High precision spectral functions from discrete imaginary time Green's functions

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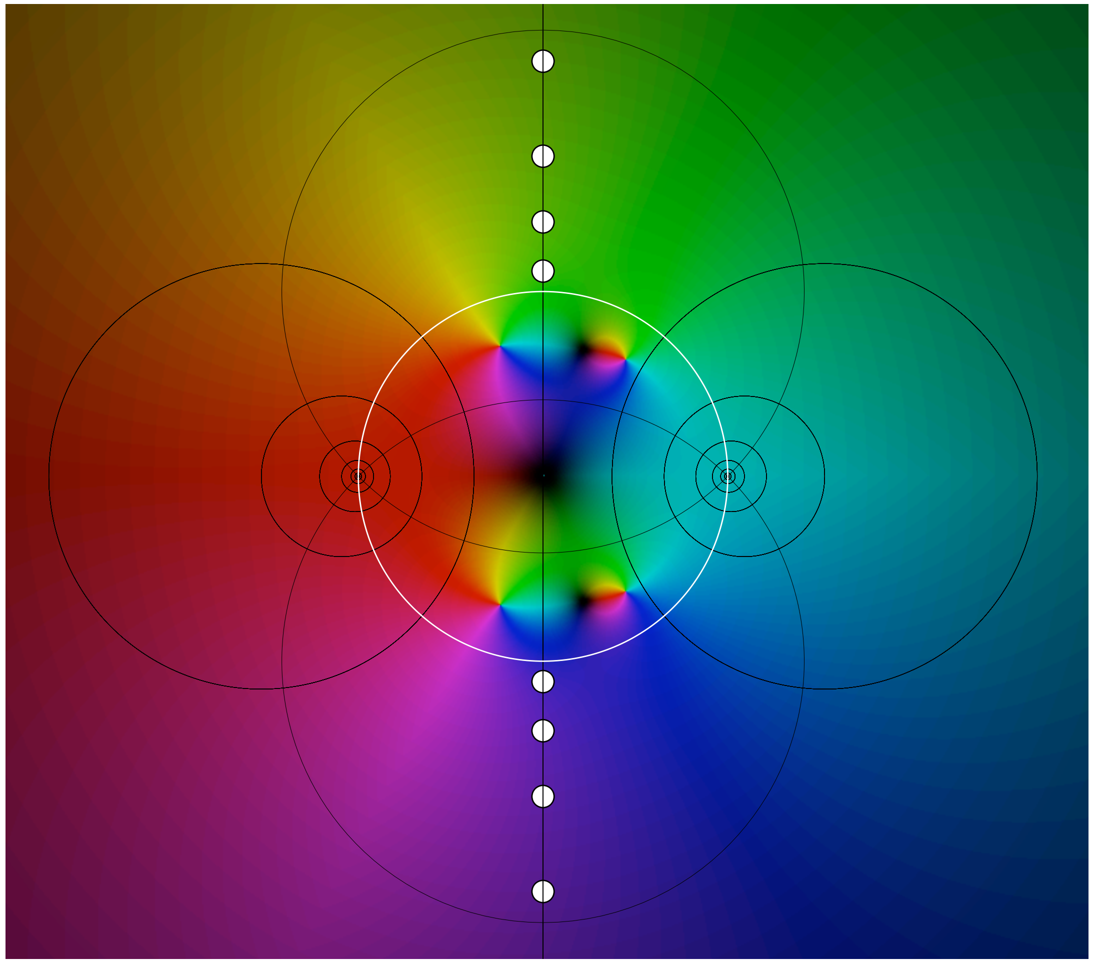

Collaborators:
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Bo Hellsing
Hugo Strand
Andro Sabashvili

