Saitama University
埼玉大学

Sparse modeling approach to analytic continuation of imaginary-time data and quantum many-body calculations

Hiroshi SHINAOKA
Saitama University, JST

TACKLING THE REAL-TIME CHALLENGE IN STRONGLY CORRELATED SYSTEMS:
SPECTRAL PROPERTIES FROM EUCLIDEAN PATH INTEGRALS

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Acknowledgements

- Saitama University
  N. Chikano
- University of Tokyo
  K. Yoshimi
  Arita's group
- Okayama University
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- Tohoku University
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- JAEA
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- Rutgers University
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  Held's group

科研費 KAKENHI

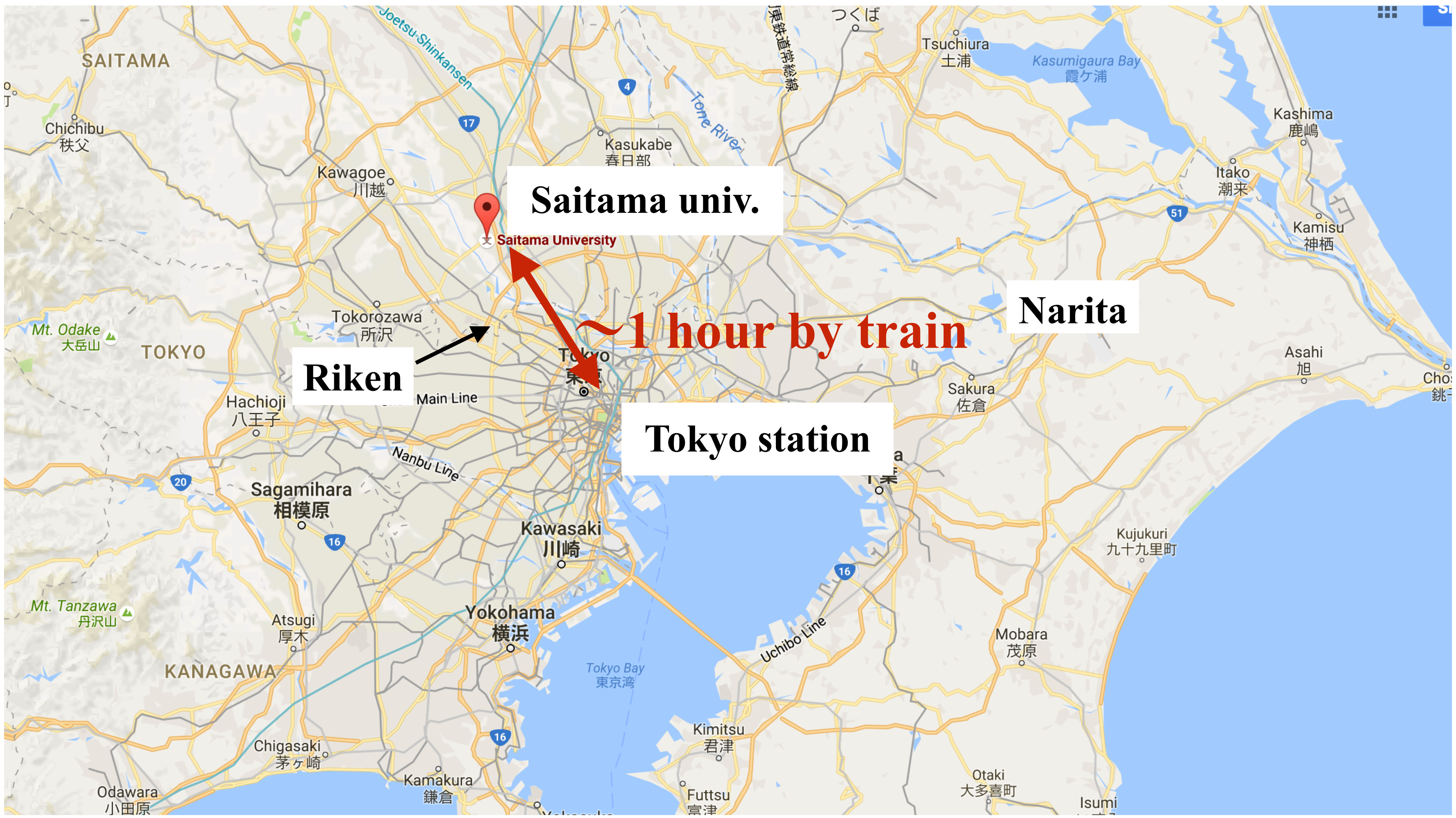
平成27~31年度 文部科学省 科学研究費補助金 新学術領域（研究領域提案型）
J-Physics：多極子伝導系の物理
J-Physics : Physics of Conductive Multipole Systems 領域番号：2704

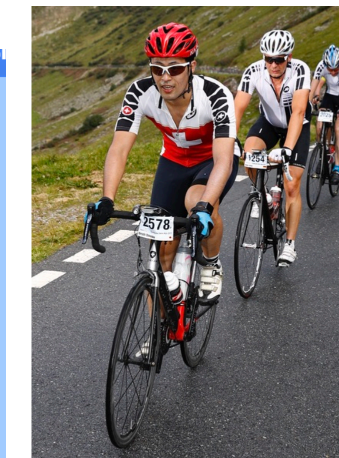
Self introduction

Developing first-principles method for correlated materials

Continuous-time quantum Monte Carlo, dynamical mean-field theory

Post doc for three years in Switzerland (Prof. M. Troyer & Prof. P. Werner)





Prof. Kajita used to be an undergraduate student of our university long time ago.

Review1: JPSJ **89**, 012001 (2020)
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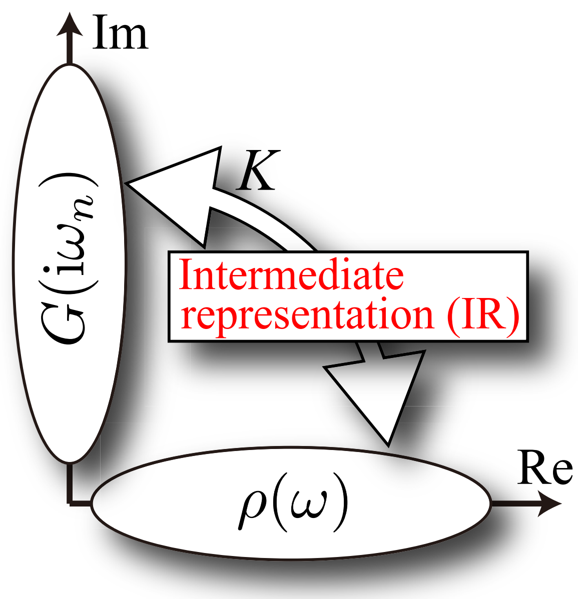
Overview



+ Sparse modeling

Stable analytic continuation

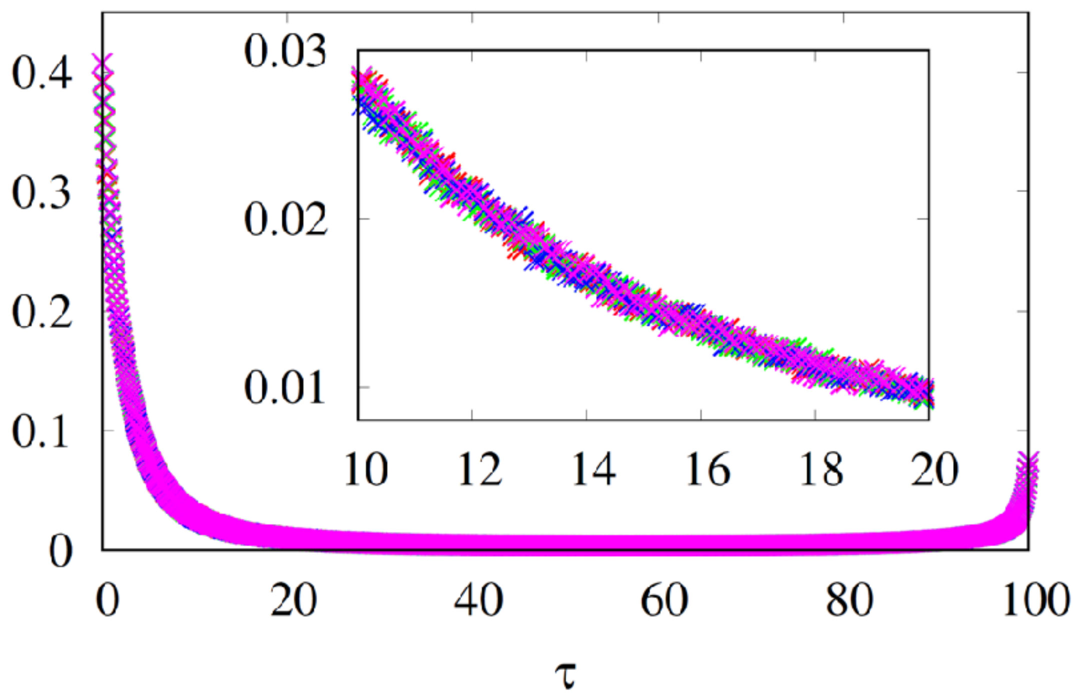
Review: J. Otsuki, M. Ohzeki, HS, K. Yoshimi, JPSJ **89**, 012001 (2020)

Efficient diagrammatic calculation

Review: HS, N. Chikano, E. Gull, J. Li, T. Nomoto, J. Otsuki, M. Wallerberger, T. Wang, K. Yoshimi, arXiv:2106.12685

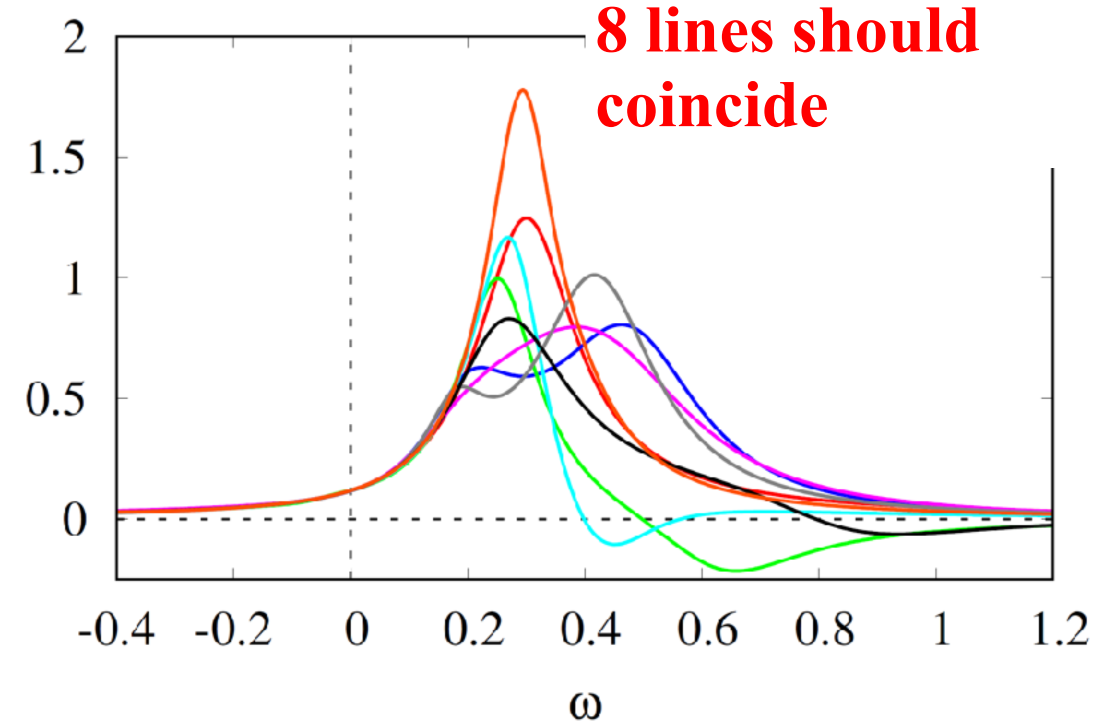
Analytic continuation is sensitive to noise

$G(\tau)$ **8-fold degenerate impurity Anderson model**



Continuous-time QMC data

$\rho(\omega)$



Padé approximation

Vidberg, Serene, 1977

Many sophisticated methods: machine-learning method, stochastic methods, *etc*.

