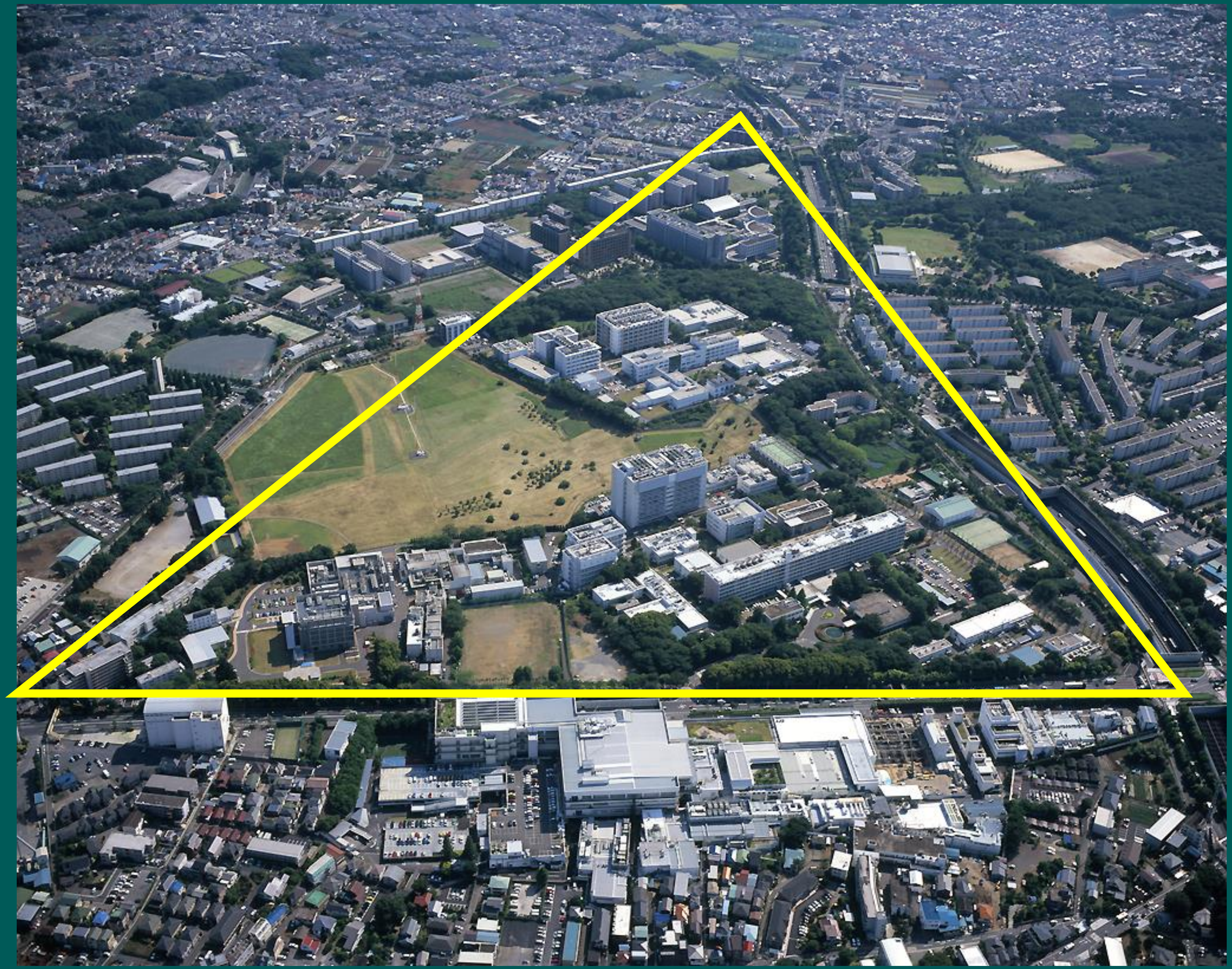
Analytic continuation. New philosophy: well-posed questions for ill-posed problem

RIKEN
Center for Emergent Matter Science
(CEMS)

理化学研究所 RIKEN

RIKEN, CEMS



A. S. Mishchenko
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Analytic continuation. New philosophy: well-posed questions for ill-posed problem

Andrey S. Mishchenko
RIKEN CEMS
(Center for Emergent Matter Science)

1. **Analytic continuation. Introduction.**

2. **Why difficult and why "ill-posed"?**

3. **The superior goal is to obtain solutions dictated SOLELY by the data, not corrupted by "useful constraints (regularization…)"**

4. **Why stochastic approach is the best? No apparent regularization for any of multiple solutions.**

5. **New philosophy. All solutions are the best! Playing linear combinations, each is the best solution too.**

Connection of many-body Monte Carlo approaches to real world.

Exact method

REAL QUANTITY

$$G_{\mathbf{k}}(\tau) = \int_0^{\infty} d\omega \, L_{\mathbf{k}}(\omega) \, e^{-\omega\tau}$$

MANY problems

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

In theoretical physics

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

$$\boxed{K(\tau_m,\omega) = \frac{1}{\pi}\frac{\omega \exp(-\tau_m \omega)}{1-\exp(-\beta\omega)}}$$

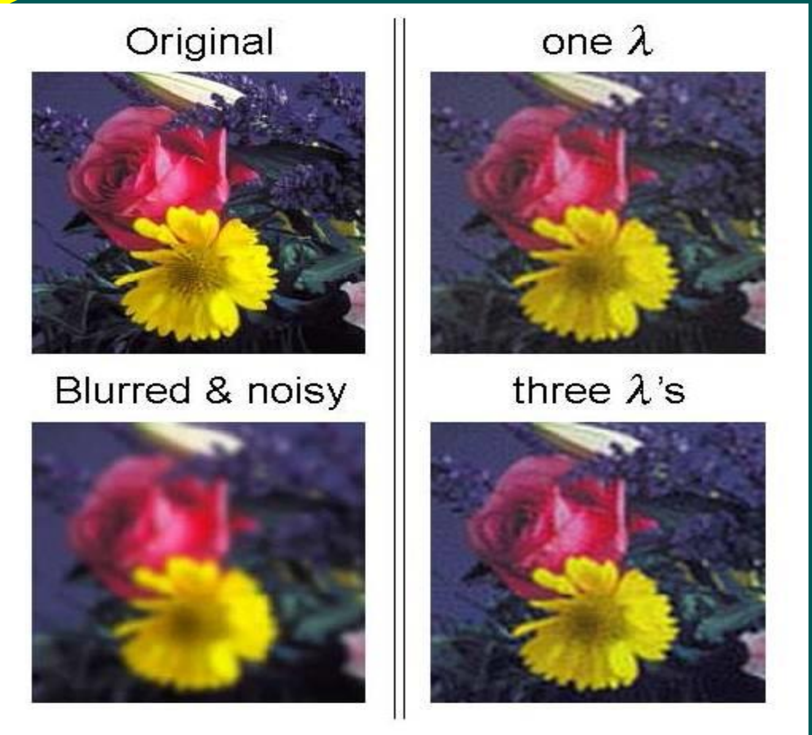
And
in real
life

Image deblurring

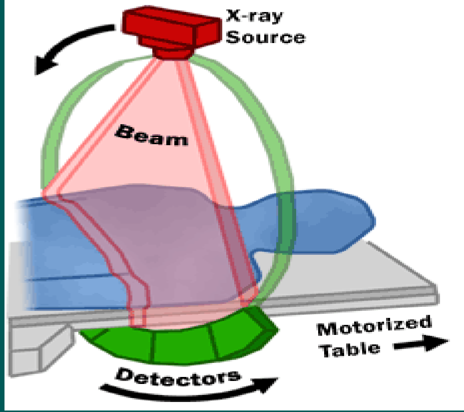
$$G(m) = \int_{-\infty}^{\infty} d\omega \; K(m,\omega) \; A(\omega)$$

m and ω are 2D vectors

K(m,ω) is a 2D x 2D noise distributon function



Medical tomography: MRI



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

m and ω are 2D vectors

K(m,ω) is a 2D x 2D distribution function

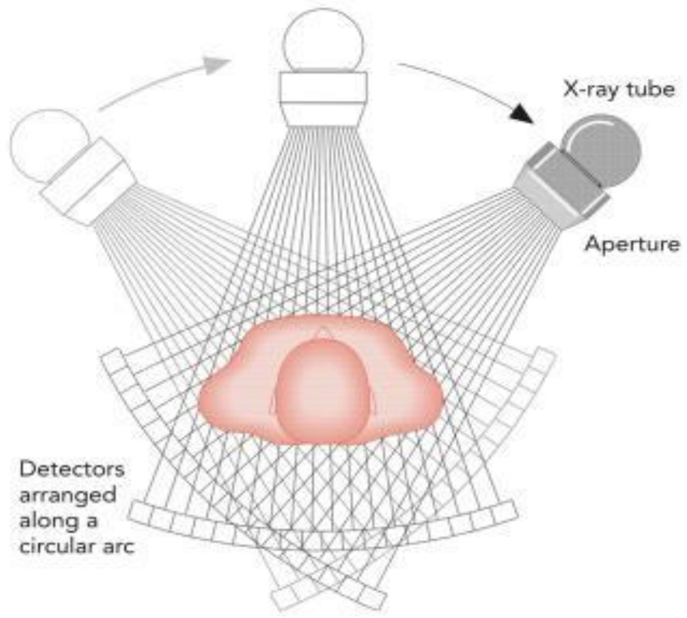


Figure 7-10 Computer tomography

Ill defined problem

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

Aircraft stability

Nuclear reactor

Maps

etc…

Ill defined problem

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

Aircraft stability

Nuclear reactor

Maps

etc…

What is the problem?

Ill defined problem

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

1. No exact solution due to noise (even processor floating point operations)

2. No exact solution et al!!!!!!!!!!

Ill defined problem

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

What to do?

1. No exact solution due to noise (even processor floating point operations)

2. No exact solution et al!!!!!!!!!!

Ill defined problem

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

What to do?

BEFORE: one search for a SINGLE approximate solution which is considered as being best by some artificially chosen criterion.

Ill defined problem

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

What to do?

BEFORE: one search for a SINGLE approximate solution which is considered as being best by some artificially chosen criterion.

Now: Each solution dictated by input data is “the best”. Let play with linear combination of “the best” solutions.

Ill defined

Another players:
CC, Pade, ….

Next player:
stochastic methods

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

Physics department:
Max Ent.
Pade approx...
Sparse …

Statistical department:
ridge regression

Engineering department:
Tikhonov Regularization

Ill defined

Another players:
CC, Pade, ….

Next player:
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$$G(m) = \int_{-\infty}^{\infty} d\omega \, K(m,\omega) \, A(\omega)$$

Physics department:
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Ill defined

Another players:
CC, Pade, ….

Next player:
stochastic
Methods
Of linear
combinations

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

Physics department:
Max Ent.
Pade approx...
Sparse …

Statistical department:
ridge regression

Engineering department:
Tikhonov Regularization

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

There is no exact solution!!!

$$G(m) = \sum_{n=1}^{N} \mathcal{K}(m,\omega_n) A(\omega_n) \;,\; m = 1, \ldots, M$$

Let us minimize!

Best solution?

