Analytic Continuation by Sobolev Method

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Linear response theory

tells you the transformation from spectral function to correlation function.

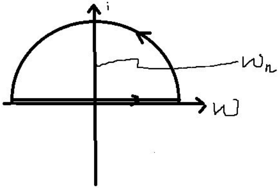
$$G(i\omega_n) = \int_{-\infty}^{\infty} d\omega' \frac{A(\omega')}{i\omega_n - \omega'} \tag{1}$$

where ω_n is a Matsubara frequency: $(2n+1)\pi/\beta$.

Analytic Continuation

From Kroma-Kronig Theorem we know that for a complex analytic function $\chi(\omega, \omega_n)$

$$\chi(0, \omega_n) = \frac{1}{i2\pi} P \int_{-\infty}^{\infty} \frac{\chi(\omega', 0)}{\omega' - i\omega_n} d\omega'$$



In comparison with equation1 we could see that these correlation function and spectral function all come from an analytic complex function G:

$$G(\omega_n) = G(0, \omega_n)$$

$$A(\omega) = -\frac{1}{2\pi} ImG(\omega, 0)$$

That's why we call it analytic continuation problem.

Discretization

The first thing: we need to transform the integration to a summation.

$$G(i\omega_n) = \sum_{i=-M}^{M} \frac{-1}{2\pi} \frac{A(\omega_i)}{i\omega_n - \omega_i} \Delta\omega_i$$

Sperate it into real part and imaginary part:

$$ReG = \frac{1}{2\pi} \sum_i \frac{\omega_i}{\omega_n^2 + \omega_i^2} A(\omega_i) \Delta\omega_i$$

$$ImG = \frac{1}{2\pi} \sum \frac{\omega_n}{\omega_n^2 + \omega_i^2} A(\omega_i) \Delta\omega_i = K_{ni} A_i$$

All the problems come from the matrix...

An example:

$$A(\omega) = \frac{1}{2}\left(e^{-\frac{1}{2}(\omega-4)^2}/\sqrt{2\pi} + e^{-\frac{1}{2}(\omega+4)^2}/\sqrt{2\pi}\right)$$

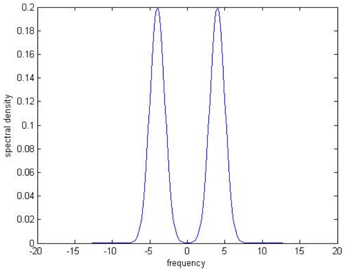


Figure: $A(\omega)$

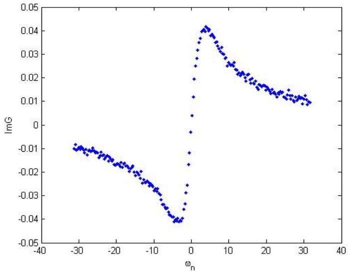


Figure: $G(i\omega_n)$

Let's do the inverse of the matrix...

$$K = UDU^{-1}$$

$$A = UD^{-1}U^{-1}ImG$$

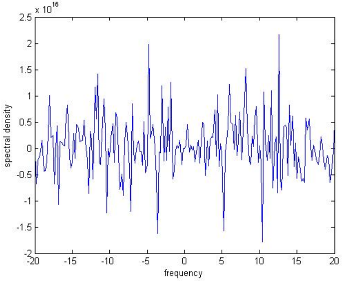


Figure: A(ω)

$$D = \begin{pmatrix} \lambda_1 & & & & \\ & \lambda_2 & & & \\ & & \ddots & & \\ & & & \sim 0 & \\ & & & & \sim 0 \end{pmatrix}$$

$ImG = K * f$

- This ill-conditioned matrix leave this problem ill-posed. There could be a large number of solutions that could fit the correlation data with in the error bars.

- Our goal is to find the most smooth solution among these candidates by adding some hypotheses or methods of evaluations.
- Stochastic-optimization method — taking average of large number of noisy solutions.
- Maximum Entropy method — the most likely function which maximizes the entropy of the system.
- Method of Consistent Constraint— smoothest curve respecting the error bars on correlation data.

Sobolev Method

So we need an objective which could evaluate not only the deviation from the data but also the smoothness of the fitting curves.

$$O = \sum_{n=0}^{N-1}\left(\frac{\sum_i K_{ni} f_i - ImG_n}{\sigma_n}\right)^2 + \sum_{j=0}^{M-1} A_j |f(\omega_j)|^2 \Delta\omega_j$$
$$+\lambda\left\{\sum_{j=1}^{M-2}\left[\left(\frac{f_{j+1}-f_{j-1}}{2\Delta\omega_j}\right)^2 \Delta\omega_j + \frac{4}{\Delta\omega_j^3}\left(f_j - \frac{f_{j+1}+f_{j-1}}{2}\right)^2\right]\right\} \quad (2)$$

We call it Sobolev method because we choose the norm from Sobolev space

$$\left(\int |f|^2 d\omega + \int |f'|^2 d\omega + \int |f''|^2 d\omega\right)$$

to describe the roughness of the curves.