<u>Question</u> What information remains in imaginary-time data?
Can we extract the relevant information?

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

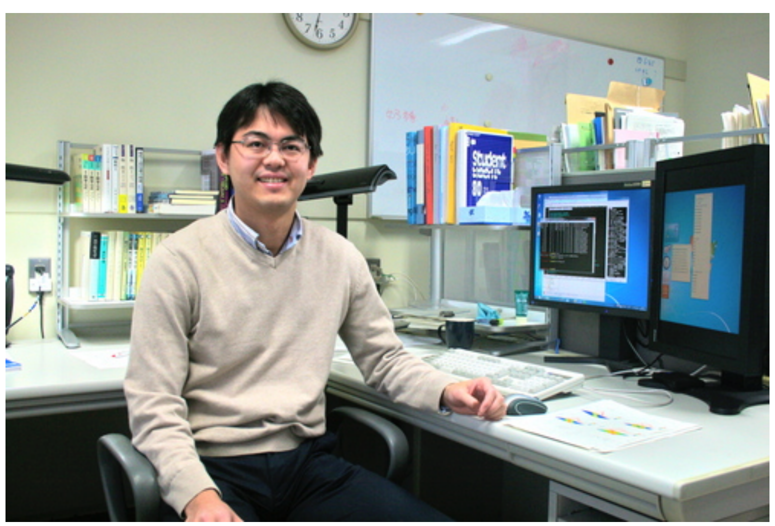
Sparse modeling of imaginary-time Green's functions

J. Otsuki, M. Ohzeki, H. Shinaoka, K. Yoshimi, PRE **95**, 061302(R) (2017)

Junya Otsuki
Tohoku univ.→Okayama univ.

Masayuki Ohzeki
Tohoku univ.

Kazuyoshi Yoshimi
Univ. Tokyo



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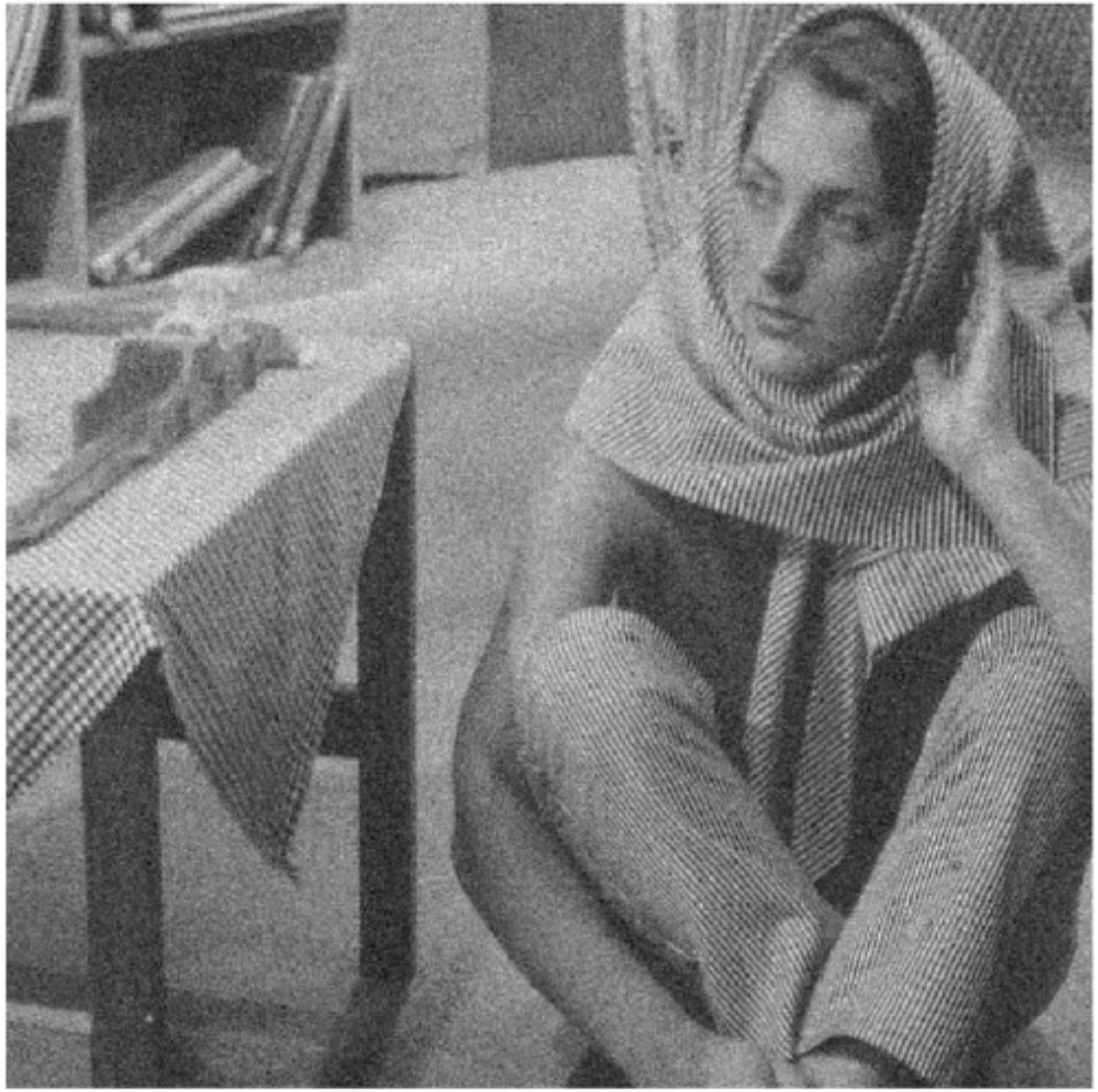
Review2: arXiv:2106.12685

Sparse modeling in data science

M. Elad and M. Aharon, IEEE Transactions on Image Processing **15**, 3736 (2006)

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Sparse modeling in data science



Noise

M. Elad and M. Aharon, IEEE Transactions on Image Processing **15**, 3736 (2006)

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

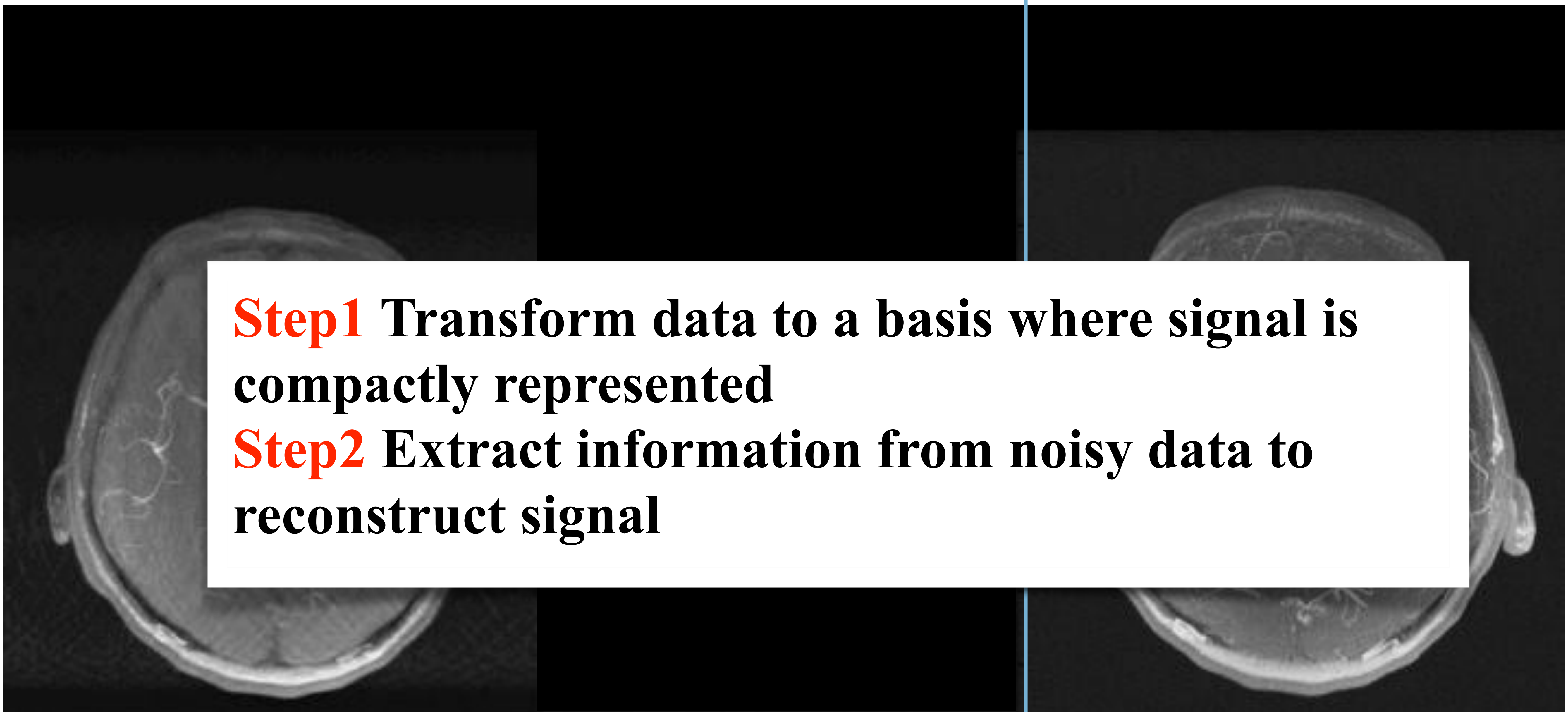
Sparse modeling in data science

Denoised

M. Elad and M. Aharon, IEEE Transactions on Image Processing **15**, 3736 (2006)

MRI

1/4 measurement time | **Full measurement time**



Step1 Transform data to a basis where signal is compactly represented
Step2 Extract information from noisy data to reconstruct signal