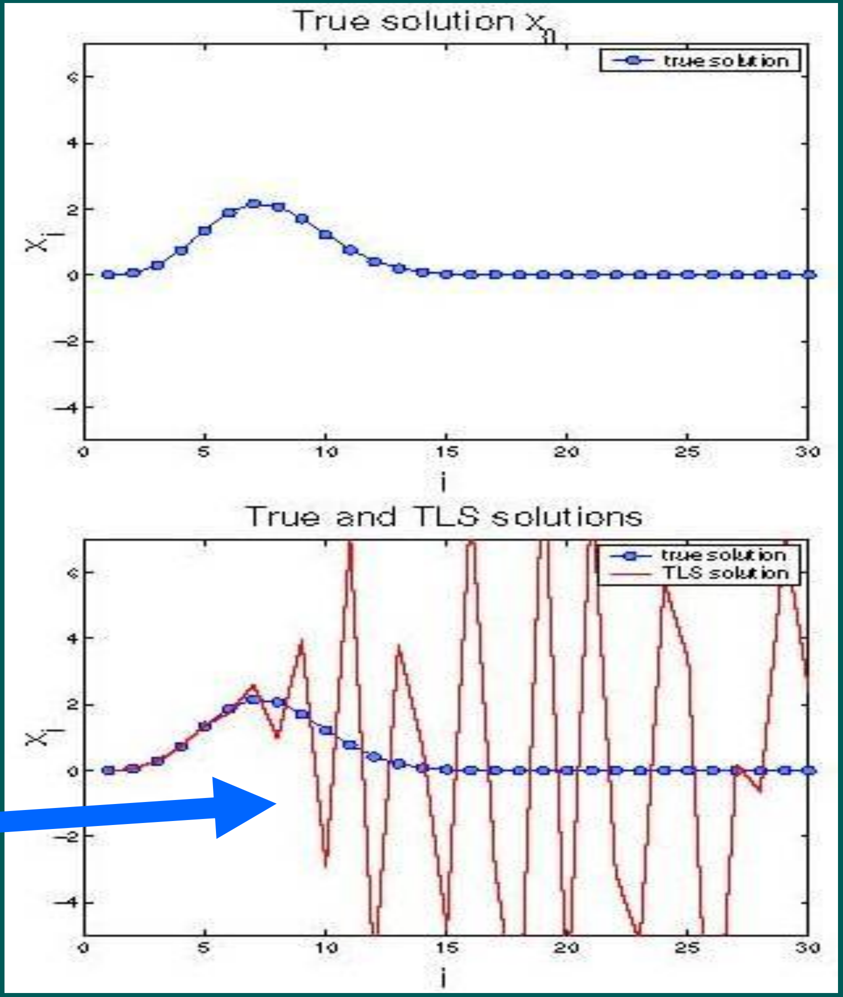
$$\| \widehat{\mathcal{K}} \vec{A} - \vec{G} \|^2 = \sum_{m=1}^{M} \left| \sum_{n=1}^{N} \mathcal{K}(m,\omega_n) A(\omega_n) - G(m) \right|^2$$

$$\| \hat{K}\vec{A} - \vec{G} \|^2 = \sum_{m=1}^{M} \left| \sum_{n=1}^{N} K(m,\omega_n)A(\omega_n) - G(m) \right|^2$$

Ill defined

Exact solution?!

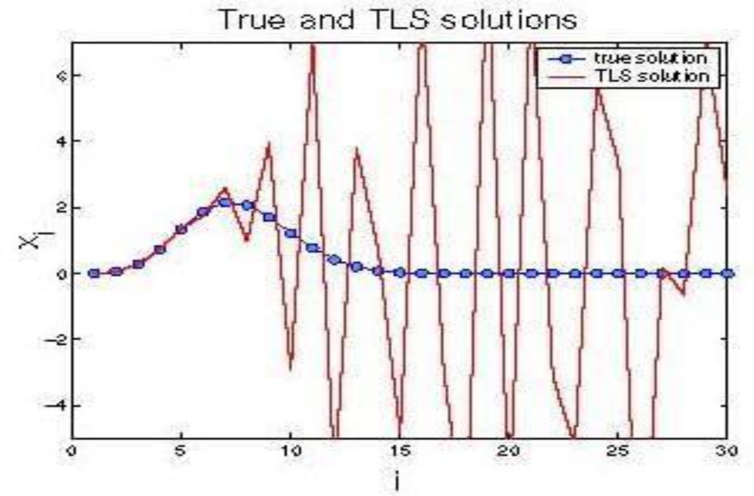
$$\boxed{\vec{A} = \sum_{i=1}^{r} \frac{\vec{u}_i^{\dagger} \otimes \vec{v}_i}{\sigma_i} \vec{G}}$$



Saw-tooth instability

$$\| \widehat{K}\vec{A} - \vec{G} \|^2 = \sum_{m=1}^{M} \left| \sum_{n=1}^{N} K(m,\omega_n)A(\omega_n) - G(m) \right|^2$$

+ Испортили



Tikhonov Regularization 1941 Moscow

$$\vec{A} = \sum_{i=1}^{r} \frac{\vec{u}_i^{\dagger} \otimes \vec{v}_i}{\sigma_i}\vec{G} \rightarrow \vec{A} = \sum_{i=1}^{r} \boxed{\left\{ \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2} \right\}} \frac{\vec{u}_i^{\dagger} \otimes \vec{v}_i}{\sigma_i}\vec{G}$$

REGULARIZATION

- In every scheme one minimizes not just

a |M| measure dictated by data but add some extra conditions which somehow corrupt the measure |M|

May schemes: cut of small eigenstates, filters, ban for large derivatives, - all methods CORRUPT RESULT

$$\| \widehat{K}\vec{A} - \vec{G} \|^2 = \sum_{m=1}^{M} \left| \sum_{n=1}^{N} K(m,\omega_n)A(\omega_n) - G(m) \right|^2$$

+F(A)

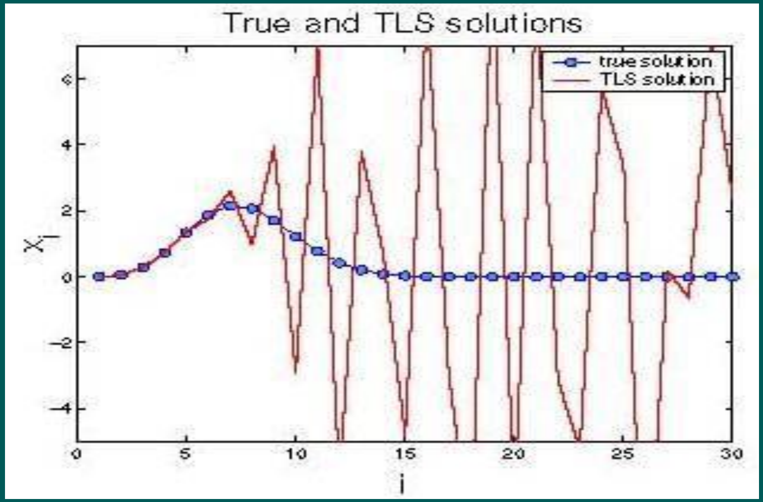
+ F(A)

Corrupted!!!!!

Tikhonov

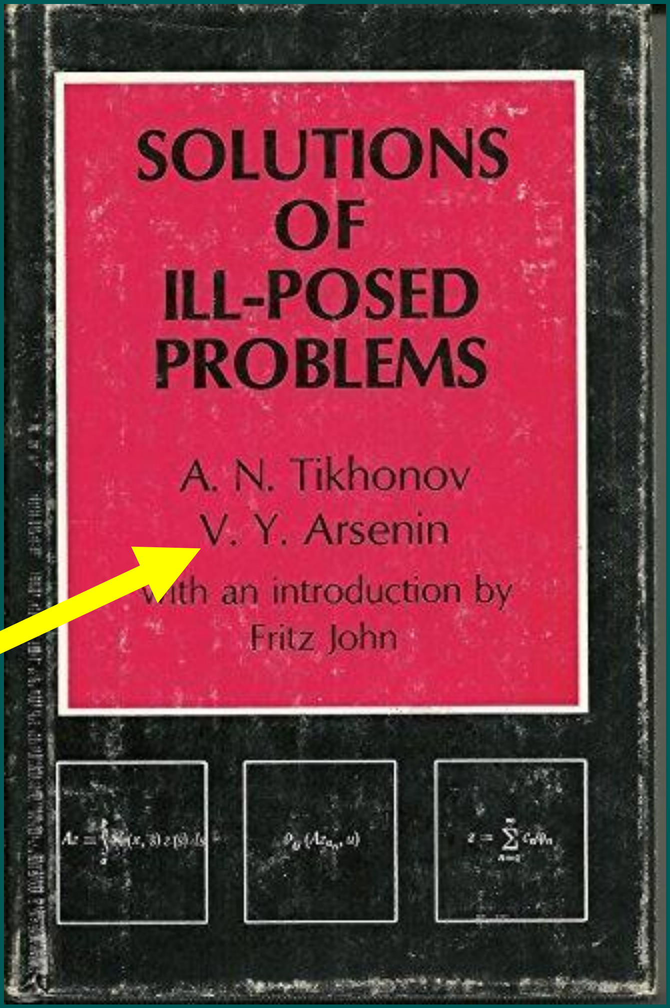
Regilarization

1941



$$\vec{A} = \sum_{i=1}^{r} \frac{\vec{u}_i^{\dagger} \otimes \vec{v}_i}{\sigma_i} \vec{G} \rightarrow \vec{A} = \sum_{i=1}^{r} \boxed{\left\{ \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2} \right\}} \frac{\vec{u}_i^{\dagger} \otimes \vec{v}_i}{\sigma_i} \vec{G}$$

All regularization methods are bad



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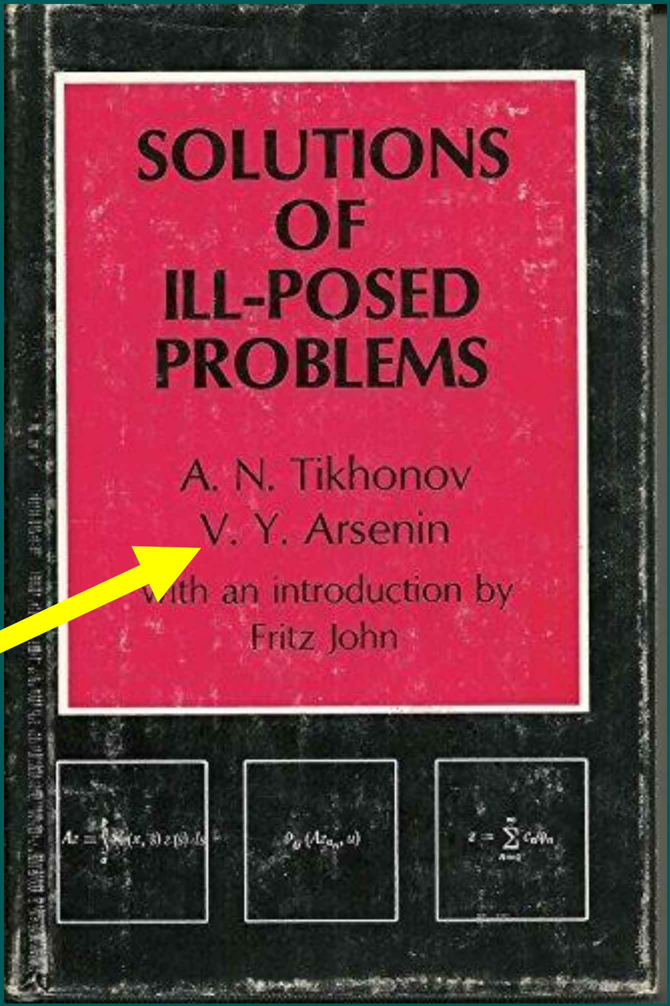
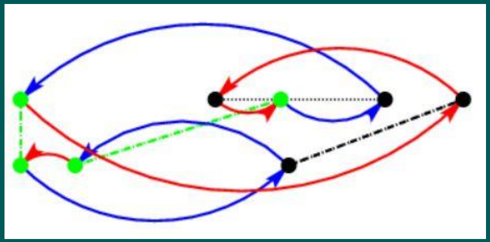
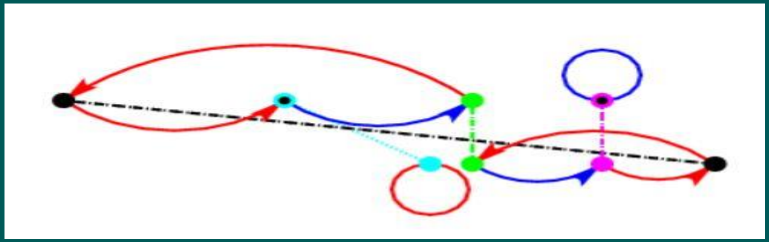


