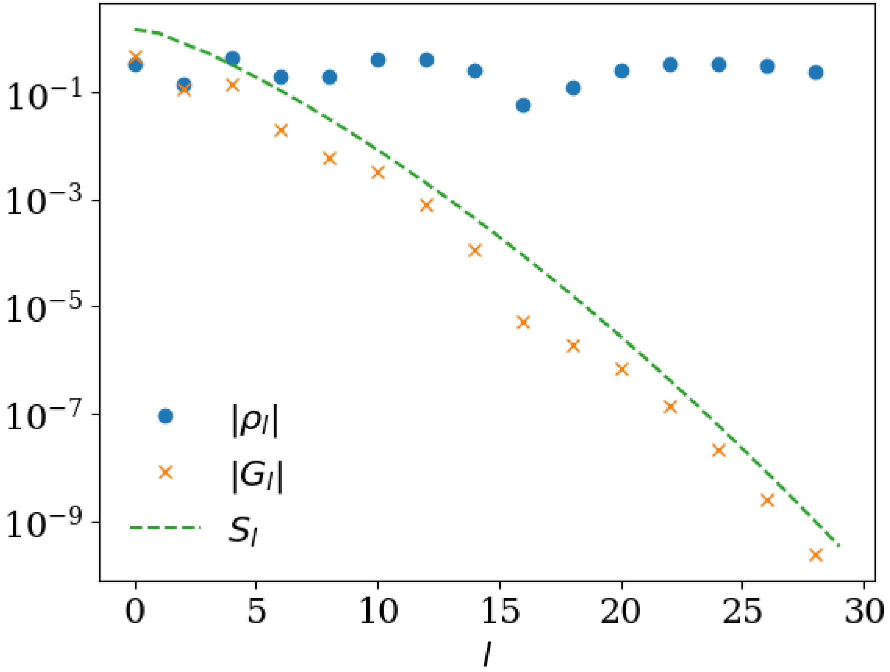
$|G_l|$ converges as fast as S_l.

Example:

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

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

$\beta = 100, \omega_{\mathrm{max}} = 1.$



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 $\Sigma(\mathrm{i}\omega)$:

$$G(\mathrm{i}\omega) = (G_0^{-1}(\mathrm{i}\omega) + \Sigma(\mathrm{i}\omega))^{-1}$$

$$G_l = \sum_{n=-\infty}^{+\infty} U_l^*(\mathrm{i}\omega_n) G(\mathrm{i}\omega_n)$$

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

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

Dense mesh in τ?

Second-order self-energy (Hubbard U):