ZDNet Japan 大関真之
https://japan.zdnet.com/article/35074052/4/

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Step 1: basis transformation

Lehmann representation

$$G(\tau) = \int_{-\infty}^{\infty} d\omega K_{\pm}(\tau,\omega)\rho(\omega)$$

$$K_{\pm}(\tau,\omega) = \frac{e^{-\tau\omega}}{1 \pm e^{-\beta\omega}}$$

Fermion (+), boson (-)

Discretization

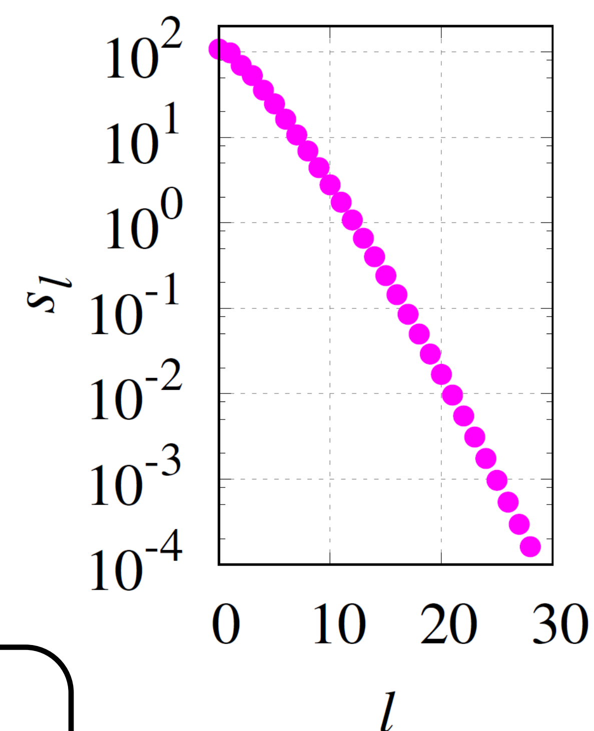
$$\boldsymbol{G} = \boldsymbol{K}\boldsymbol{\rho}$$

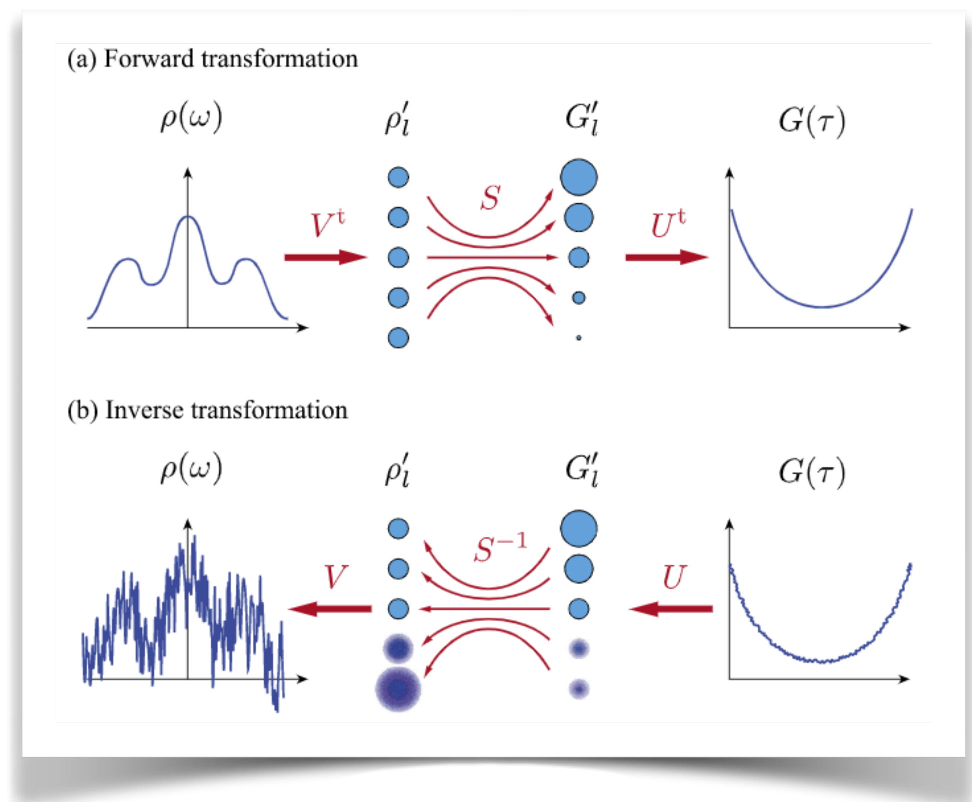
Singular value decomposition (SVD)

$$K = USV^{\mathrm{t}}$$

$$G' \equiv U^t G,\ \rho' \equiv V^t \rho$$

$$G'_l = s_l \rho'_l$$

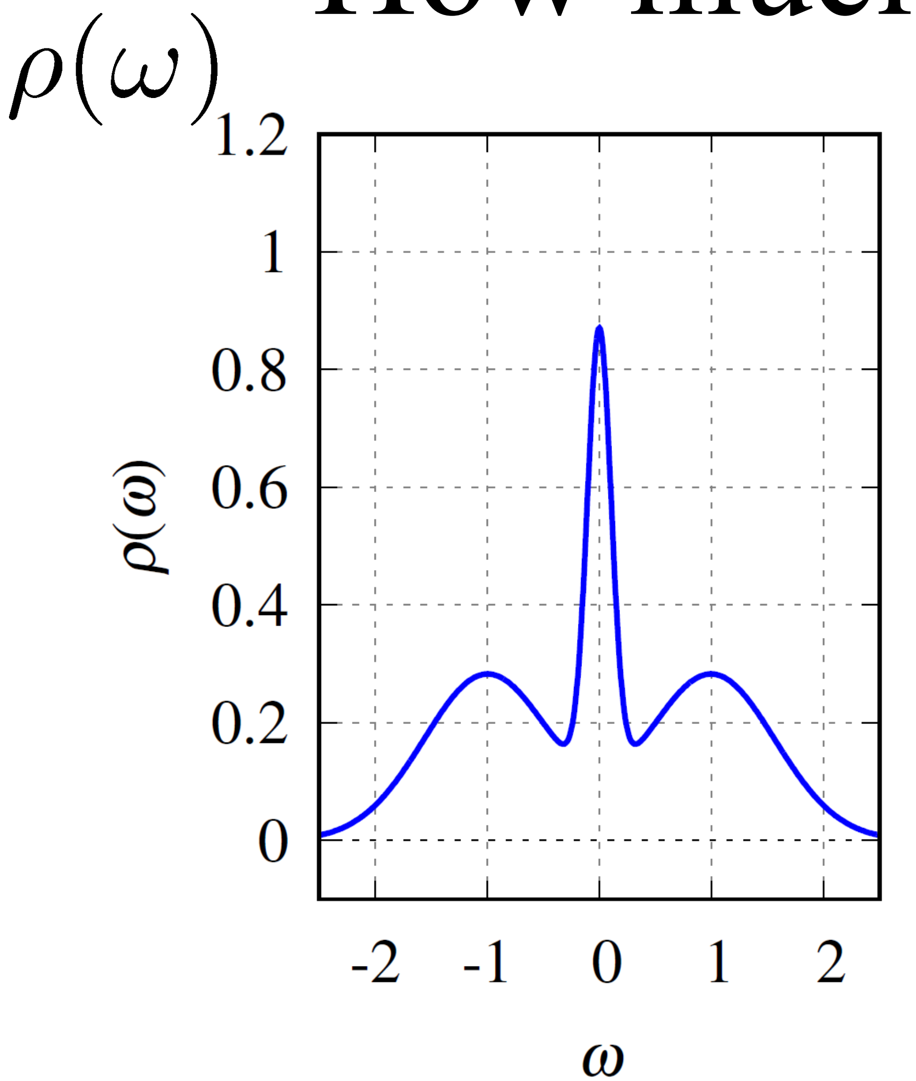


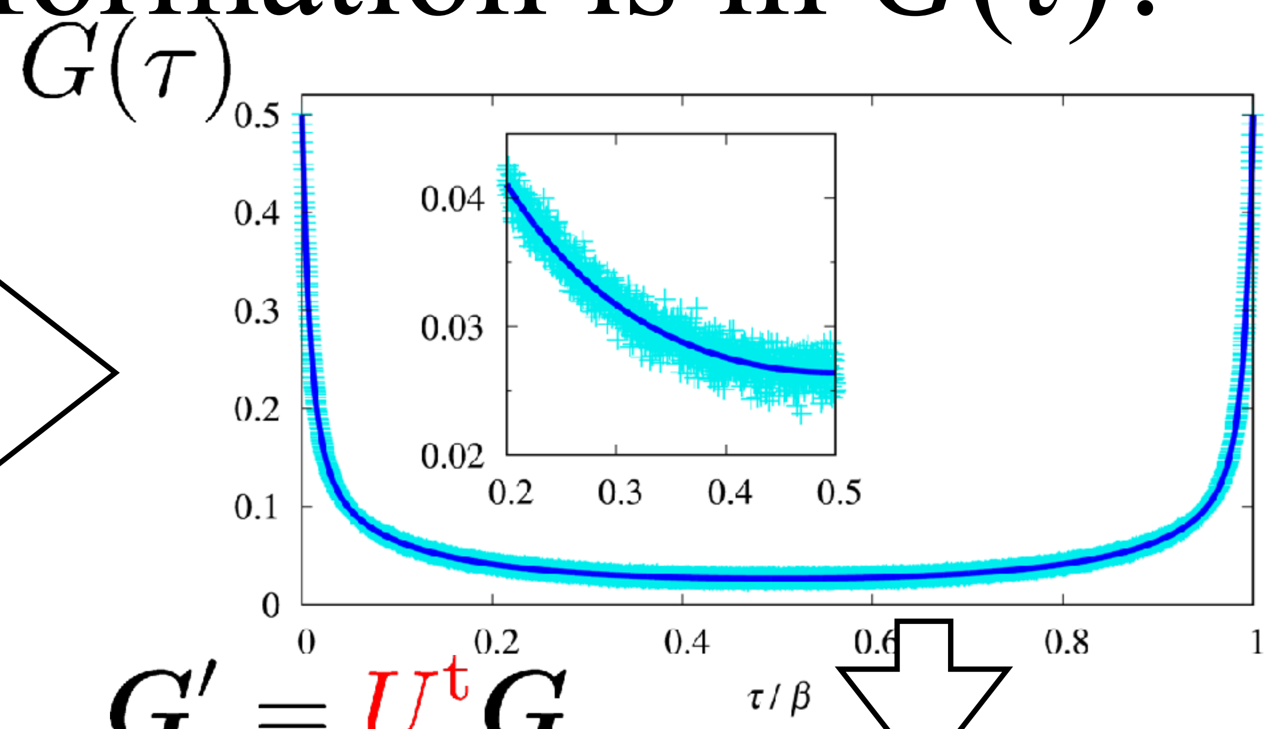


Information in G is carried by a few coefficients.