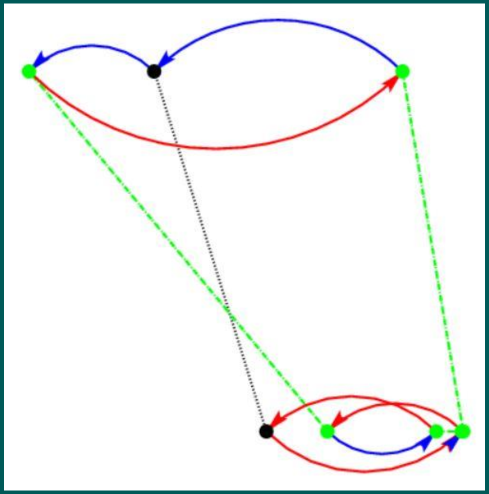
Let's avoid regularization!

Diagrammatic Monte Carlo

- Exact summation of Feynman diagrams for Green and correlation functions.





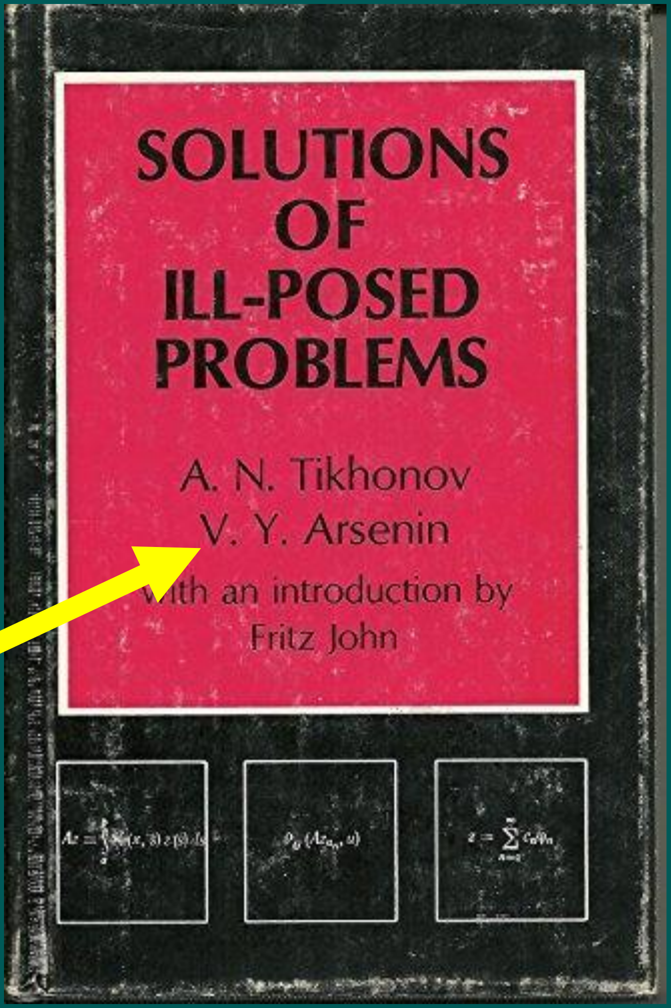


AM, Tupitsyn, Nagaosa, and Prokof'ev,
Scientific Reports 11, 9699 (2021)
AM, Pollet, Prokofev, Kumar, Maslov, and Nagaosa,
Phys. Rev. Lett., 123, 076601 (2019)
AM, Nagaosa, and Prokof'ev,
Phys. Rev. Lett. 113, 166402 (2014).

Simons Collaboration

Exact: but on imaginary time or Matsubara frequencies

All regularization methods are bad



Let's avoid regularization!

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- Chose configuration (no predefined parametrization)

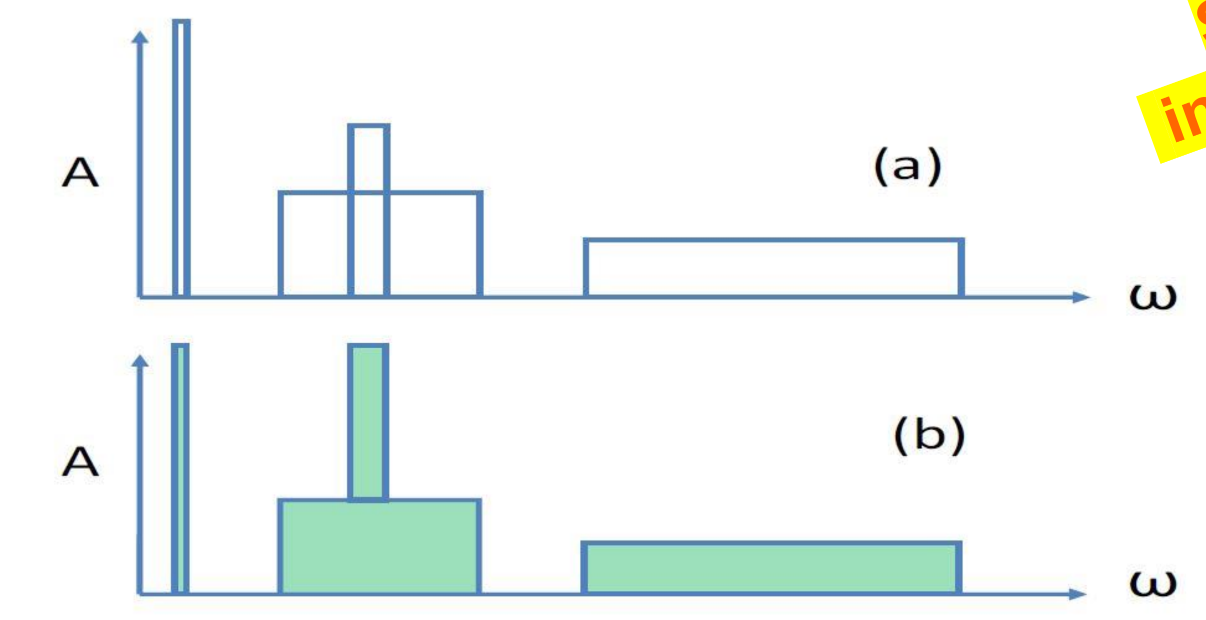

Fig. 2: *An example of configuration with $K = 4$. Panel (b) shows how the intersection of rectangles in panel (a) is treated.*

Statistical independence

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- Chose configuration
- Naive measure minimization

Statistical independence

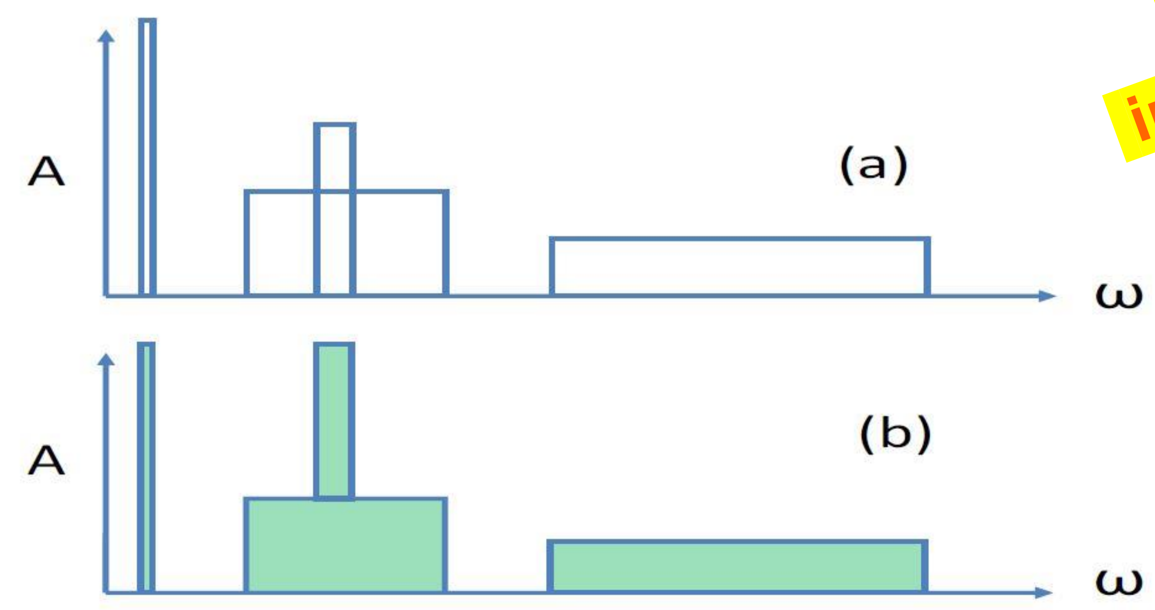
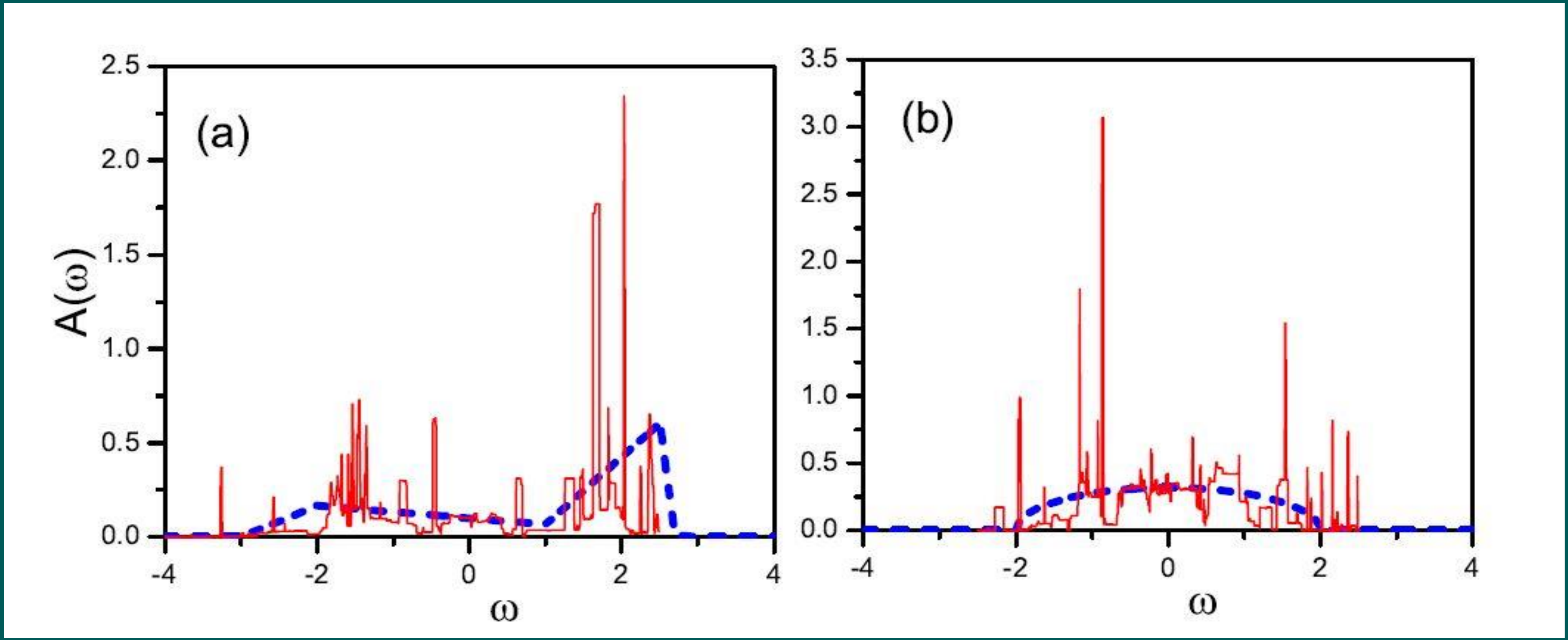