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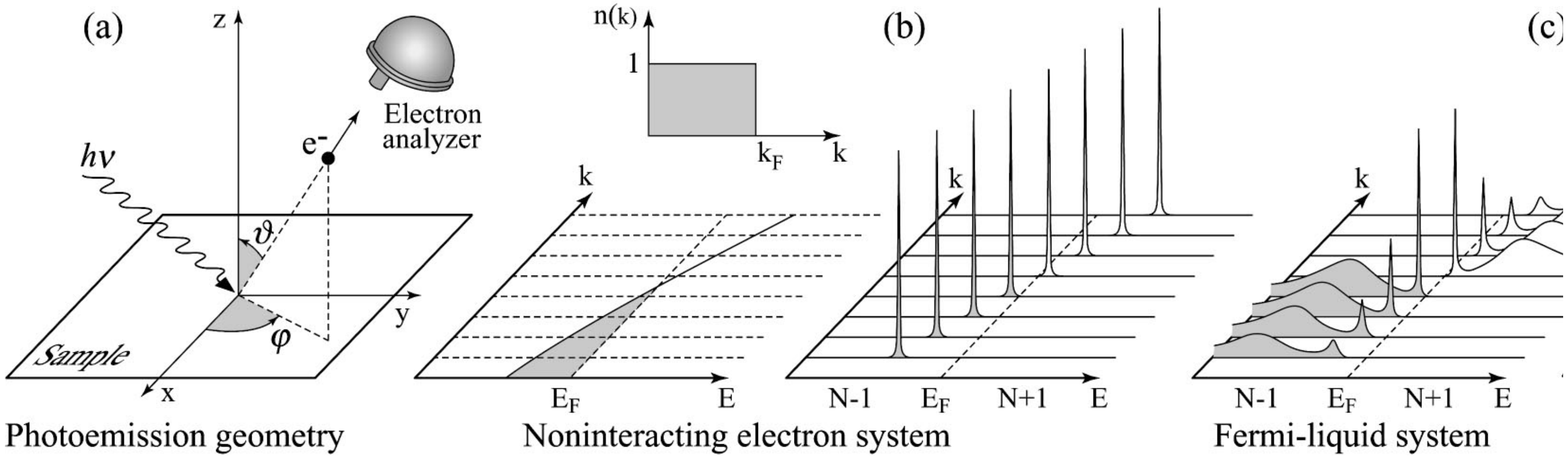
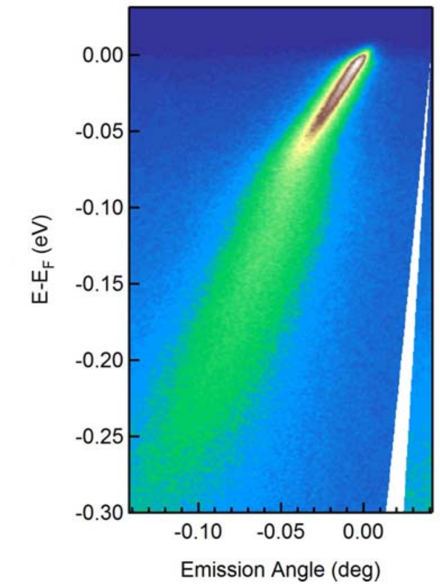
Spectral function



Damascelli, et al. Rev. Mod. Phys. 2003



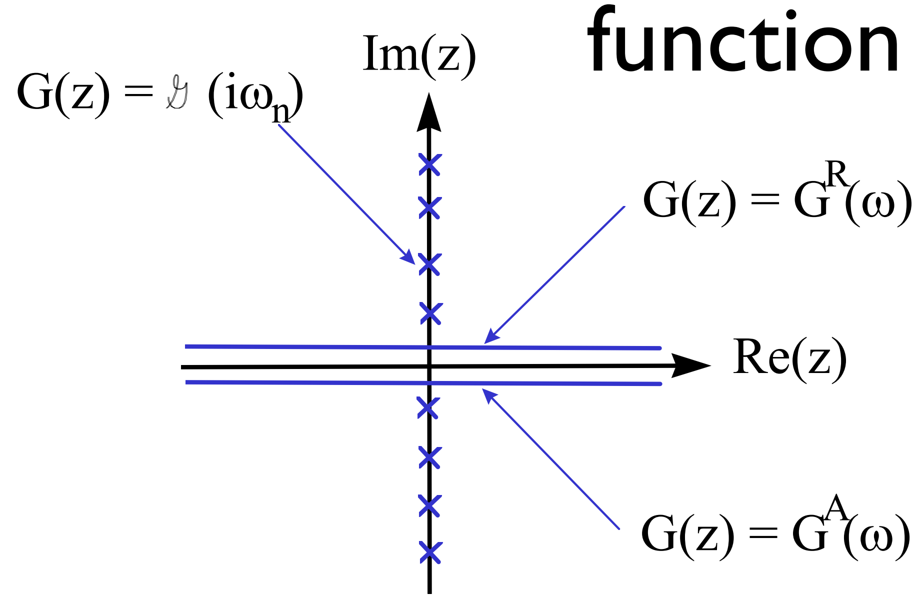
Z.X. Shen

Numerical challenge, find real frequency Green's function from Matsubara GF

$$G_k(\tau) = -<T(c_k(\tau)c_k^\dagger(0))>$$

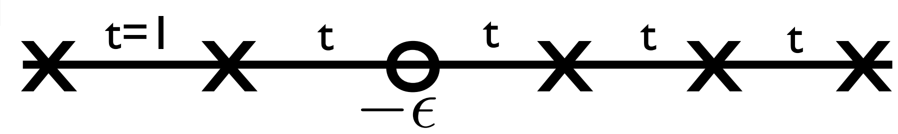
$$G_k(i\omega_n) = \int_0^\beta d\tau e^{i\omega_n\tau} G_k(\tau)$$