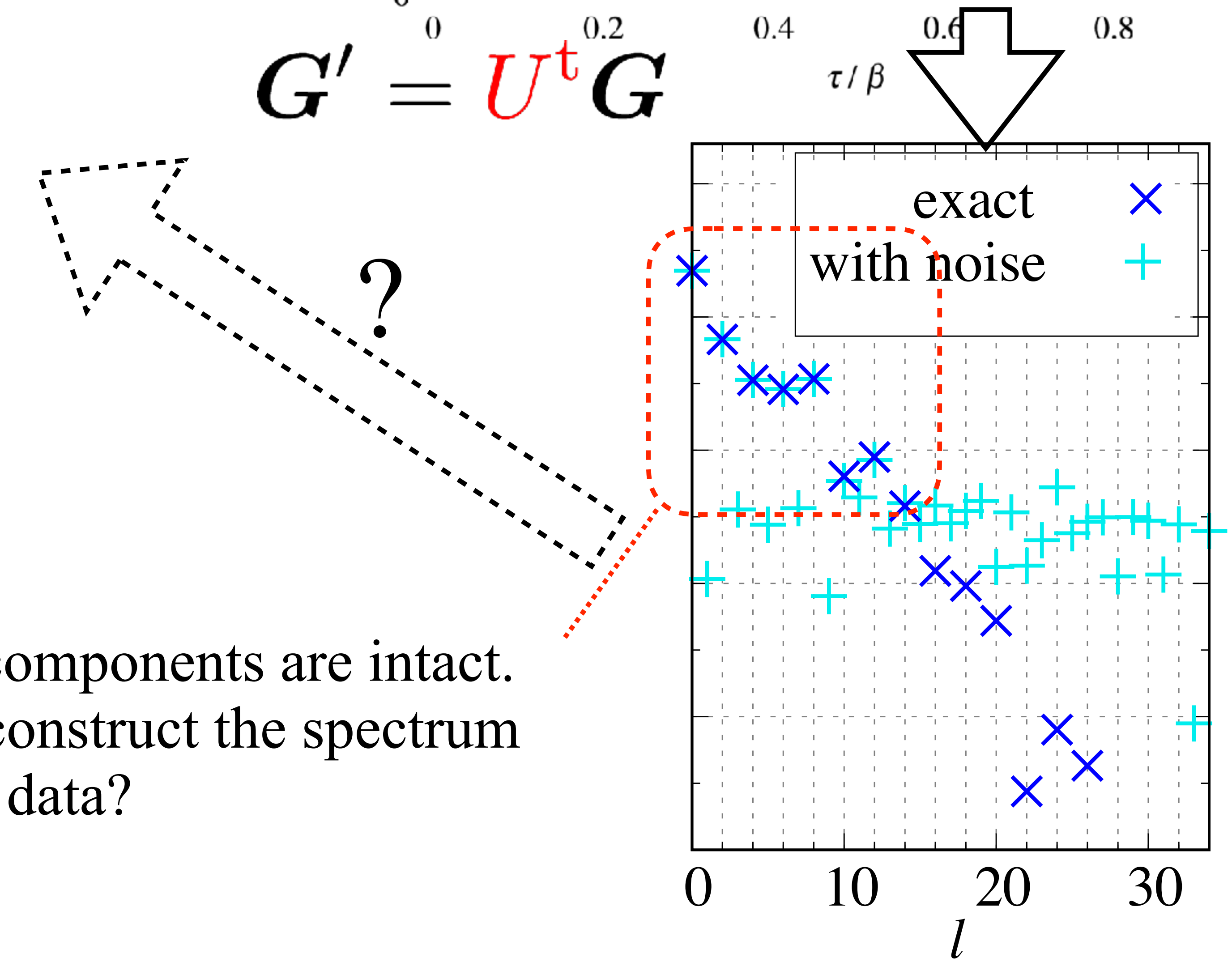
Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

How much information is in $G(\tau)$?





$$G' = U^{t} G$$



Only few components are intact.
Can we reconstruct the spectrum from these data?

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Step 2: extract signal

The least absolute shrinkage and selection operator (LASSO)

R. Tibshirani, Stat. Soc., Ser. B**58**, 267 (1996)

Minimize $$\frac{1}{2}\|\boldsymbol{G}' - S\boldsymbol{\rho}'\|_2^2 + \lambda\|\boldsymbol{\rho}'\|_1$$

Data fit

Sparseness of solution

$$\|\boldsymbol{\rho}'\|_1 \equiv \sum_l |\rho_l'|$$

L1 regularization

with

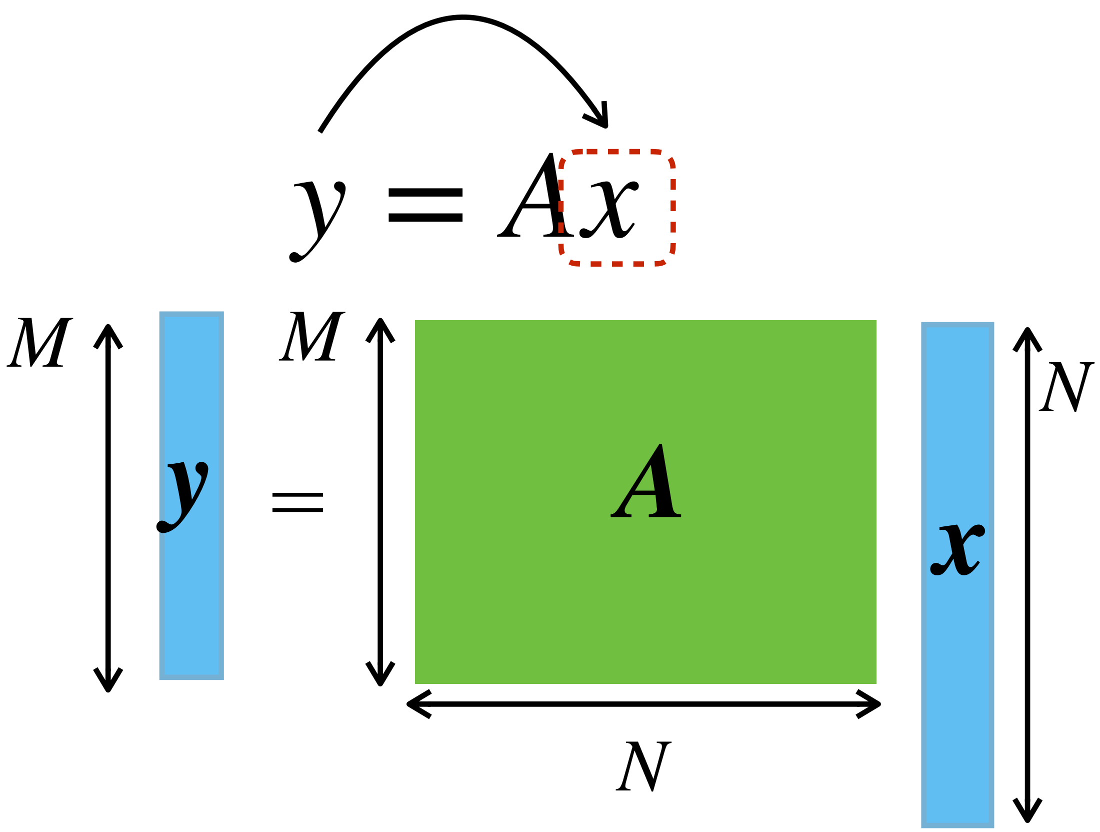
Positivenes $\rho_i \geq 0,$ Sum rule $\sum_i \rho_i = 1$

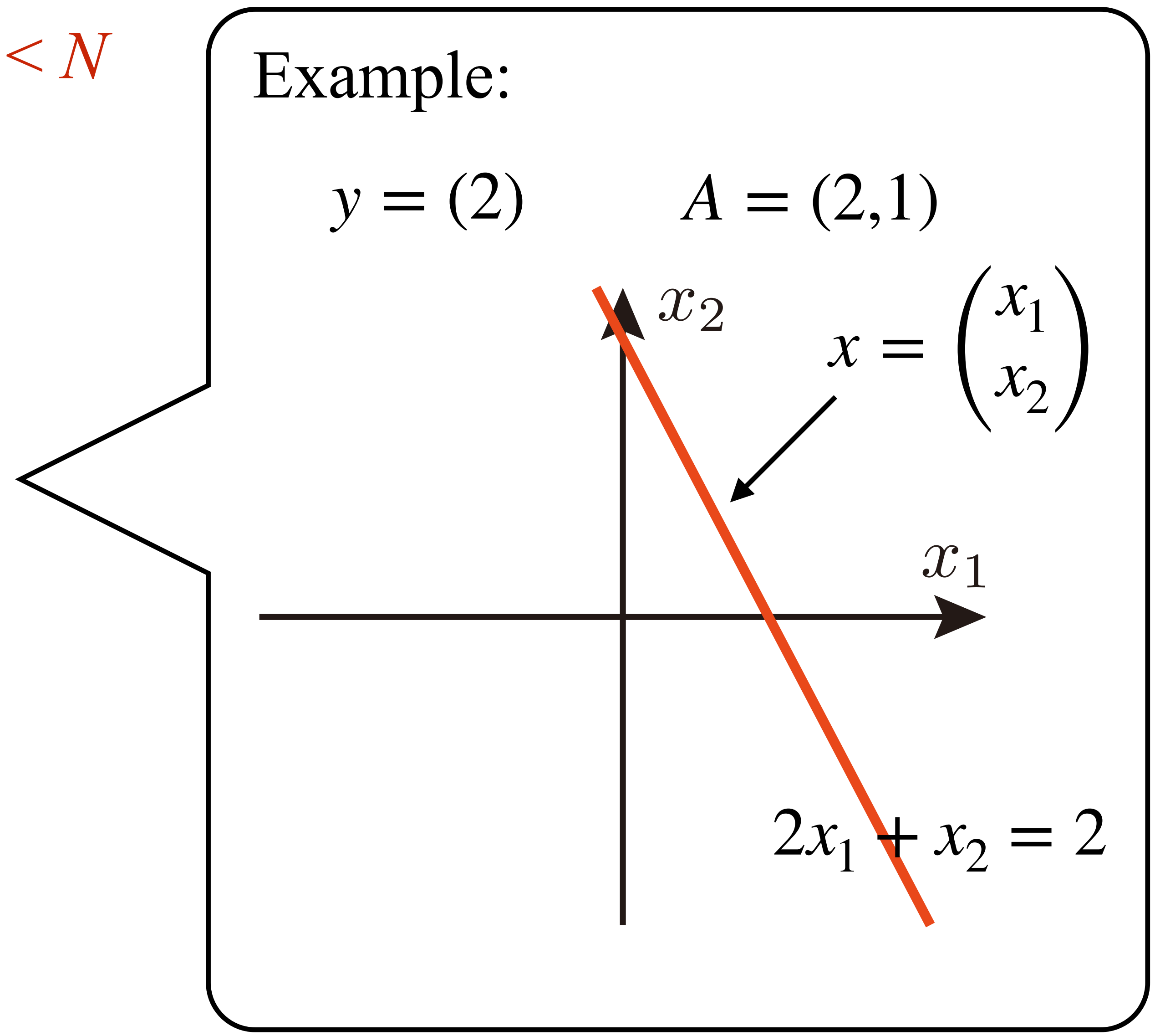
- Convex optimization problem → fast & stable
- No default model like Maximum entropy method
- λ can be optimized automatically.