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

$$G_l = \int_0^\beta d\tau U_l(\tau)G(\tau)$$

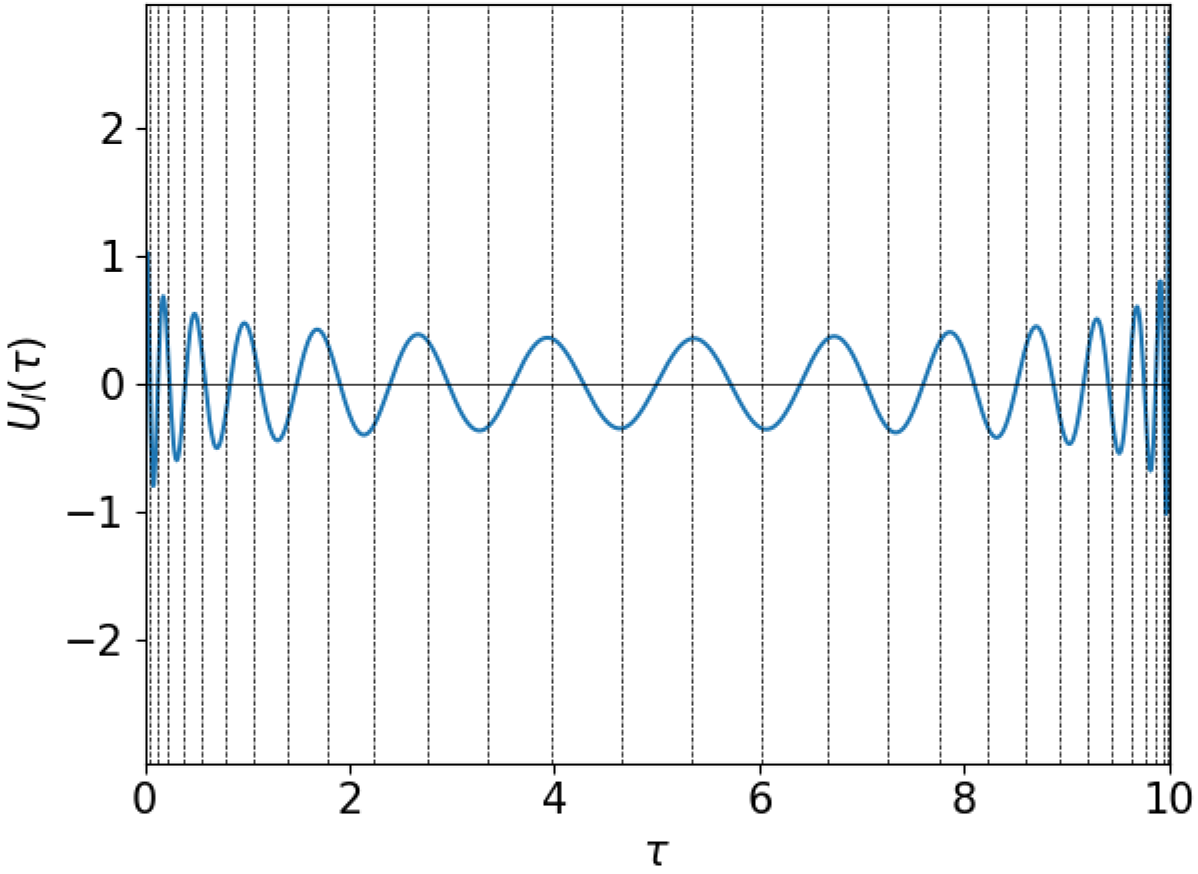
Q: Need to compute $G(\tau)$ on a dense mesh of τ?

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

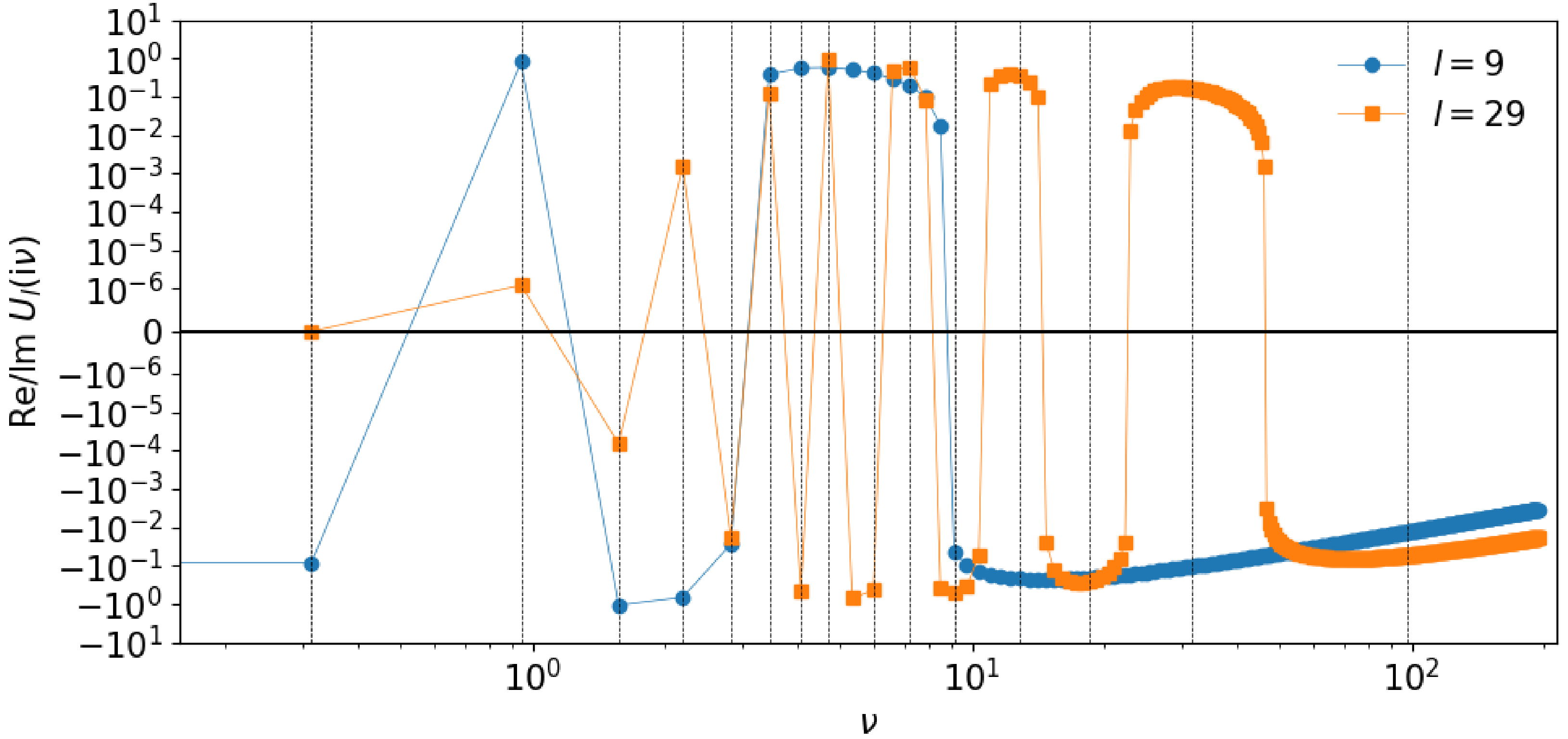
$\beta = 10, \omega_{\max} = 10, L = 30$:



Sampling points

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

$\beta = 10, \omega_{\mathrm{max}} = 10, L = 30$:



Transform from time/frequency to IR

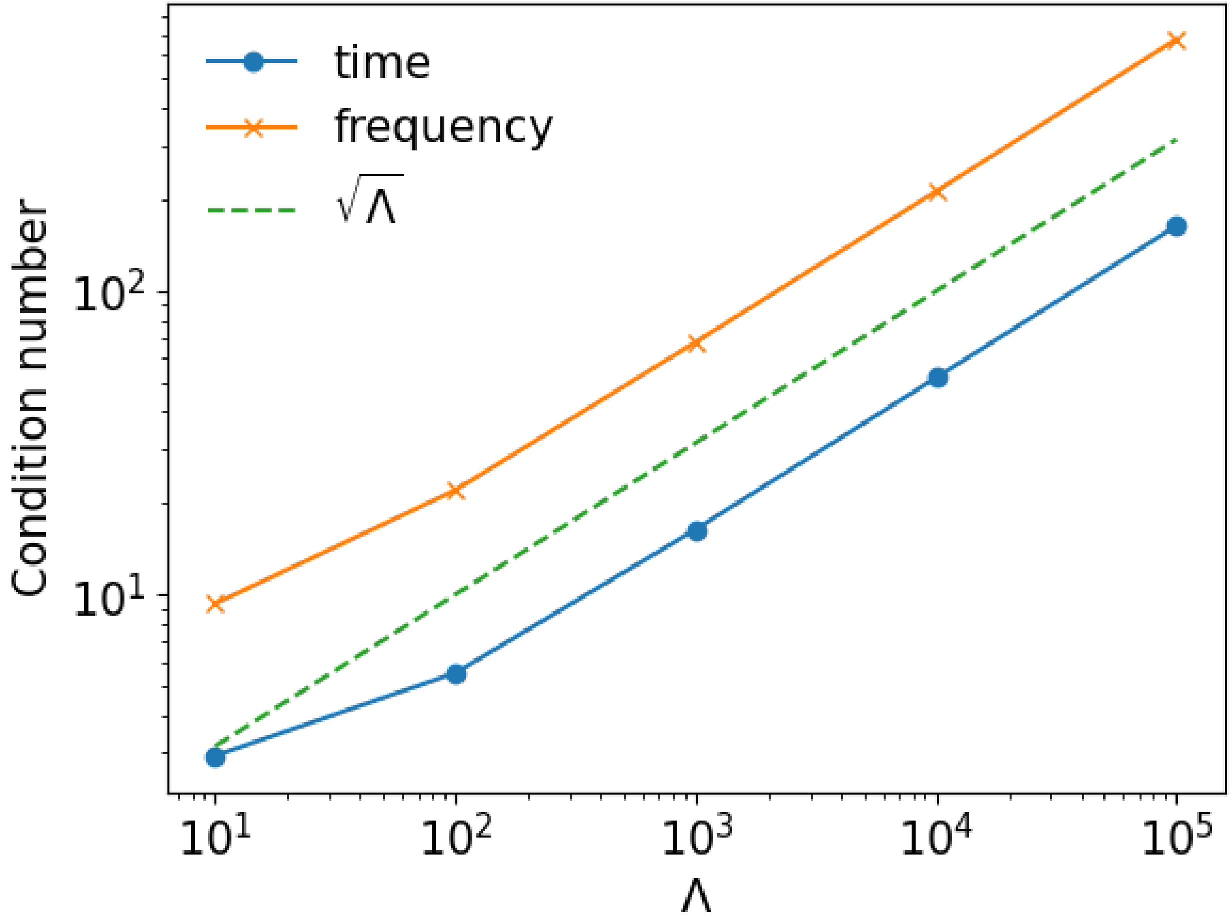
- Well conditioned fitting problem
- Implemented in sparse-ir as stable linear transform