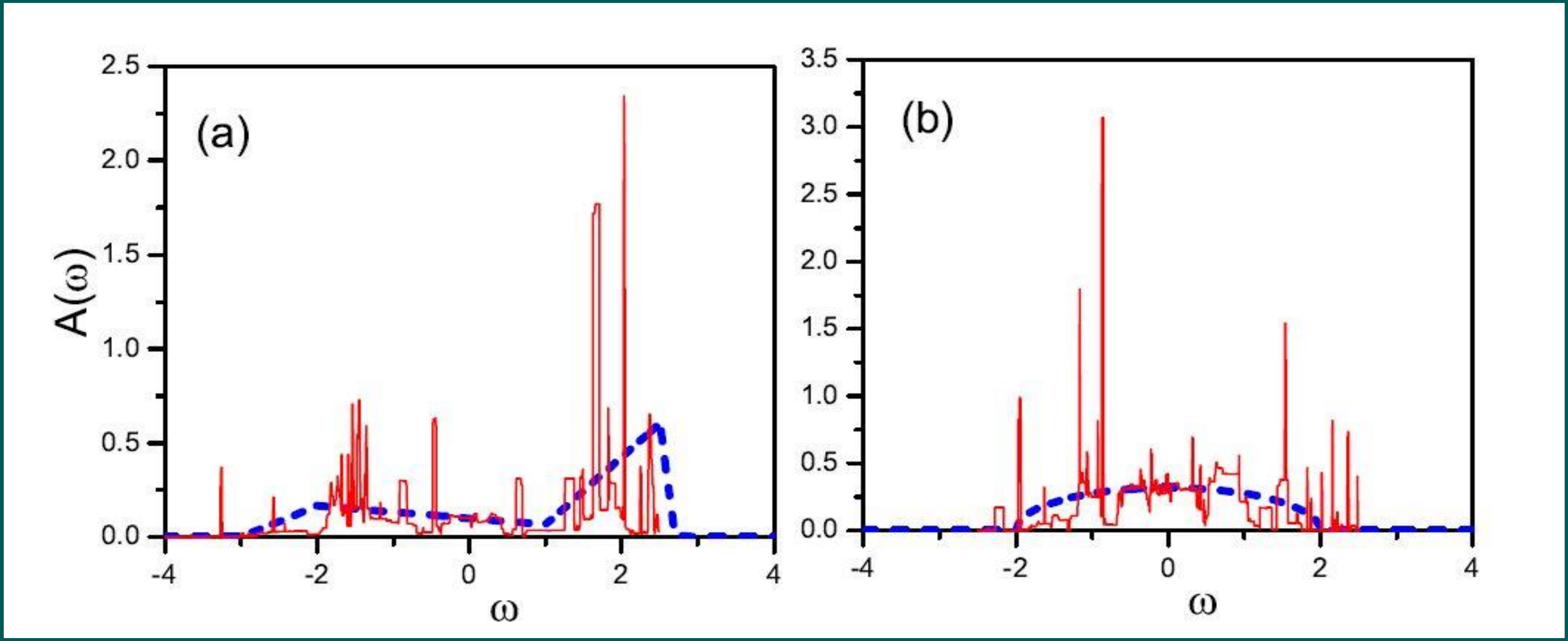
Fig. 2: *An example of configuration with $K = 4$. Panel (b) shows how the intersection of rectangles in panel (a) is treated.*

- We get Saw tooth instability (STI)



Indeed, regularization is to fight the STI.

- We get Saw tooth instability (STI)
- Chose another initial configuration and again get STI



Indeed, regularization is to fight the STI.

STI decreases when average solutions even when every solution is with STI!

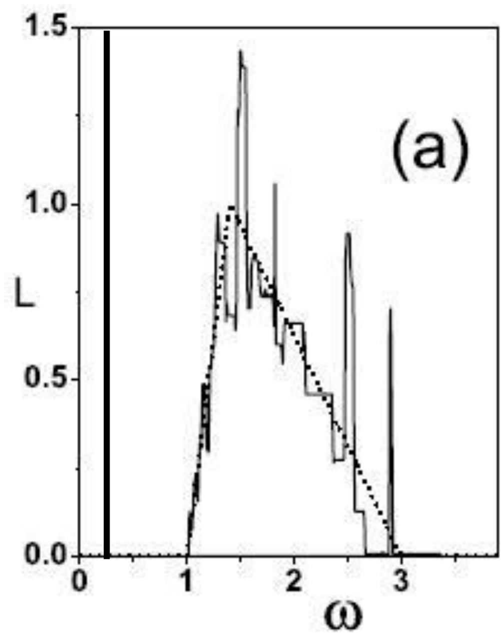
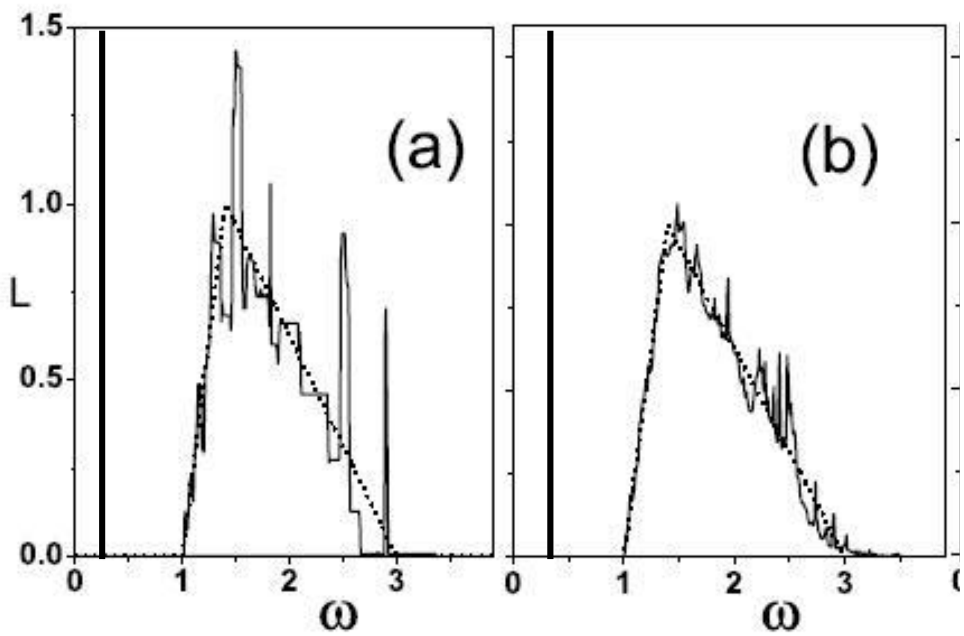


Fig. 7. Comparison of the actual spectral function (dashed line) with the results of spectral analysis after averaging over (a) $M = 4$, (b) $M = 28$, and (c) $M = 500$ particular solutions.

STI decreases when average solutions even when every solution is with STI!



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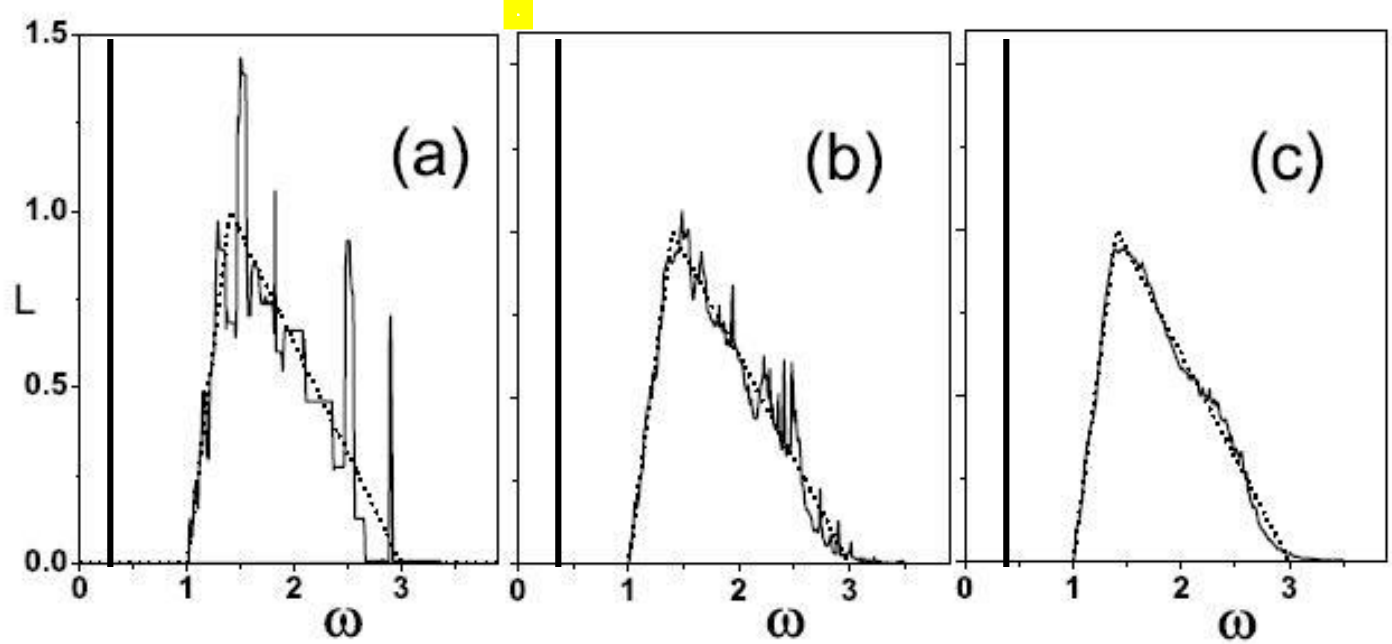


Fig. 7. Comparison of the actual spectral function (dashed line) with the results of spectral analysis after averaging over (a) $M = 4$, (b) $M = 28$, and (c) $M = 500$ particular solutions.

No regularization in each solution – it is dictated by data only!!