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Regularizing ill-conditioned inverse problem

Ill-conditioned inverse problem for $M < N$





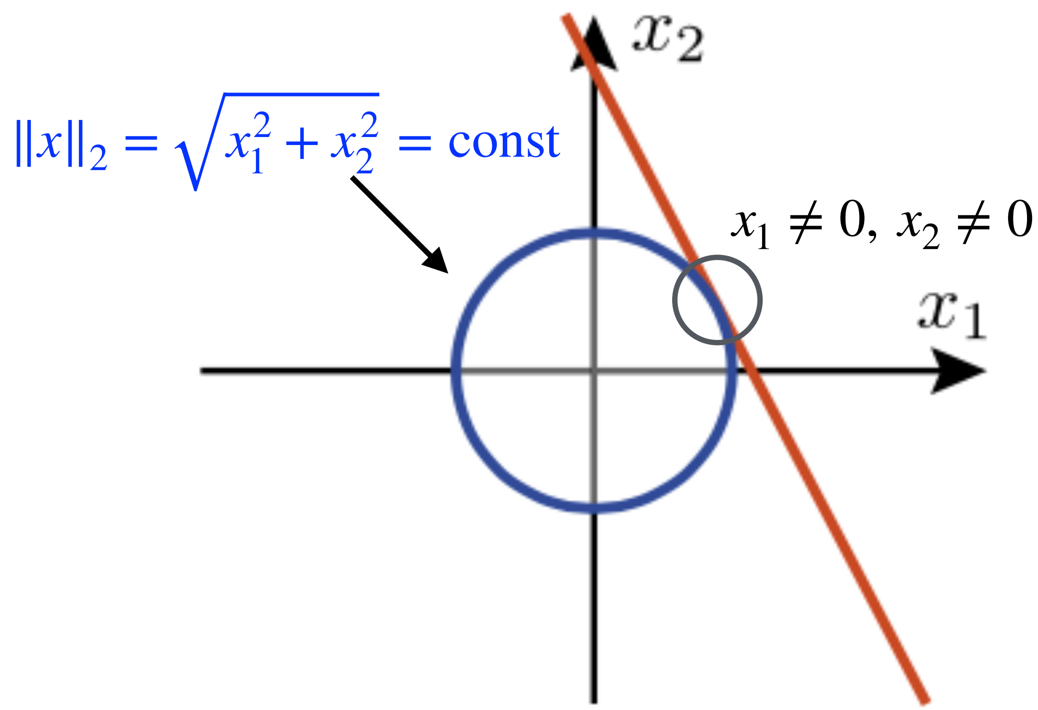
Select out a unique solution out of degenerate solutions → Regularization

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

L1 vs L2 regularization

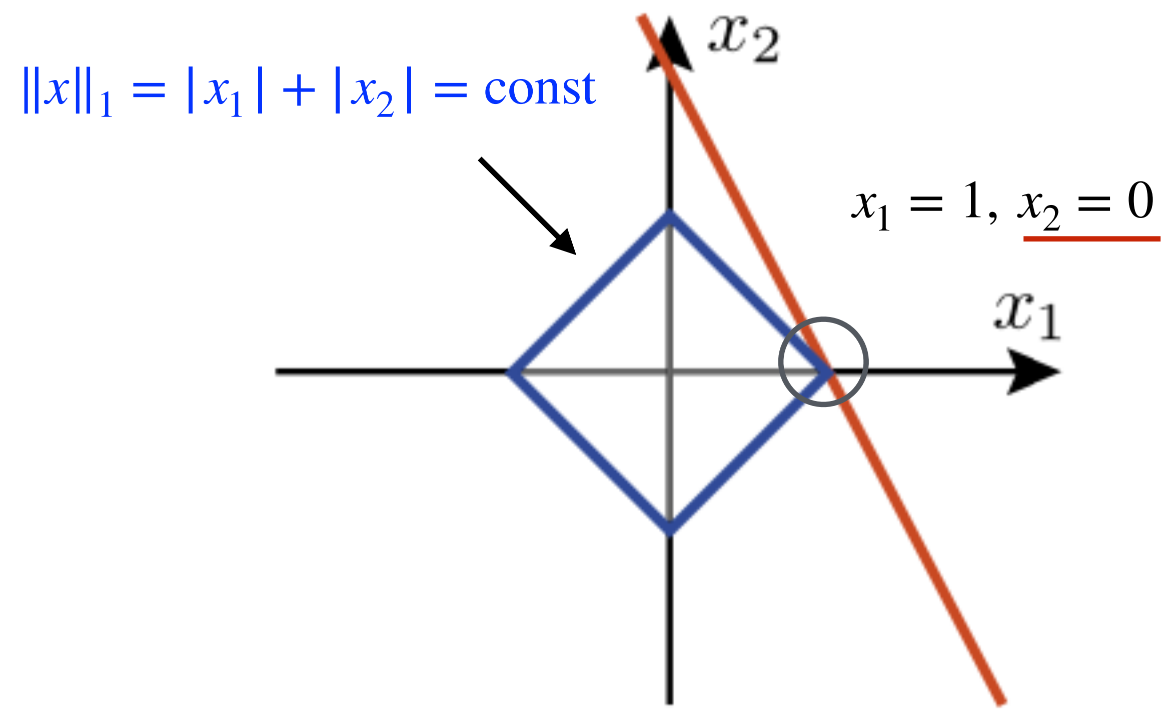
Let us adopt the solution minimizing L1/L2 norm of the solution…

L2 regularization



Known as Ridge/Tikhonov regularization

L1 regularization

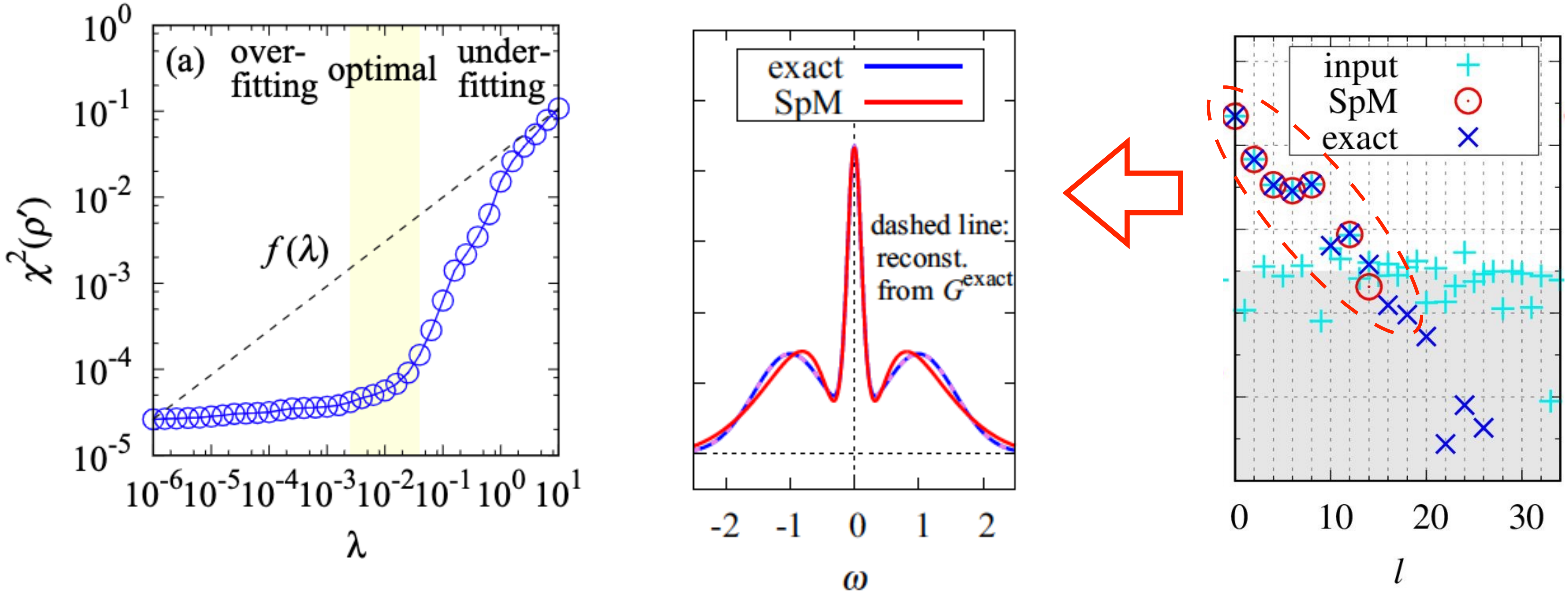


In general, L1 regularization suppresses irrelevant parameters to exactly zero.

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Step 2: extract signal

$$\text{Minimize} \quad \frac{1}{2}\|\boldsymbol{G}' - S\boldsymbol{\rho}'\|_2^2 + \lambda\|\boldsymbol{\rho}'\|_1$$



Relevant parameters are selected out automatically.

Possible extensions:

- Covariance
- Matrix-valued correlation functions

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Open-source implementation

https://github.com/SpM-lab/SpM

SpM

Welcome to SpM's documentation!

This is a documentation of Sparse Modeling (SpM) tool for analytical continuation.

Navigation

1. How to install
2. Tutorials
3. Algorithm
4. Calculation flow
5. Input files
6. Output files

Quick search

Go

What is SpM ?

A sparse-modeling tool for computing the spectral function from the imaginary-time Green function. It removes statistical errors in quantum Monte Carlo data, and performs a stable analytical continuation. The obtained spectral function fulfills the non-negativity and the sum rule. The computation is fast and free from tuning parameters.