$$
\begin{aligned}
G_l &= \underset{G_l}{\mathrm{argmin}} \sum_k \left| G(\bar{\tau}_k) - \sum_{l=0}^{N_\mathrm{smpl}-1} U_l(\bar{\tau}_k) G_l \right|^2 \\
&= (\mathbf{F}^+ \boldsymbol{G})_l,
\end{aligned}
$$

where we define $(\mathbf{F})_{kl} = U_l(\bar{\tau}_k)$ and $\mathbf{F}^+$ is its pseudo inverse.

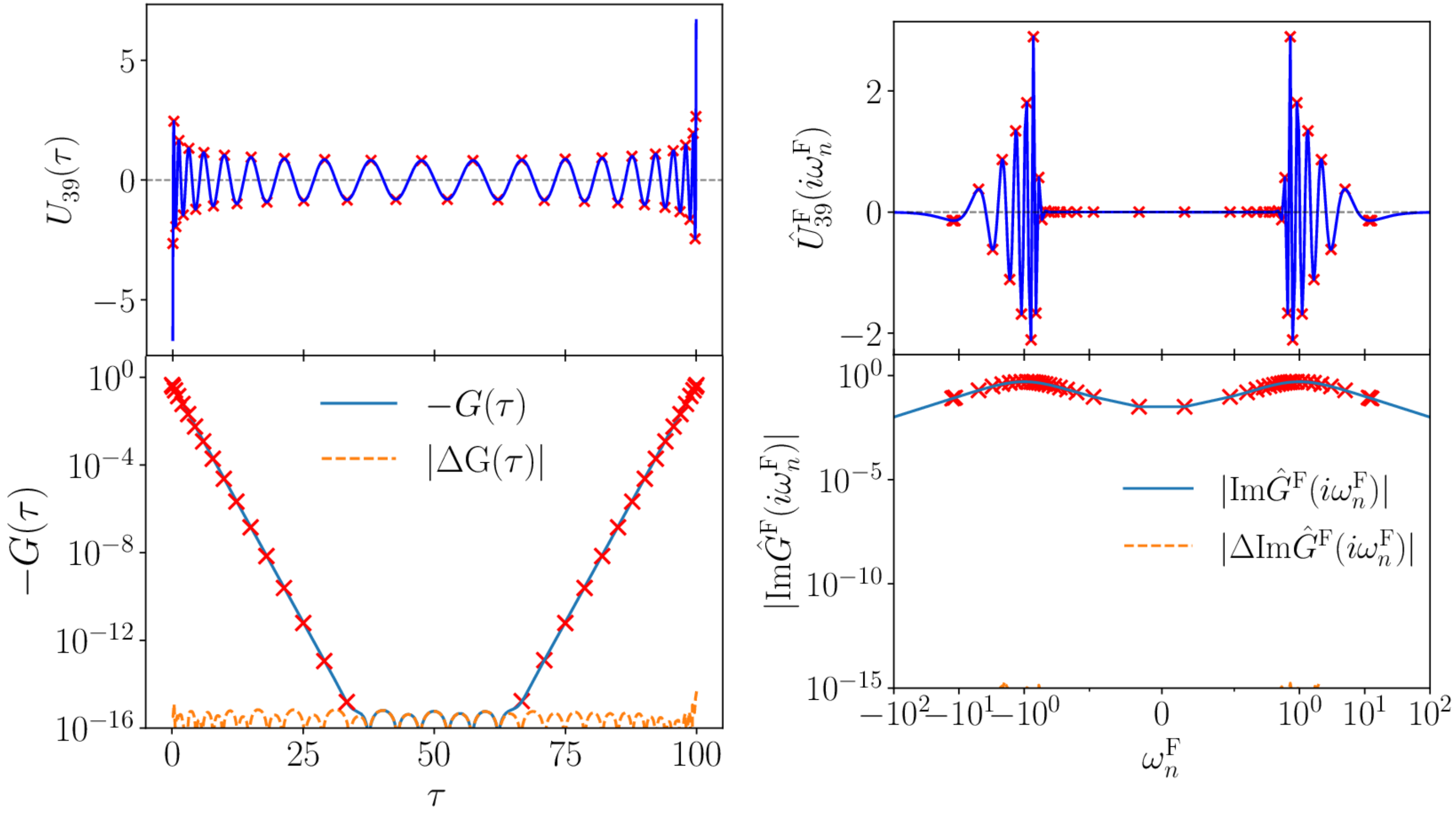
Condition number

- Small condition number of $\mathbf{F}$
- If condition number is 10^p, you may loos p digits in transformation (three out of 16 digits)

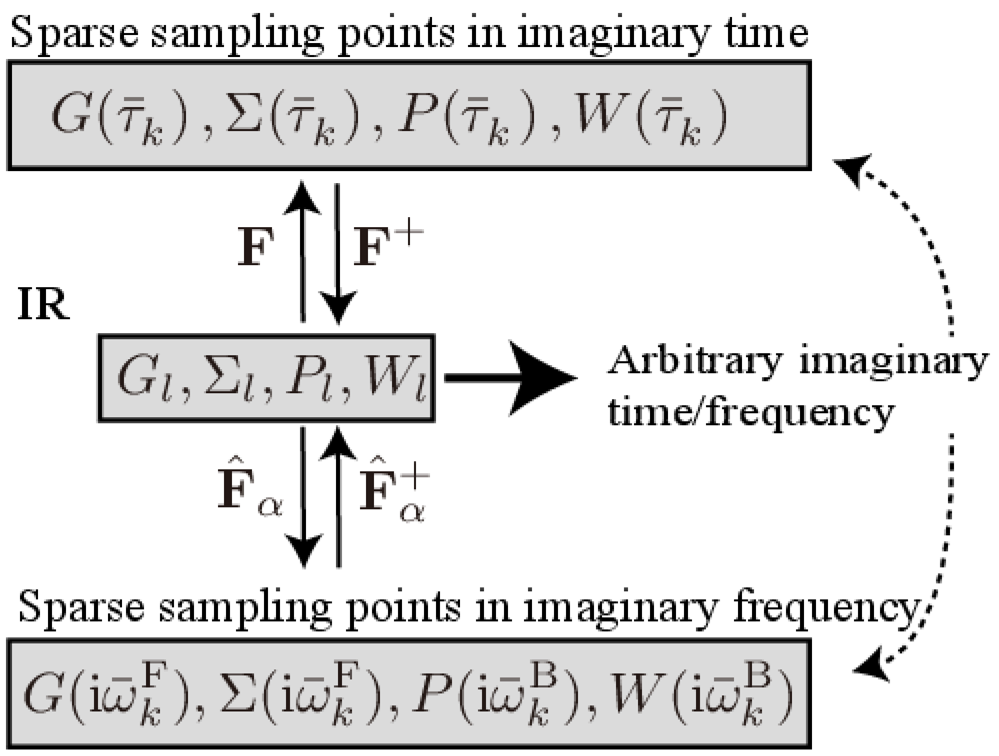


Numerical demonstration

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



Stable and efficient numerical transform



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

$$G(\mathrm{i}\nu, \boldsymbol{k}) = \frac{1}{\mathrm{i}\nu - \epsilon(\boldsymbol{k}) + \mu - \Sigma(\mathrm{i}\nu, \boldsymbol{k})} \tag{1}$$

$$\downarrow$$

$$\downarrow (\mathrm{i}\nu \to \tau, \boldsymbol{k} \to \boldsymbol{r})$$

$$\downarrow$$

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

$$\downarrow$$

$$\downarrow (\tau \to \mathrm{i}\nu, \boldsymbol{r} \to \boldsymbol{k})$$

$$\downarrow$$

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

Self-consistent equations (sparse sampling)

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

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

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

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