- We call these *As and* λ penalties because they limit the expansion and curvature of the solutions.
- The most smooth function is the one that minimizes the objective under appropriate penalties.
- The penalties are adjusted so that the

$$\chi^2 = \frac{1}{N}\sum_{n=0}^{N-1}\left(\frac{\sum_i K_{ni} f_i - ImG_n}{\sigma_n}\right)^2 \approx 1$$

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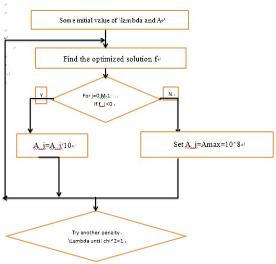


Figure: find the appropriate penalties through iterations and binary search

The optimized solution can be derived by the variational method.

$$\partial O/\partial f_j = 0 \qquad j = 0, 1, \ldots M-1 \tag{3}$$

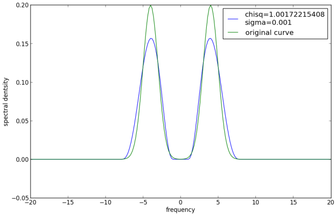
We can wrote these M equations into the form of matrix

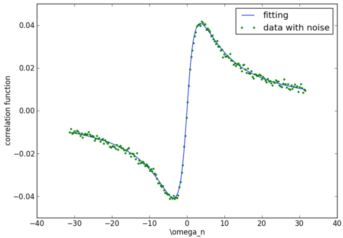
$$B * f = F^{\dagger} \begin{pmatrix} 1/\sigma_0^2 & & \cdots \\ & 1/\sigma_1^2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} ImG$$

where $F_{nj} = K_{nj} * \Delta\omega_j$ and

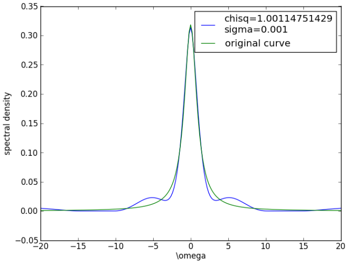
$$\begin{aligned} B \quad = \quad & F^{\dagger} \begin{pmatrix} 1/\sigma_0^2 & & \cdots \\ & 1/\sigma_1^2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} F + \begin{pmatrix} A_0\Delta\omega_0 & & \\ & A_1\Delta\omega_1 & \\ & & \ddots \end{pmatrix} \\ & +\lambda \begin{pmatrix} \frac{1}{4\Delta\omega_1} + \frac{1}{\Delta\omega_1^3} & -\frac{2}{\Delta\omega_1^3} & \cdots \\ -\frac{2}{\Delta\omega_1^3} & \frac{1}{4\Delta\omega_2} + \frac{1}{\Delta\omega_2^3} + \frac{4}{\Delta\omega_1^3} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \end{aligned} \tag{4}$$

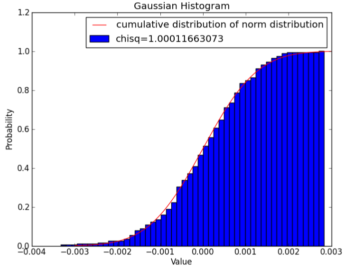
Double gaussian curve revisited

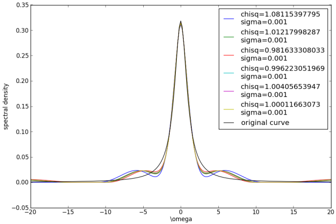




Loretzian Curve: $f = \frac{1}{\pi(1+\omega^2)}$



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chisq=1.01217998287
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sigma=0.001
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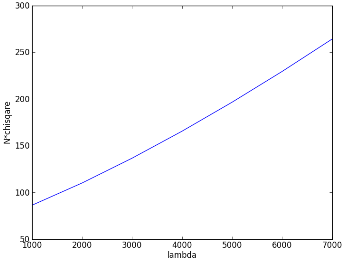
sigma=0.001
original curve
spectral density
\omega


N*chisqare
lambda

Problem unsolved and further plan

- How to define error of this method?
- Making comparison with the other method, for example MaxEnt method.
- Attack the real data, use it to analyze physical problems

Thanks for professor Emanuel Gull's instructions and help!