License

This package is distributed under GNU General Public License version 3 (GPL v3).

We kindly ask you to cite the article

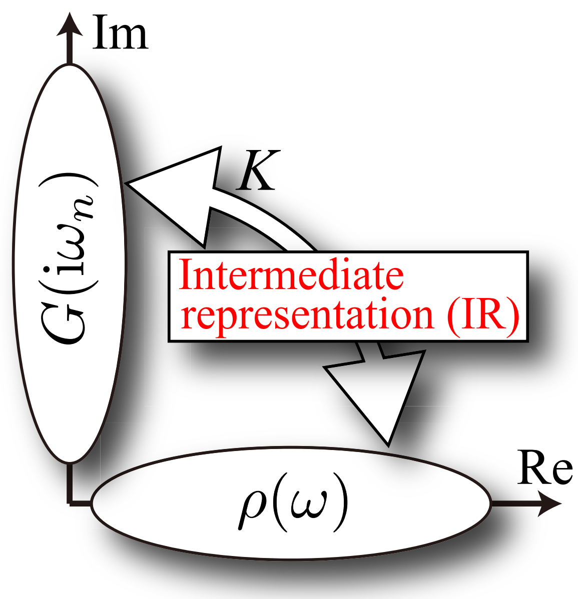
> J. Otsuki, M. Ohzeki, H. Shinaoka, K. Yoshimi, "*Sparse modeling approach to analytical continuation of imaginary-time quantum Monte Carlo data*" Phys. Rev. E 95, 061302(R) (2017).

in publications that includes results obtained using this package.

Version 2 will be released soon! (Improved stability for boson, improved determination of hyper parameter)

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Overview



+ Sparse modeling

Stable analytic continuation

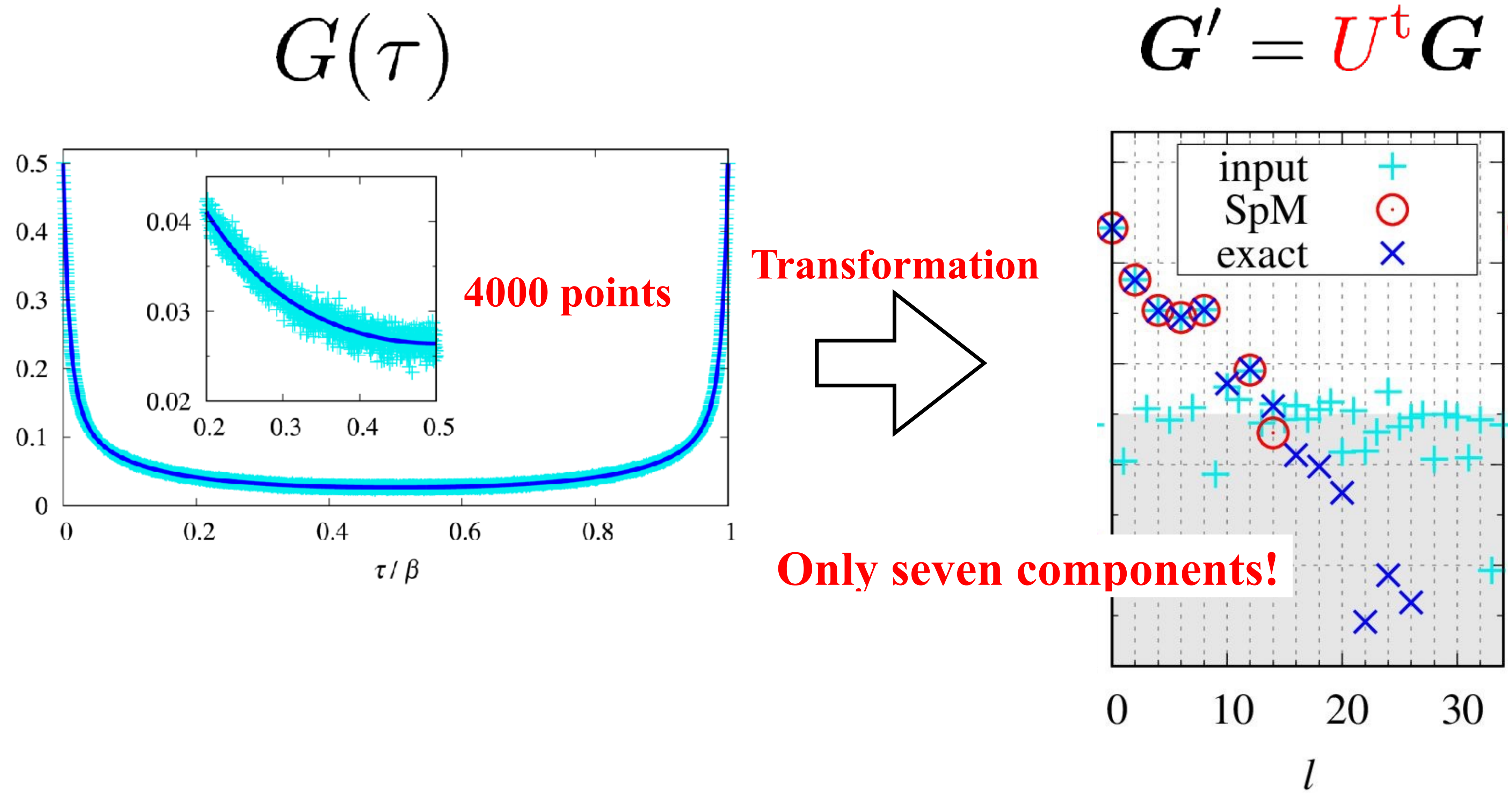
Efficient diagrammatic calculation

Review: J. Otsuki, M. Ohzeki, HS, K. Yoshimi, JPSJ **89**, 012001 (2020)

Review: HS, N. Chikano, E. Gull, J. Li, T. Nomoto, J. Otsuki, M. Wallerberger, T. Wang, K. Yoshimi, arXiv:2106.12685

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

You saw that …



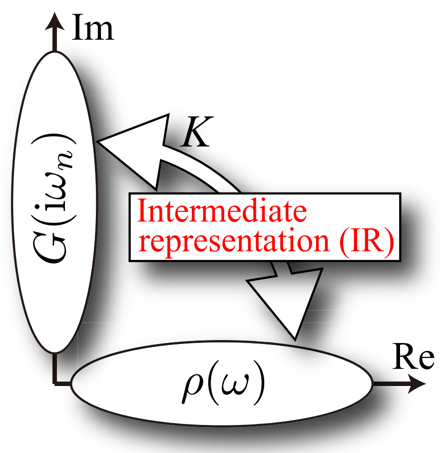
- How the SVD basis functions look like?
- Can we use the compactness of the SVD basis in many-body calculations?

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Intermediate representation (IR)

HS, J. Otsuki, M. Ohzeki, K. Yoshimi, PRB **96**, 035147 (2017)
HS, N. Chikano, E. Gull, J. Li, T. Nomoto, J. Otsuki, M. Wallerberger, T. Wang, K. Yoshimi, arXiv:2106.12685v1

$$G(\tau) = \int_{-\omega_{\max}}^{\omega_{\max}} d\omega\ K^{\alpha}(\tau,\omega)\rho(\omega)$$



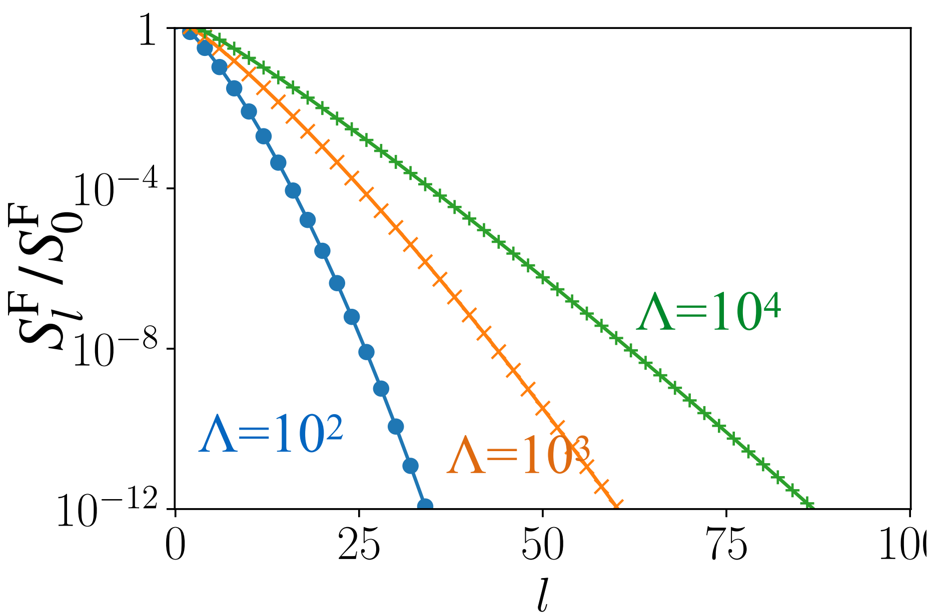
α = F (fermion), B (boson)

Singular value expansion

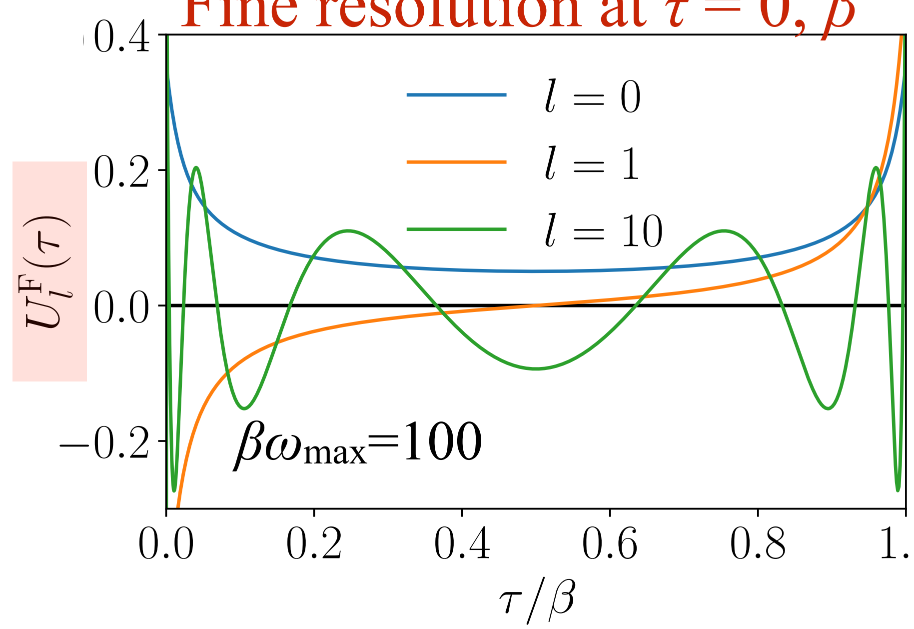
$$K^{\alpha}(\tau,\omega) = \sum_{l=0}^{\infty} S_l^{\alpha} U_l^{\alpha}(\tau) V_l^{\alpha}(\omega)$$