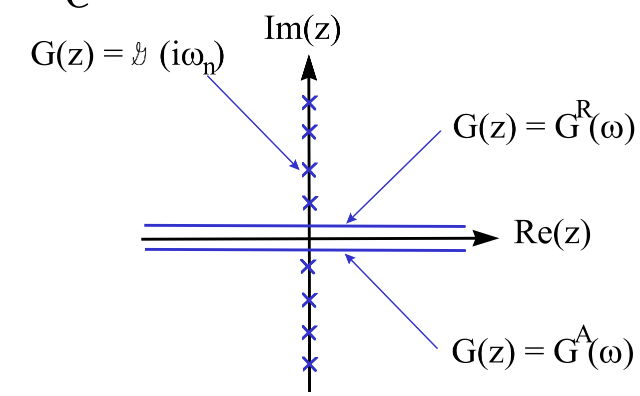
$$A_k(\omega) = -\frac{1}{\pi} Im G_k^R(\omega)$$



A.-M. Tremblay

Example: non-interacting Anderson impurity

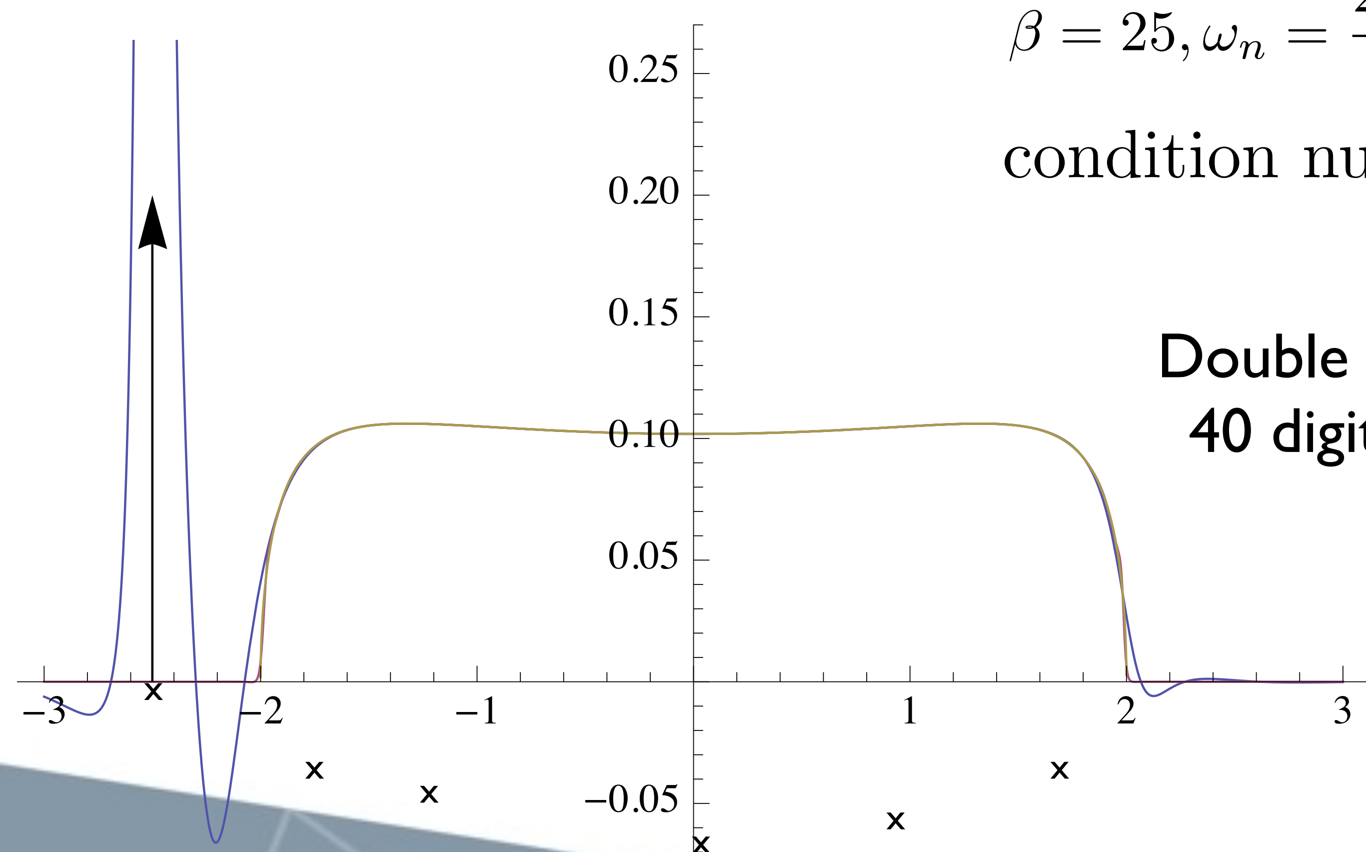




$$A(r=0,\omega) = \frac{1}{\pi}\frac{\sqrt{4-\omega^2}}{4-\omega^2+\epsilon^2}\Theta(|\omega|-2) + \frac{\epsilon}{\sqrt{4+\epsilon^2}}\delta(\omega+\sqrt{4+\epsilon^2})$$

$$G(0,i\omega_n) = \int d\omega \frac{A(0,\omega)}{i\omega_n - \omega}$$

$$\frac{P(z)}{Q(z)} = \frac{a_0 + a_1 z + \ldots + a_{m-1}z^{m-1}}{1 + b_1 + \ldots + b_m z^m} \qquad G(i\omega_n) = \frac{P(i\omega_n)}{Q(i\omega_n)}$$



$$\beta = 25, \omega_n = \frac{2\pi}{\beta}(n+\frac{1}{2}), n_{max} = 40$$

$$\text{condition number } |\lambda_{max}/\lambda_{min}| \sim 10^{50}$$

Double precision cannot capture the peak
40 digit precision does (width 10^(-10))

see also, Karrasch, Meden, Schönhammer, PRB 2010