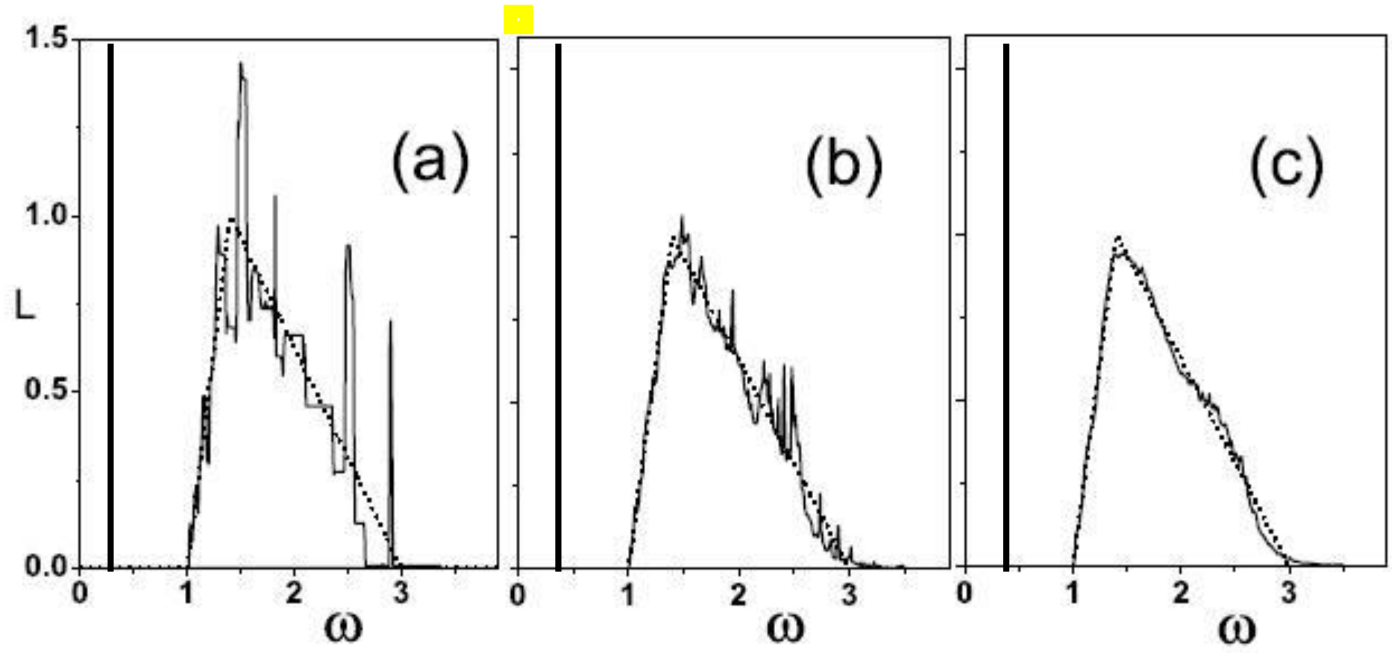
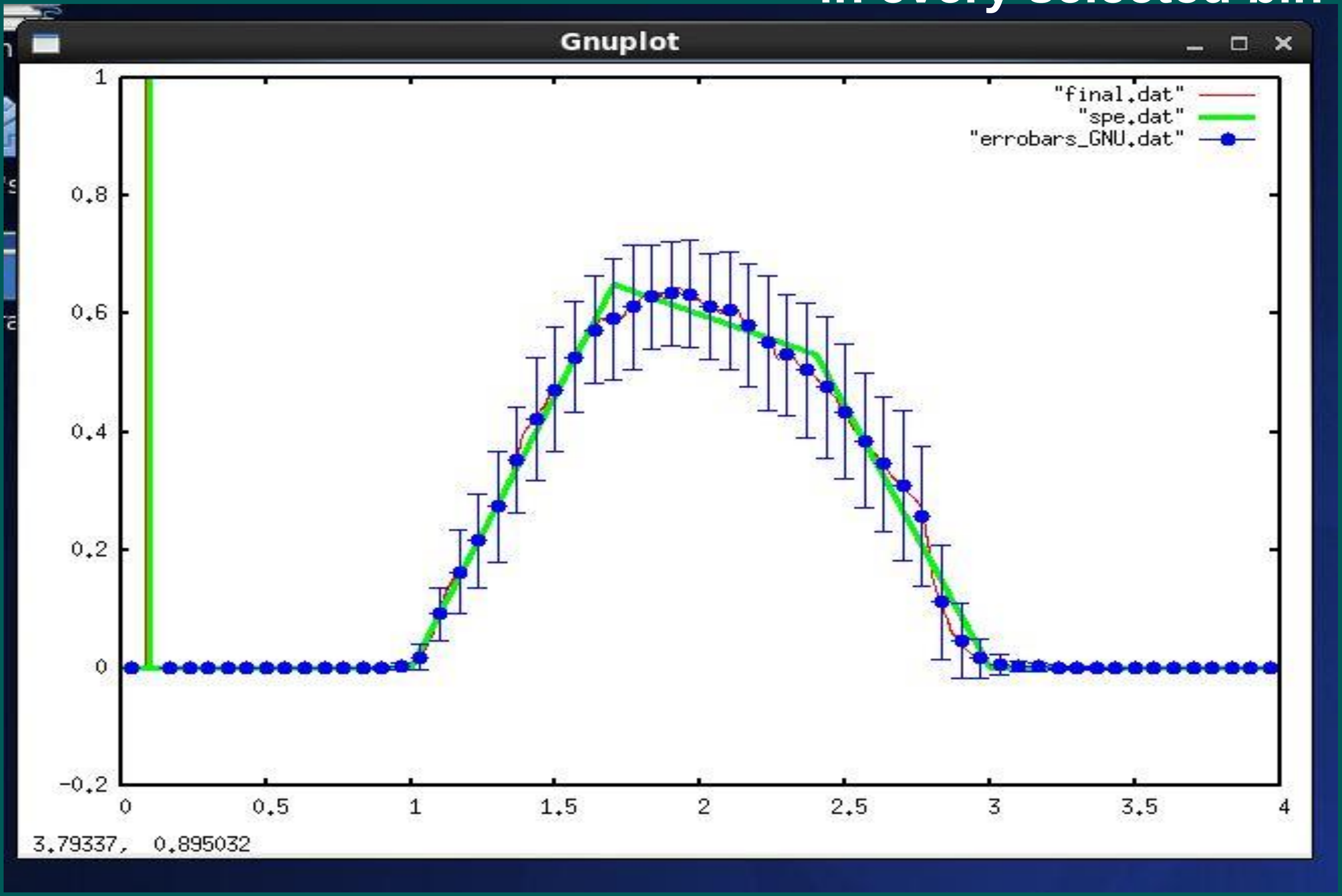


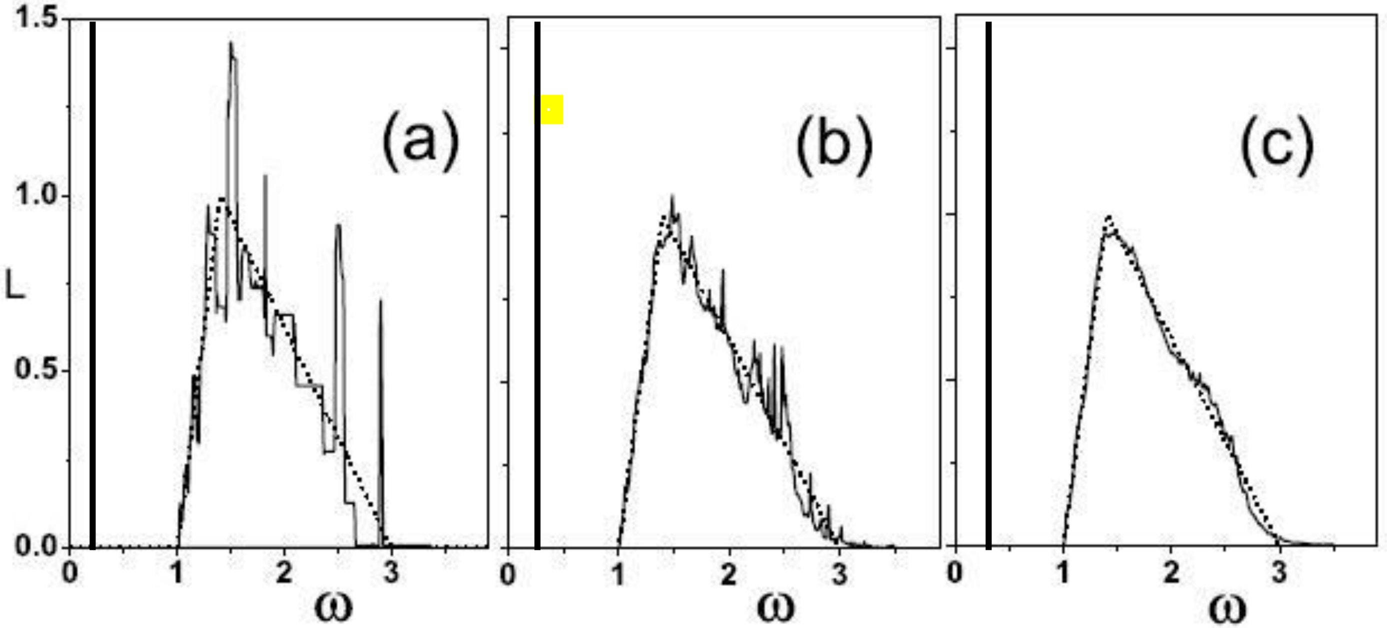
Fig. 7. Comparison of the actual spectral function (dashed line) with the results of spectral analysis after averaging over (a) $M = 4$, (b) $M = 28$, and (c) $\boxed{M = 500}$ particular solutions.

Errorbars estimate

Expectation and standard deviation in every selected bin



Self-averaging of the saw-tooth noise.



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AM, N.V. Prokof'ev, A. Sakamoto and B.V. Svistunov: Diagrammatic quantum Monte Carlo study of the Frohlich polaron, Phys. Rev. B, 62, 6317-6336, (2000)

AM: Stochastic optimization method for analytic continuation, contribution to "Correlated Electrons: From Models to Materials", ed. by E. Pavarini, W. Koch, F. Anders and M. Jarrell, pp. 14.1-14.28, (Forschungszentrum Julich GmbH, Julich, 2012).

Many solutions.
All are the best!!!

$$R_i(x)$$

We are not going to chose the best. All are the best.

O. Goulko, AM, L. Pollet, N. Prokof'ev, and B. Svistunov: Numerical analytic continuation: answers to well-posed questions, Phys. Rev. B 95, 014102 (2017).

Many solutions.
All are the best!!!