Singular values   IR basis functions

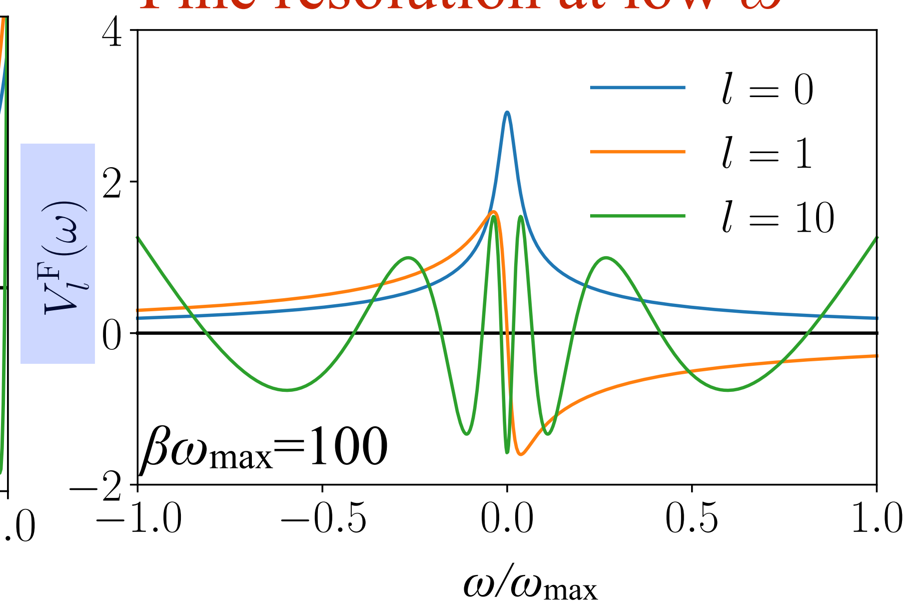
$\Lambda \equiv \beta\omega_{\max}$



Fine resolution at $\tau = 0, \beta$

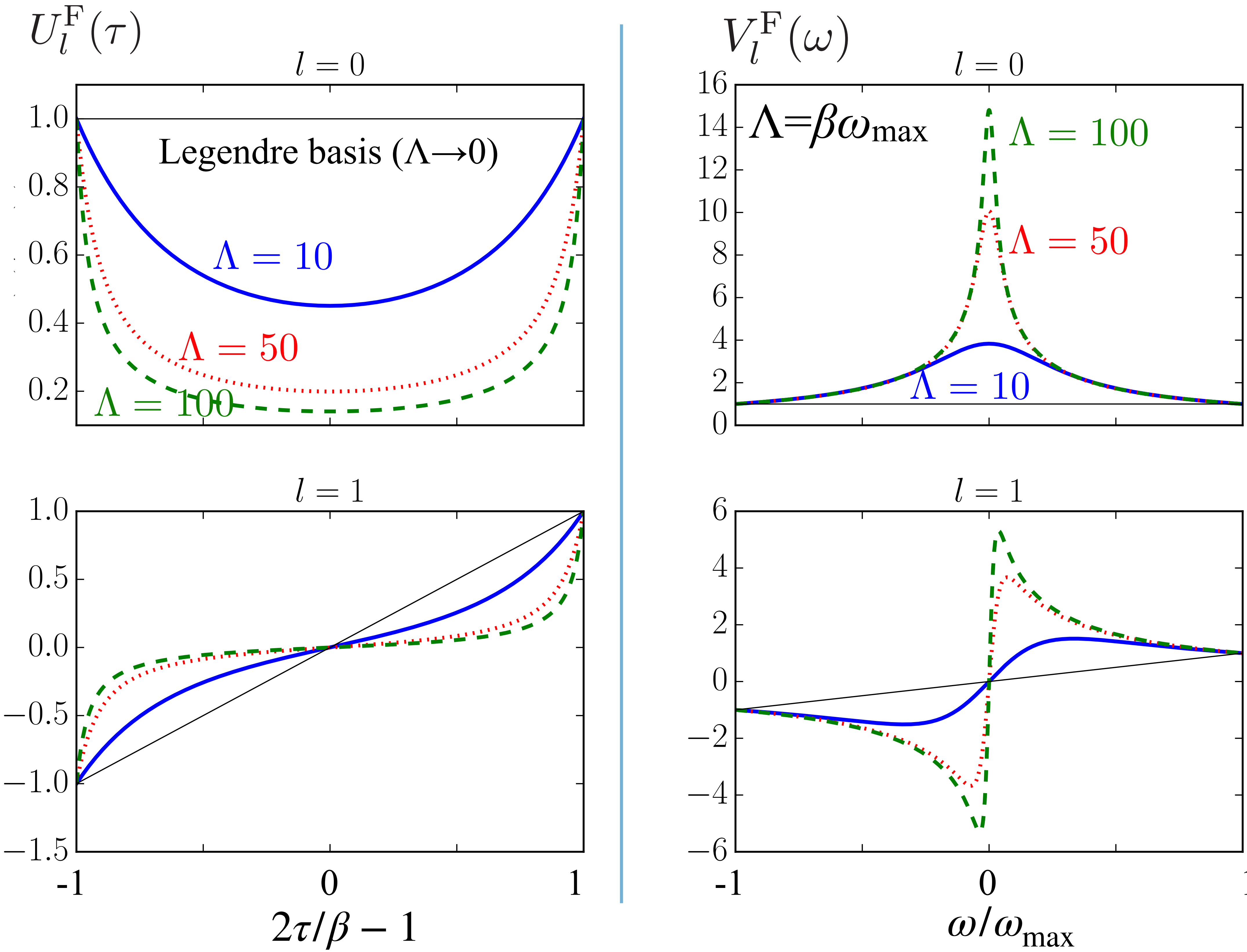


Fine resolution at low ω



IR basis functions

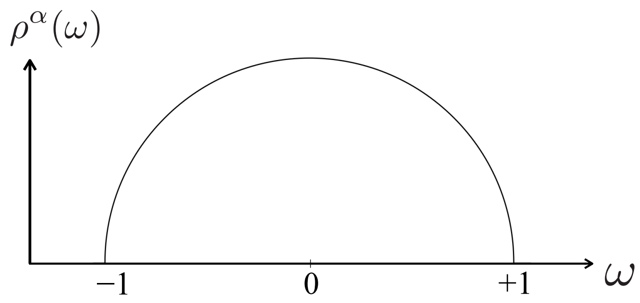
$\Lambda \equiv \beta\omega_{\mathrm{max}}$

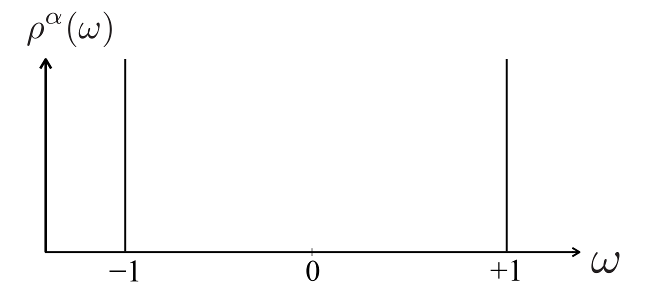


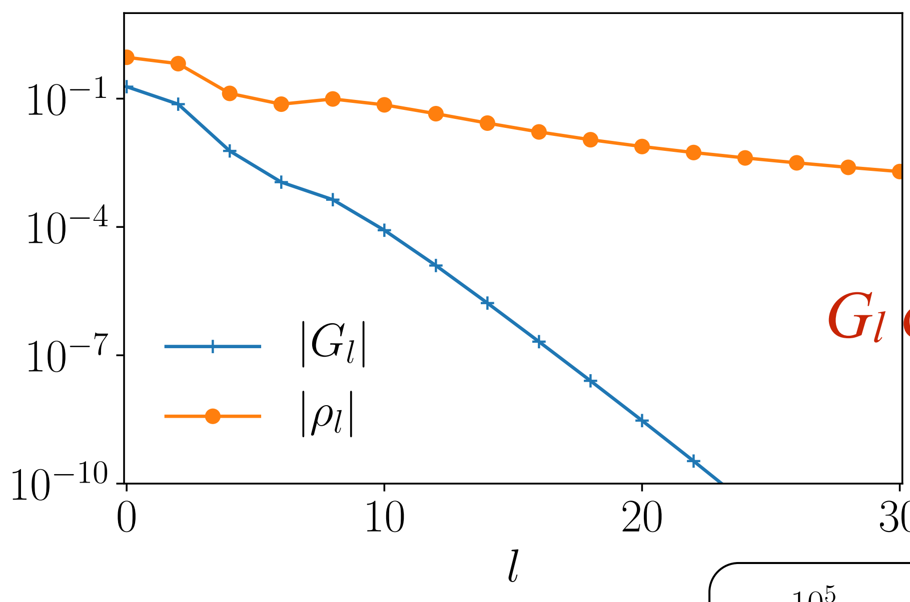
Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Compactness of IR

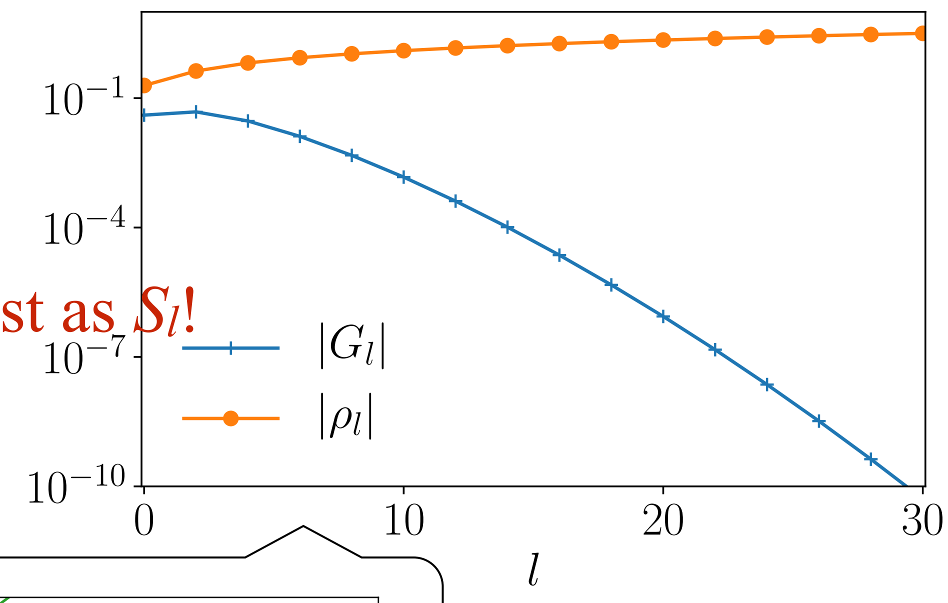
$\omega_{\max} = 1,\ \beta = 100$ (fermion)