High precision self-consistent Green's function calculations

High precision calculations requires a finite basis (?)

Can we work with a finite set of imaginary frequencies?

We discretize imaginary time: the GF of the diagrammatic expansion, not the path integral directly.

Advantage: non-interacting GF and spectral function can be captured exactly.

Spectral weight conservation can be build into the formalism.

$$G(\tau - \tau') = G_0(\tau - \tau') + \int d\tau_1 d\tau_2 G_0(\tau - \tau_1)\Sigma(\tau_1 - \tau_2)G_0(\tau_2 - \tau') + ...$$

$$\boxed{\tau_j = \frac{\beta}{N} j}$$

$$\Downarrow$$

$$G(\tau_i - \tau_j) = G_0(\tau_i - \tau_j) + (\frac{\beta}{N})^2 \sum_{l,l'=0}^{N-1} G_0(\tau_i - \tau_l)\Sigma(\tau_l - \tau_{l'})G_0(\tau_{l'} - \tau_j) + ...$$

$$(\text{ambiguity at } \tau_i - \tau_j = 0)$$

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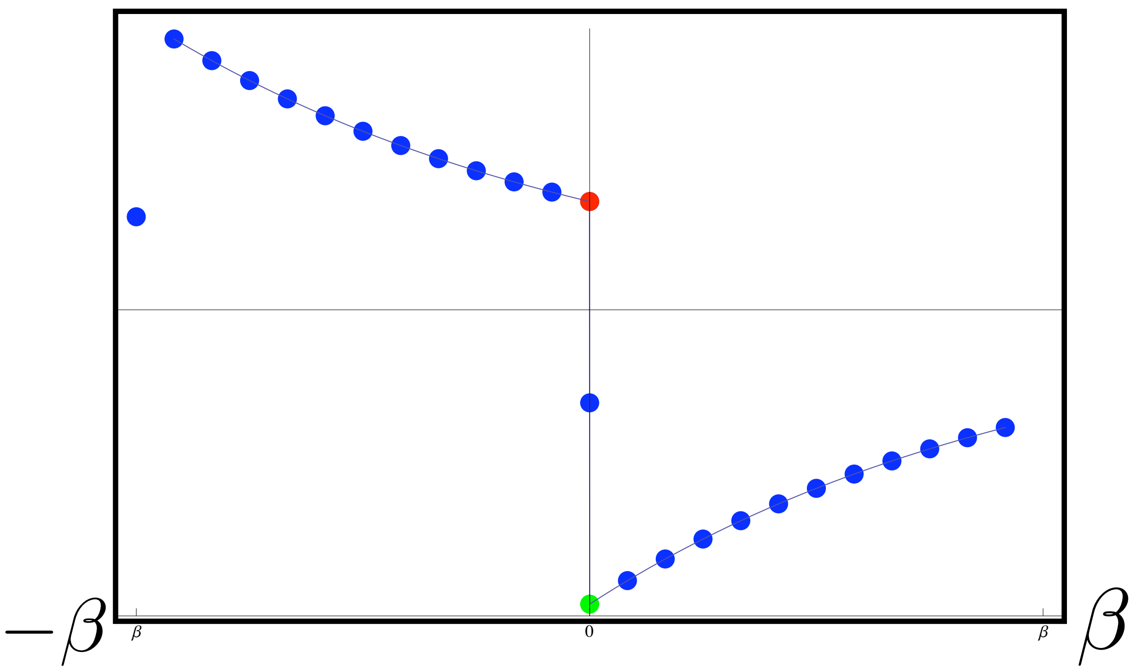
Non-interacting GF