- $F(x) = \sum_i (1/N)\, R_i(x)$

Average – the simplest way

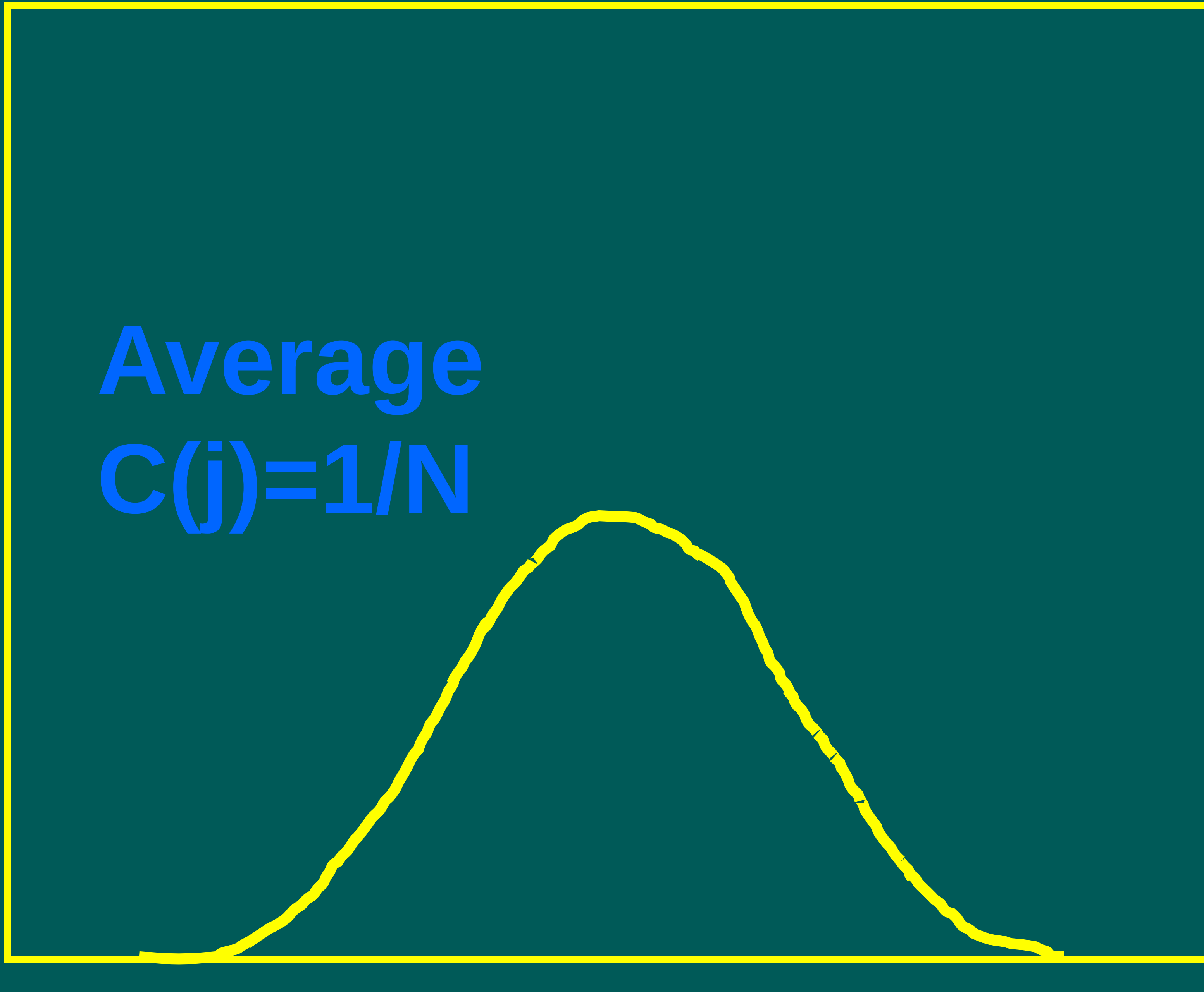
Many solutions.
All are the best!!!

- $F(x) = \sum_i C(i)\, R_i(x)$

Let's play?