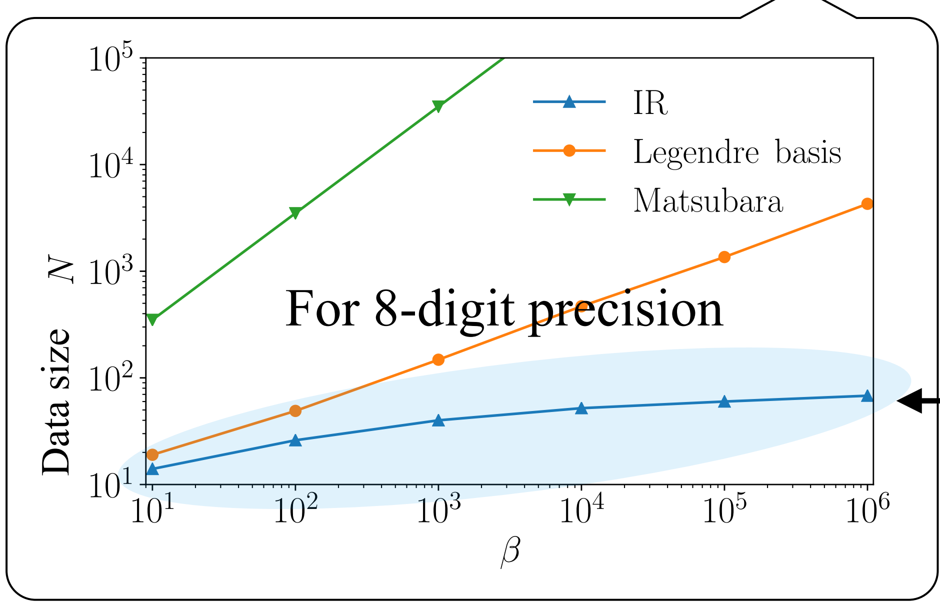






G_l decay as fast as S_l!





Most compact!

Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Open source software: irbasis

https://github.com/SpM-lab/irbasis

N. Chikano, K. Yoshimi, J. Otsuki, H. Shinaoka (2018) + M. Wallerberger (2019)

- Python and C++
- Step-by-step tutorial

python

Integral form

$$S_l^\alpha U_l^\alpha(\tau) = \int_{-\omega_{\max}}^{\omega_{\max}} d\omega K^\alpha(\tau,\omega) V_l^\alpha(\omega)$$

$x \equiv 2\tau/\beta - 1,\ y \equiv \omega/\omega_{\max}$

$$s_l^\alpha u_l^\alpha(x) = \int_{-1}^{1} dy k^\alpha(x,y) v_l^\alpha(y) \qquad x, y \in [-1,1]$$

Precomputed data for $\Lambda = 10, 10^2, \ldots, 10^7$

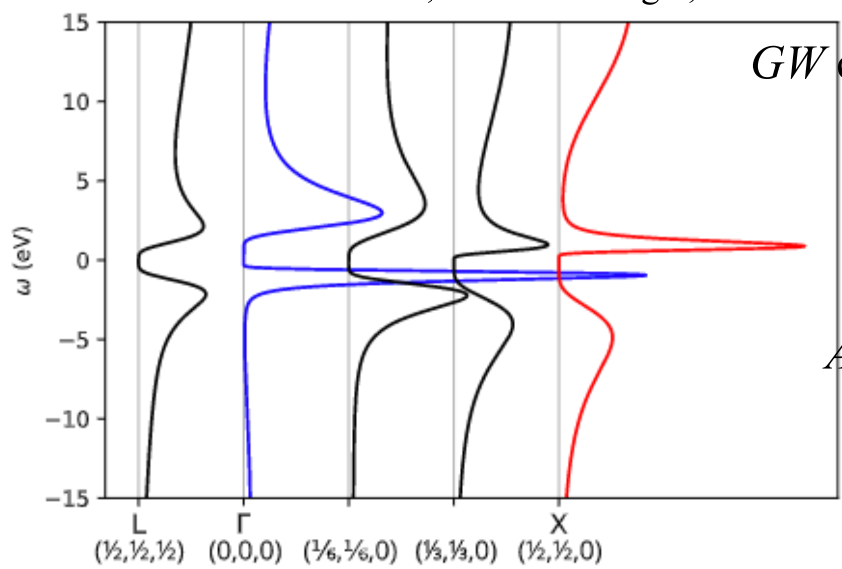
Review1: JPSJ **89**, 012001 (2020)
Review2: arXiv:2106.12685

Applications

Review: HS *et al.*, arXiv:2106.12685

Diagrammatic calculations for materials

J. Li, M. Wallerberger, C.-N. Yeh, N. Chikano, E. Gull, HS, PRB **101**, 035144 (2020)



GW calculations of silicon crystals

Ab initio calculations of superconducting materials

T. Wang, T. Nomoto, Y. Nomura, HS, J. Otsuki, T. Koretsune, and R. Arita, PRB **102**, 134503 (2020)

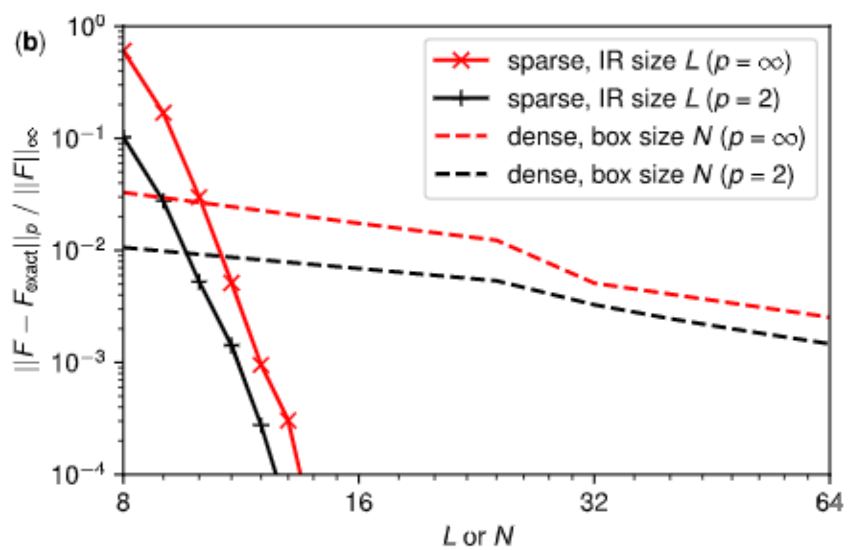
Denoiser

Y. Nagai and HS, JPSJ **88**, 064004 (2019)

Extension to two-particle quantities

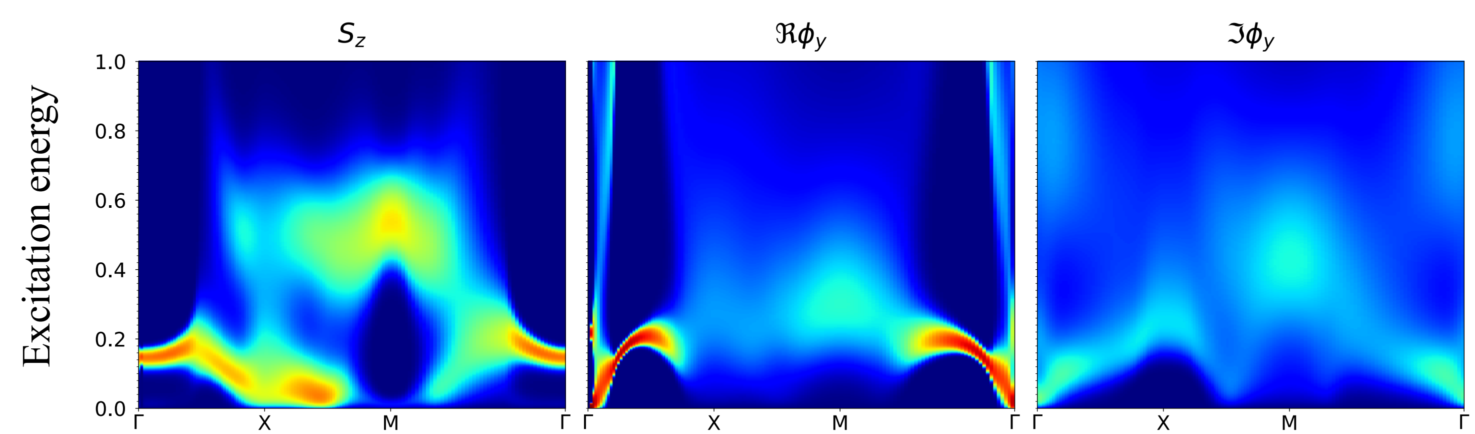
Bethe-Salpeter equation with exponential convergence

M. Wallerberger*, HS*, A. Kauch, PRR **3**, 033168 (2021)



Dynamical spin-orbital susceptibility

HS *et al.*, SciPost **8**, 12 (2020)



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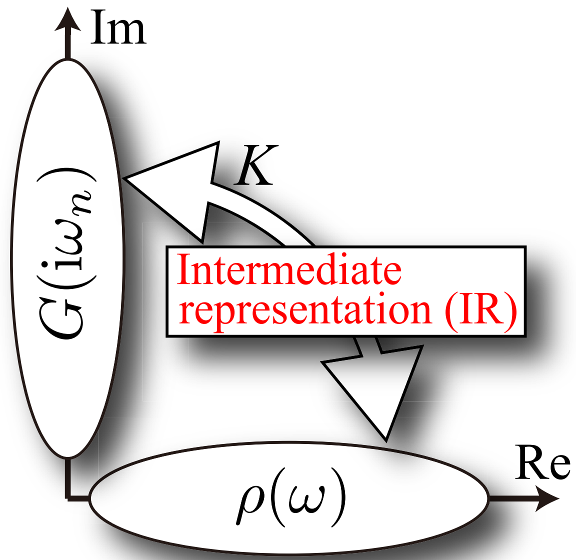
Summary



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Review: J. Otsuki, M. Ohzeki, HS, K. Yoshimi, JPSJ **89**, 012001 (2020)

Efficient diagrammatic calculation

Review: HS, N. Chikano, E. Gull, J. Li, T. Nomoto, J. Otsuki, M. Wallerberger, T. Wang, K. Yoshimi, arXiv:2106.12685

IR basis and sparse modeling may be combined with other techniques such as ML!
I am open to interdisciplinary research! h.shinaoka@gmail.com

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Review2: arXiv:2106.12685