$$G_{0,k}(\tau) = e^{-\tau\epsilon_k}[n_f(\epsilon_k)\theta(-\tau+0^+) + (n_f(\epsilon_k)-1)\theta(\tau-0^+)]$$

$$\tau_j = \frac{\beta}{N} j$$



$$G_{0,k}(\tau_j) = \frac{1}{\beta}\sum_{n=0}^{N-1} e^{-i\omega_n\tau_j} G_{0,k}(i\omega_n)$$

$$G_{0,k}(\tau_0) = n_f(\epsilon_k) - \frac{1}{2}$$

$$G_{0,k}(i\omega_n) = \frac{\beta}{N}\sum_{j=0}^{N-1} e^{i\omega_n\tau_j} G_{0,k}(\tau_j) = \frac{\beta}{2N}\coth\frac{\beta}{2N}(i\omega_n - \epsilon_k)$$

Periodic: $i\omega_n \to i\omega_n + i\Omega_N$ $\qquad \Omega_N = \frac{2\pi}{\beta}N$

Dyson equation

$$G_k(i\omega_n) = (i\omega_n - \epsilon_k - \Sigma_k(i\omega_n))^{-1}$$

$$\boxed{G_k(i\omega_n) = \frac{\beta}{2N}\text{Coth}\frac{\beta}{2N}(i\omega_n - \epsilon_k - \Sigma_k(i\omega_n))}$$

$$G_0^{\pm} = G_0 \pm \frac{\beta}{2N}$$

$$G = G_0 + G_0^{+}\Sigma G_0^{-} + G_0^{+}\Sigma G_0 \Sigma G_0^{-} + ...$$

Σ is 1PI diagrams of periodized Green's functions

$G(i\omega_n)$ is periodic $G(i\omega_n) = G(i\omega_n \pm i\Omega_N)$ with $\Omega_N = \frac{2\pi}{\beta}N$

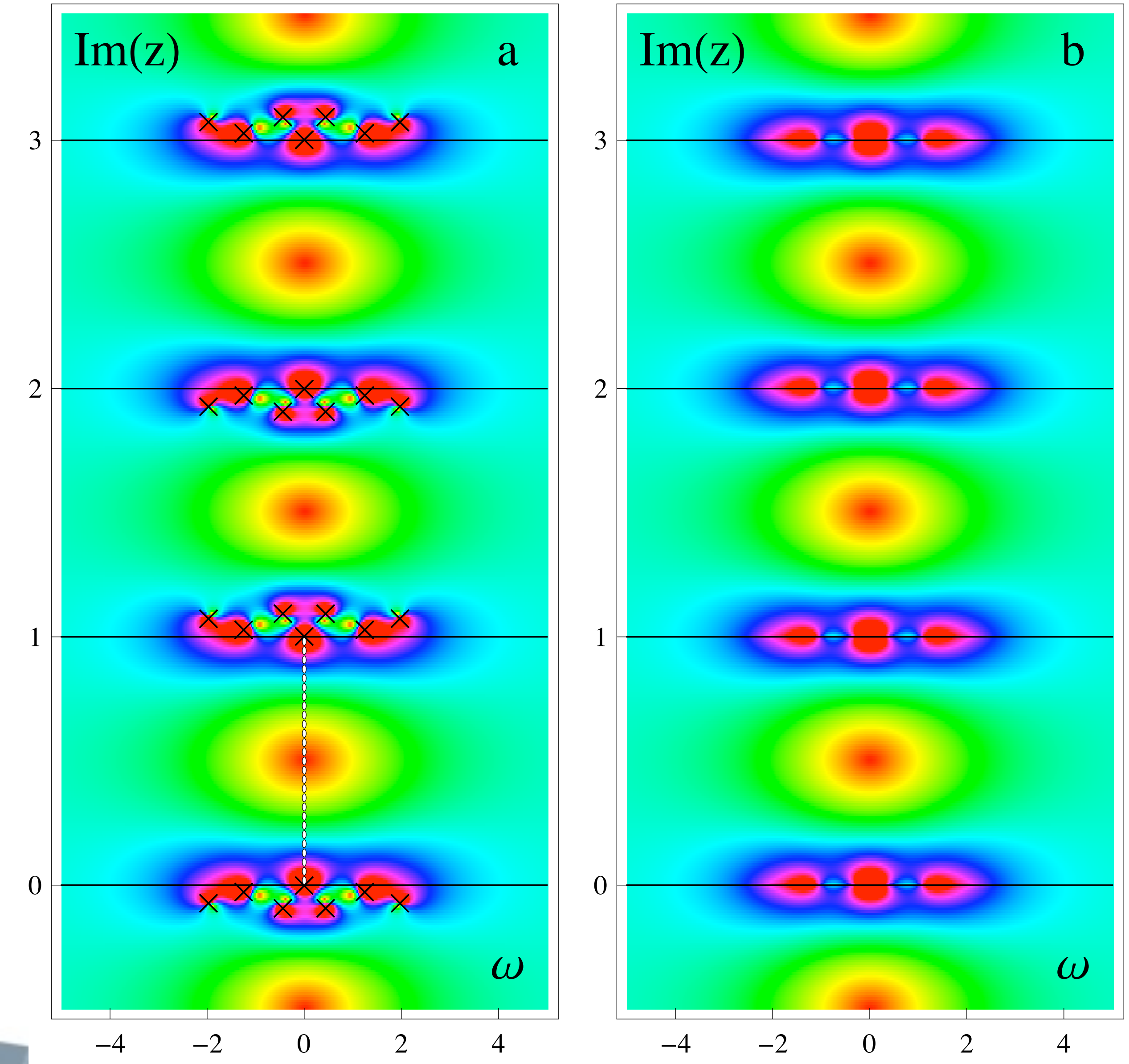
Analytic Structure/Analytic continuation