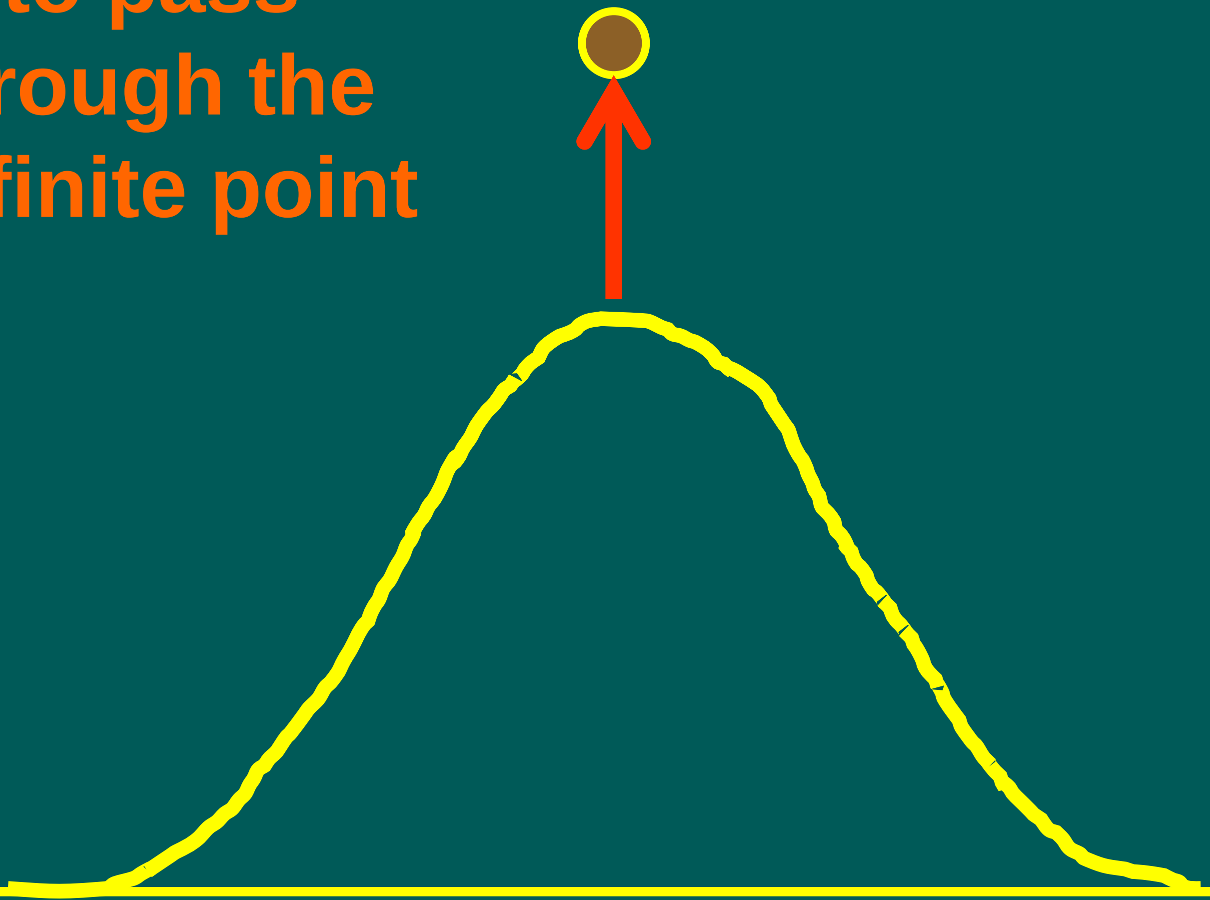
$\sum_i C(i) = 1$

A



A

Let change C(j) to pass through the definite point

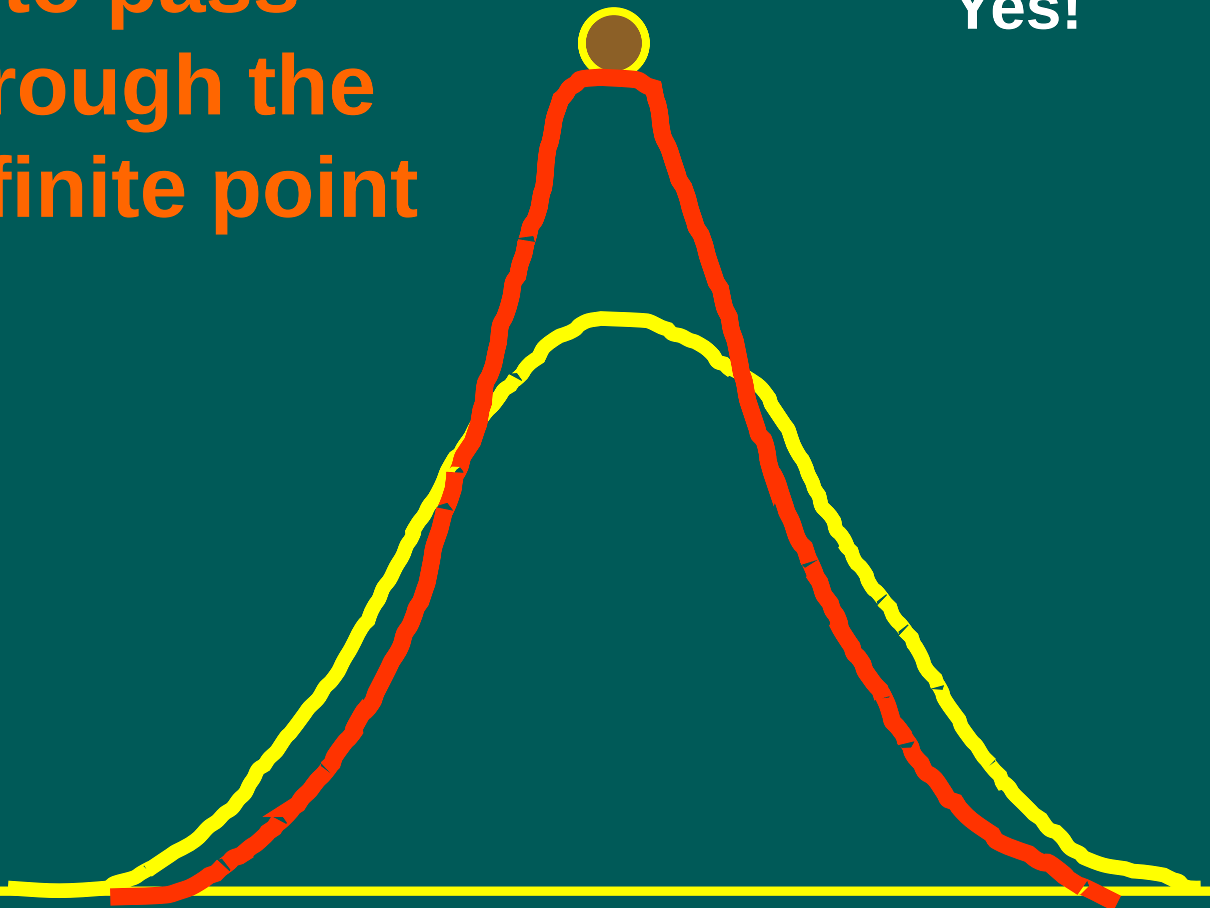


A

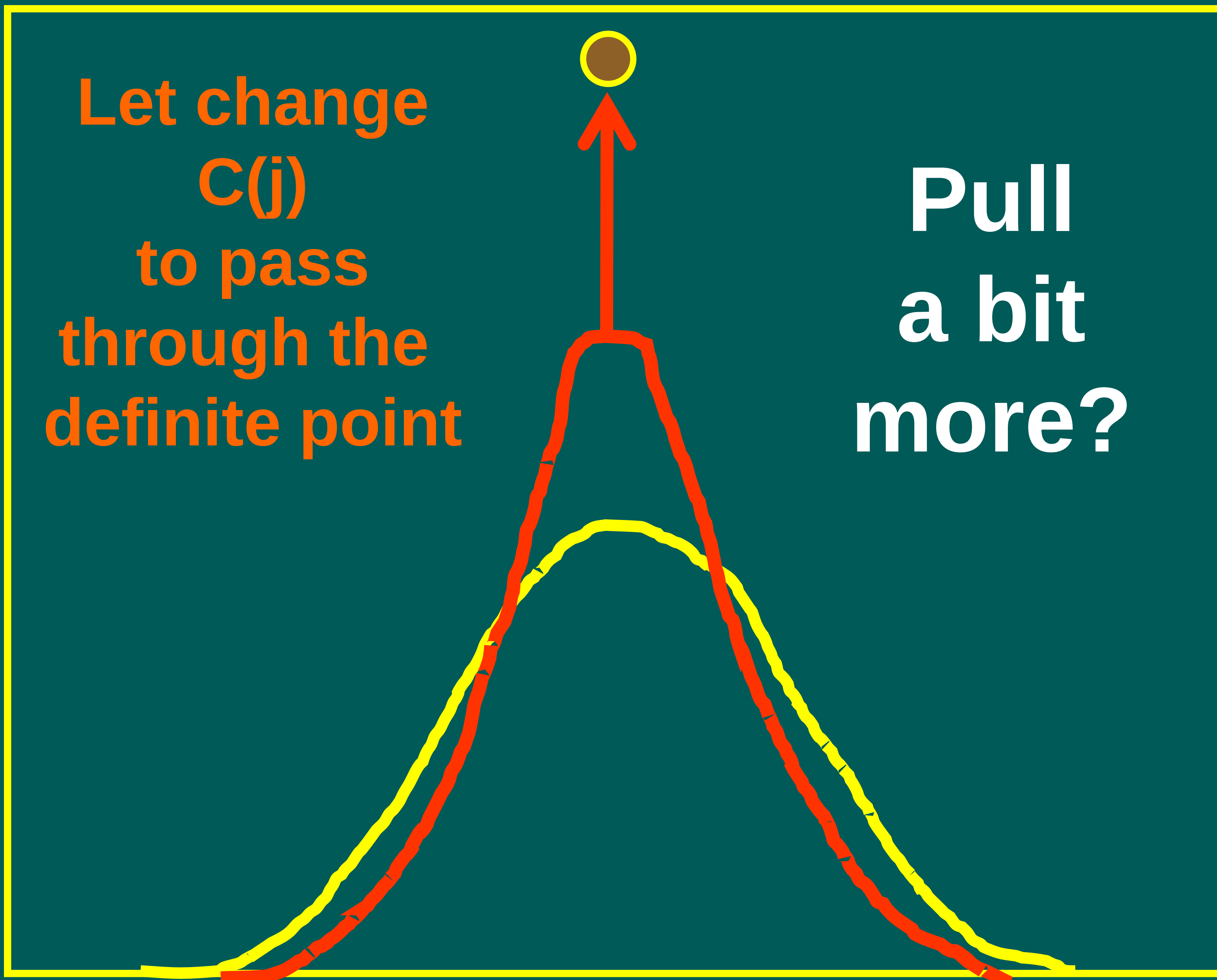
Let change C(j) to pass through the definite point

Good?

Yes!

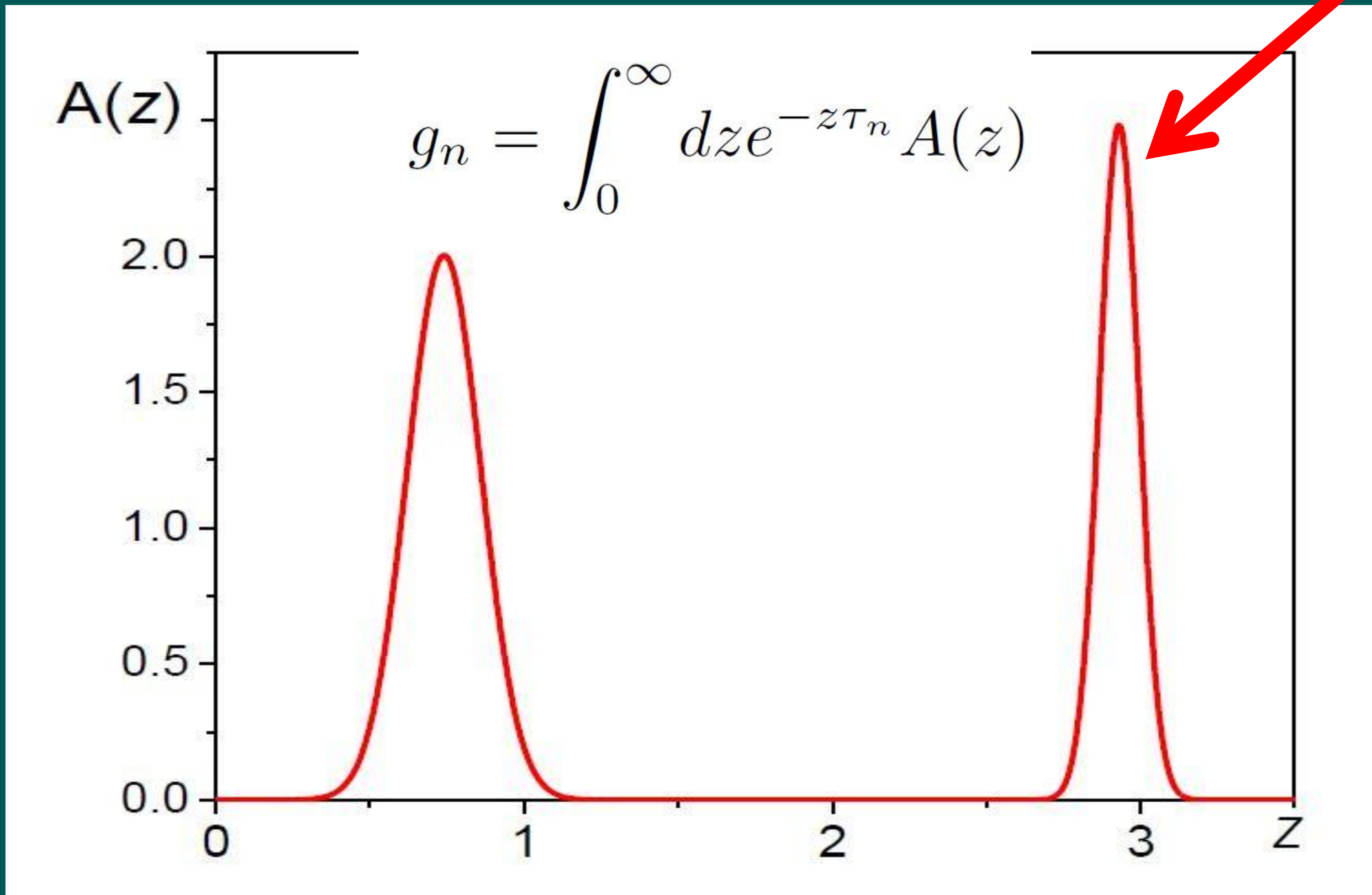


A


Let change
C(j)
to pass
through the
definite point
Pull
a bit
more?


A
GOOD?
NOT
GOOD!
Pull
a bit
more?
Extra
structures

Blind tests: how much we can say about second peak



O. Goulko et al, Phys. Rev. B **95**, 014102 (2017)

Noise level δ=10^{-3}

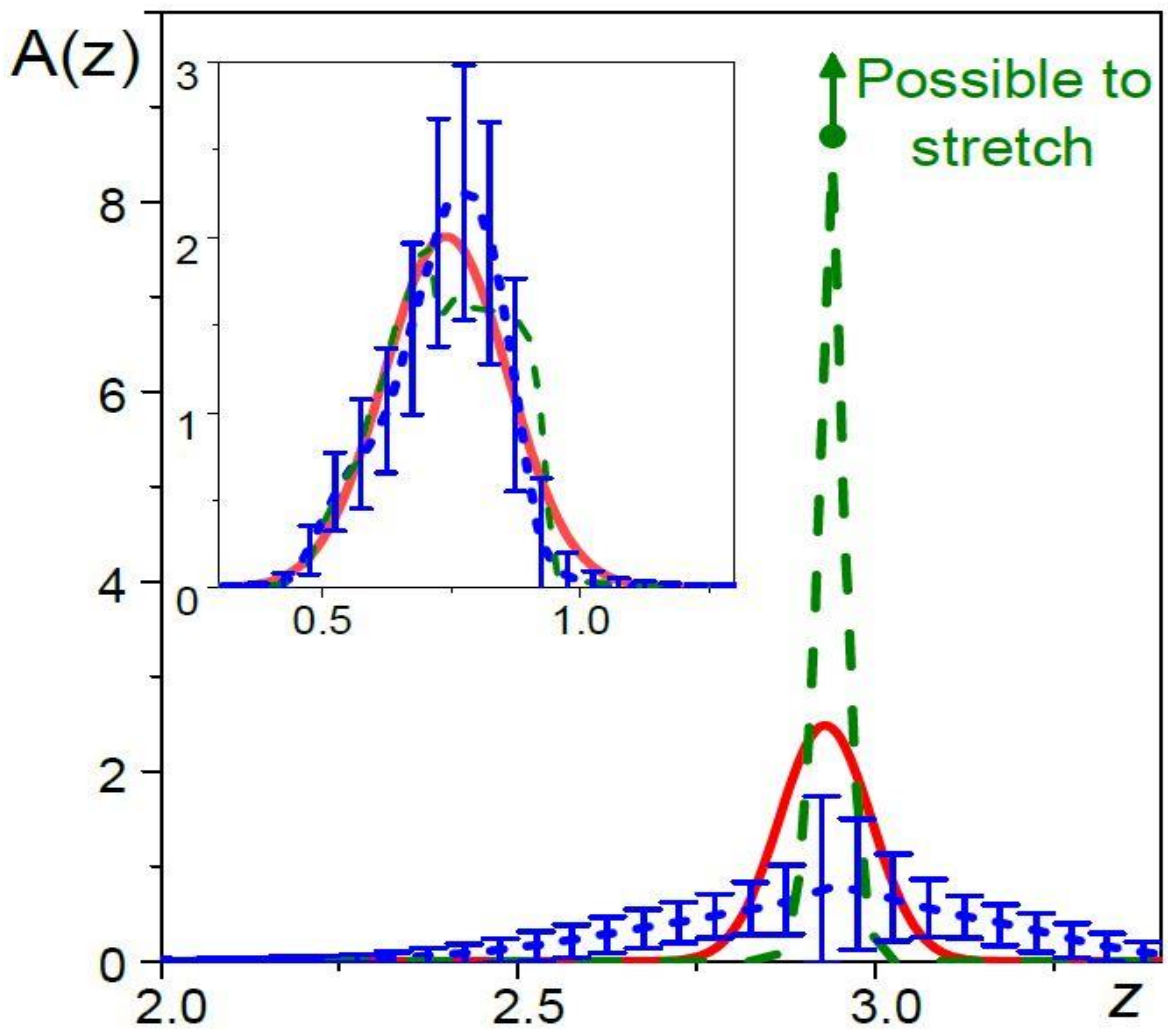


FIG. 3. (Color online.) Results for test 1, featuring two peaks of finite width with noise level 10^{-3}. Shown is the compari-