Discretize the spectral representation $G_k(\tau) = -\frac{1}{Z}\sum_{m,n} e^{-\beta E_n} e^{\tau(E_n - E_m)} |\langle m|c_k^\dagger|n\rangle|^2$

$A(k,\omega) = \frac{1}{Z}\sum_{m,n} |\langle m|c_k^\dagger|n\rangle|^2 e^{-\beta E_n}(1+e^{-\beta\omega})\delta(E_m - E_n - \omega)$

$$G_k(z) = \int d\omega A(k,\omega)\frac{\beta}{2N}\mathrm{Coth}\frac{\beta}{2N}(z-\omega)$$

Periodic $\Omega_N = \frac{2\pi}{\beta}N$



Represent spectral function in terms of a (set of) generalized Lorentzians

$$L_{\epsilon,\gamma}(\omega) = \frac{i\frac{\beta}{2N}}{\sinh\frac{\beta}{2N}(\omega-\epsilon+i\gamma)} - \frac{i\frac{\beta}{2N}}{\sinh\frac{\beta}{2N}(\omega-\epsilon-i\gamma)}$$

Reduces to Lorentzian for large N:

$$\frac{2\gamma}{(\omega-\epsilon)^2+\gamma^2}$$

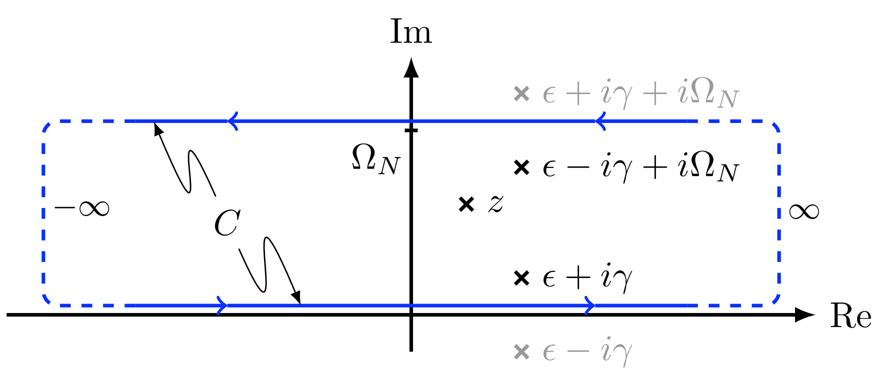
"$G^R(z)$"