Noise level $\delta=10^{-5}$

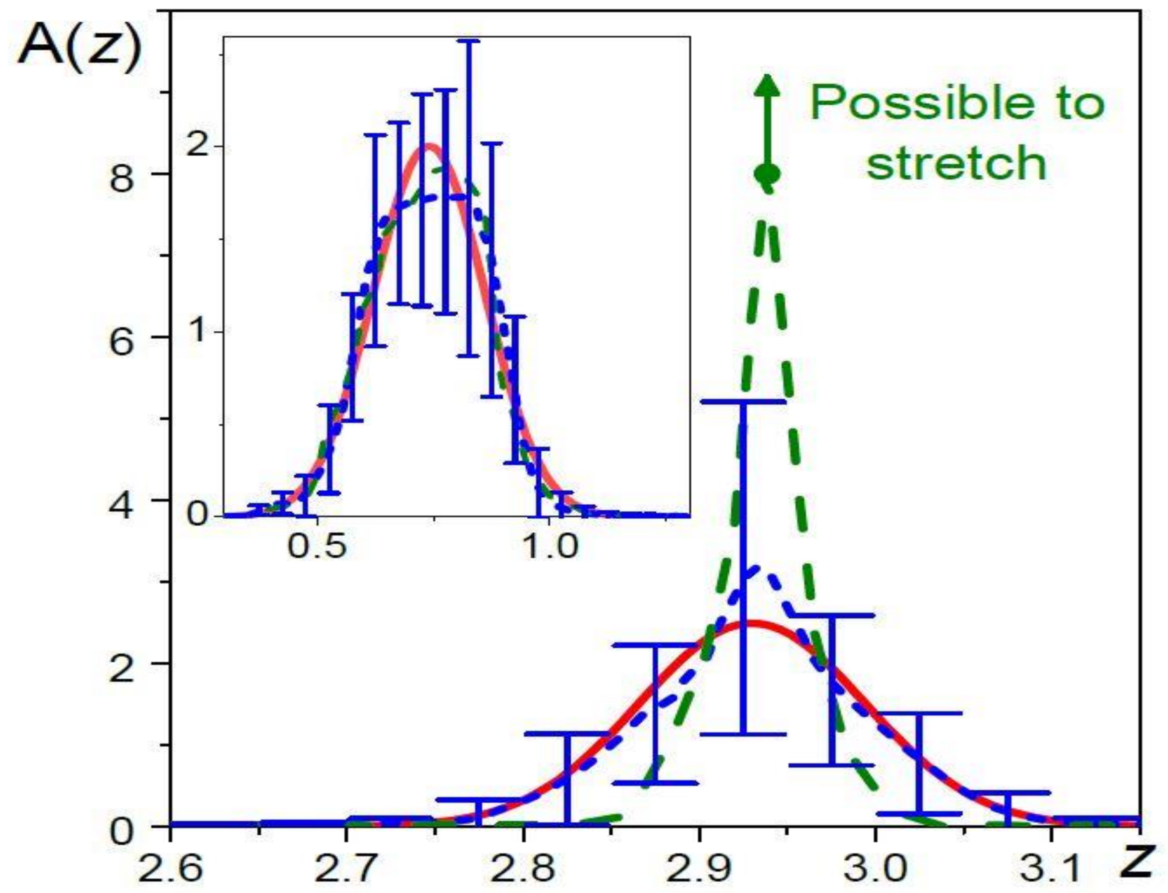


FIG. 6. (Color online.) Results for test 2, featuring two peaks of finite width with noise level 10^{-5}. Shown is the com-

Noise level δ=10^{-5}
First peak -> δ function

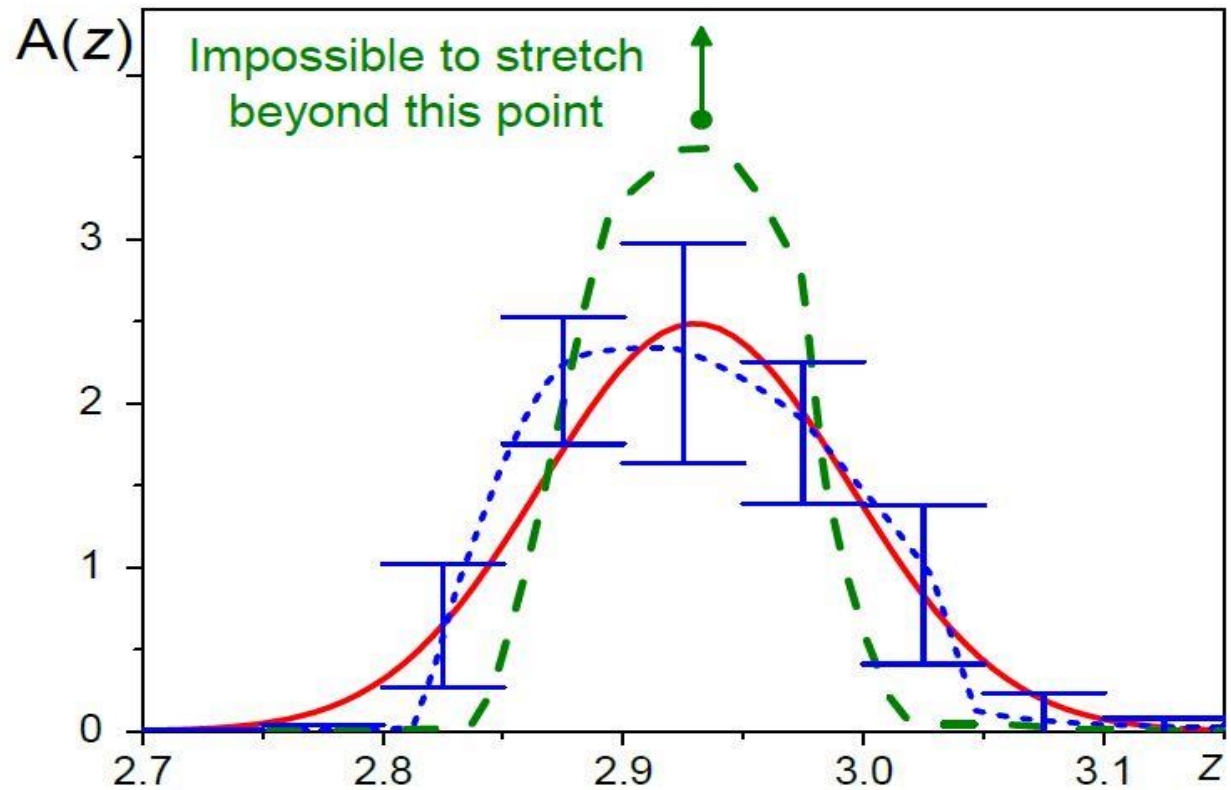


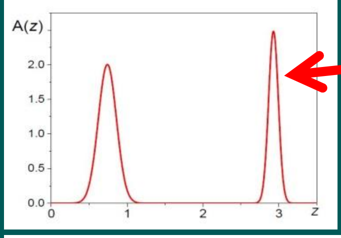
FIG. 8. (Color online.) Results for test 3, characterized by a δ-function at low frequency and a peak of finite width at high frequency with noise level 10^{-5}. Shown is the comparison be-

Conclusions. Numeric analytic continuation :
well posed answers to the ill posed problems.

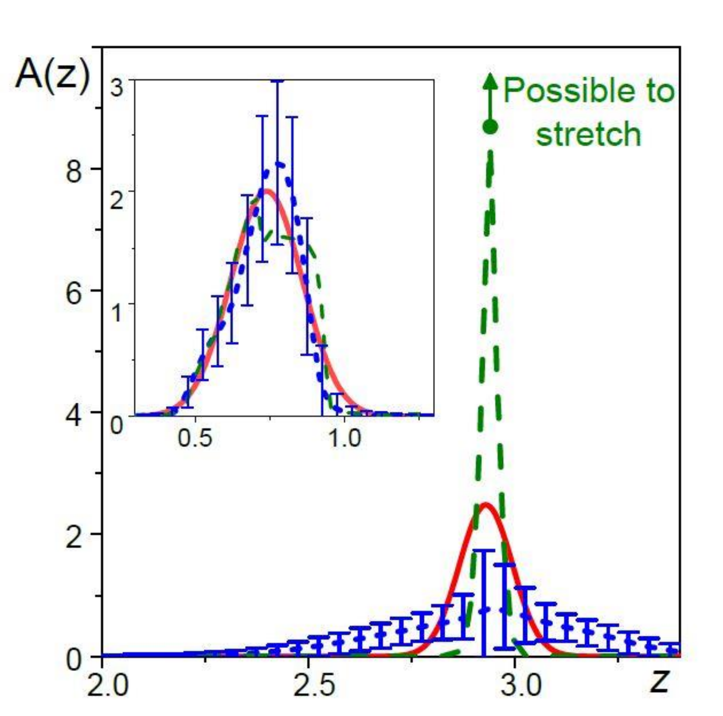
g_n – given MC data,
K[n,z] – known kernel

$$G[n,A] = \int dz\, K[n,z]\, A(z)$$

A(z) – spectral function to find



High energy peak



Objectives:

1.Stochastic optimization method (SOM) can quickly find a lot of [J>1000] solutions $\{A_j(z)\}$ each having good objective function (δ_n – error bars)

$$. .\ O_1 = \chi^2 = N^{-1}\sum_{n=1}^{N} [\ (g_n - G[n,A_j])/\ \delta_n\ ]^2 < \chi_c^2 = 1$$

Usually, final solution is obtained as average

$$\langle A(z)\rangle = J^{-1}\sum_{j=1}^{J} A_j$$

which removes saw tooth instability. However, one can search solution as

$$A_{fin}(z) = J^{-1}\sum_{j=1}^{J} c_j A_j \quad \text{where } \sum_{j=1}^{J} c_j = 1$$

where Cj<0 are possible untill $\chi^2 < \chi_c^2$.

Results

1. One can introduce one more part of objective function

$$O_5 = \sum_k\ T(k)[A_{fin}(z_k) - A_T(z_k)]^2$$

which characterizes deviation from target function $A_T(z)$.

2. It is legal to satisfy O_5 until $\chi^2 < \chi_c^2$.

3. This approach can verify which features of result are robust and which can be an artefact at given error bars δ_n. (see example where high energy peak can be made very narrow (green) or very wide (blue) in comparison with actual peak (red) without compromising the error bars). Hence, peak width is undefined.

O. Goulko et al, arXiv: 1609.01260

Stochastic approach

- 1. No corruption of data by regularization.

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- 2. Can list all possible solutions dictated solely by data.

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- 4. Why not invented before! No possibility to get thousands of independent solutions without modern computer facilities.

Stochastic Analytic Continuation

and Diagrammatic Monte Carlo

Phys. Rev. Lett., vol. 86, 4624 (2001) : Pseudo-Jahn-Teller polaron
Phys. Rev. Lett., vol. 87, 186402 (2001) : Exciton in semiconductors
Phys. Rev. Lett., vol. 91, 236401 (2003) : Optical conductivity of Frohlich polaron
Phys. Rev. Lett., vol. 93, 036402 (2004) : ARPES in high T_c cuprates
Phys. Rev. Lett., vol. 96, 136405 (2006) : Franck-Condon principle
Phys. Rev. Lett., vol. 99, 146405 (2007) : Nonlocal el-ph in high T_c cuprates
Phys. Rev. Lett., vol. 99, 226402 (2007) : ARPES in high T_c cuprates
Phys. Rev. Lett., vol. 100, 166401 (2008) : Optical conductivity in high T_c cuprates
Phys. Rev. Lett., vol. 101, 116403 (2008) : Exciton-polaron in semiconductors
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Phys. Rev. Lett., vol. 105, 266605 (2010) : SSH polaron in organic compounds
Phys. Rev. Lett., vol. 107, 076403 (2011) : Optical conductivity of Holstein polaron
Phys. Rev. Lett., vol. 109, 176402 (2012) : Time dependent Holstein-Hubbard
Phys. Rev. Lett., vol. 113, 166402 (2014) : Finite density polaron gas
Phys. Rev. Lett., vol. 114, 086601 (2015) : Conductivity in organic materials
Phys. Rev. Lett., vol. 114, 146401 (2015) : Mobility of Holstein polaron
Phys. Rev. Lett., vol. 123, 076601 (2019) : Mobility of Frohlich polaron

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Stochastic approach

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Thank you for attention

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- 2. Can list all possible solutions dictated
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  list all possible “best” solutions every of
  which is the best.
- 4. Why not invented before! No possibility to get thousands of independent solutions without modern computer facilities.