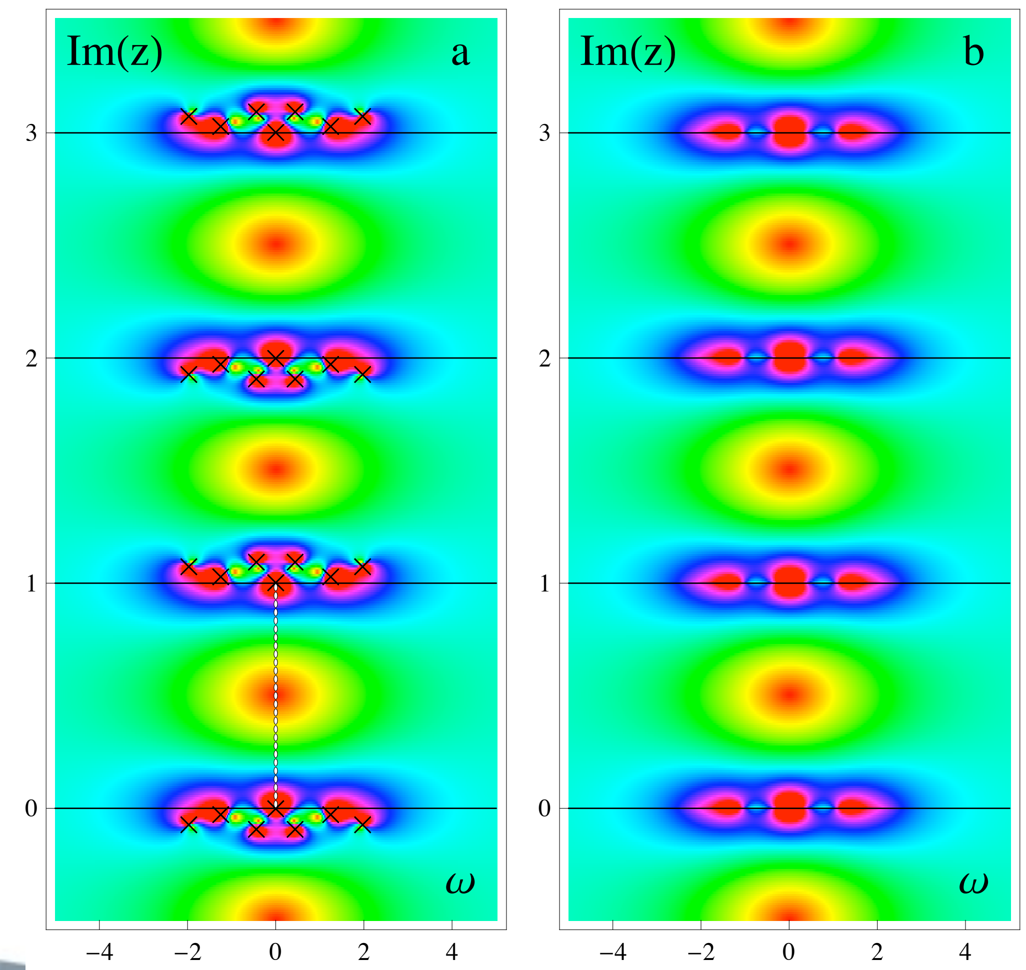
$$G(z) = \frac{1}{2}\oint_C \frac{dz'}{2\pi} L_{\epsilon,\gamma}(z')\frac{\beta}{2N}\coth\frac{\beta}{2N}(z-z') \qquad 0 < Imz < \Omega_N$$

$$= \frac{\beta}{4N}\left(\coth\frac{\beta}{4N}(z-\epsilon+i\gamma) + \tanh\frac{\beta}{4N}(z-\epsilon-i\gamma)\right)$$

Spectral weight conserving:

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}L(\omega) = 1$$





Monday, April 30, 12

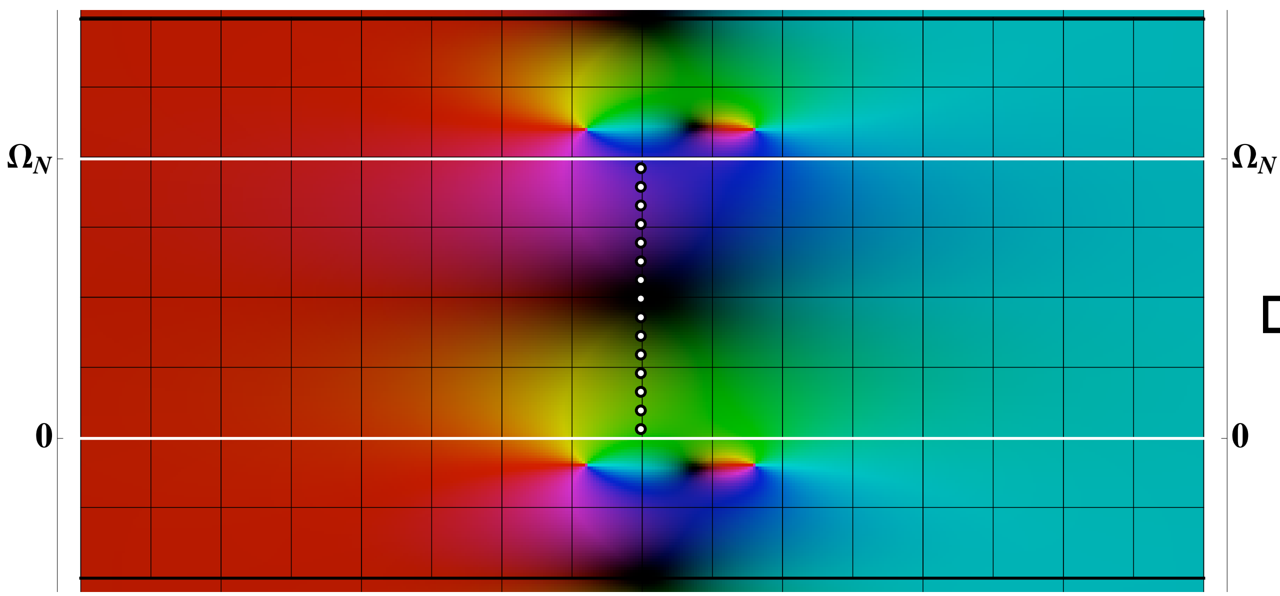
Map periodically repeated poles to single poles:

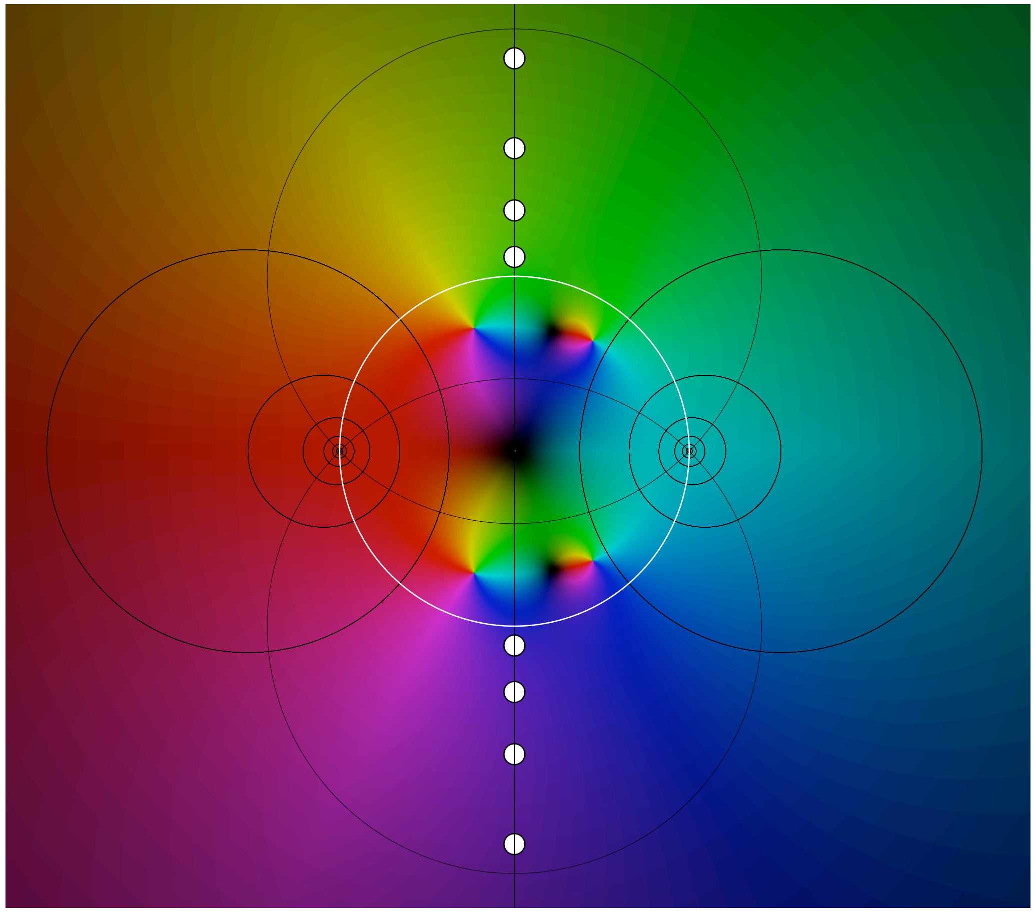
$$G(z) = \frac{\beta}{4N} \sum_\nu [a_\nu \coth \frac{\beta}{4N}(z - \epsilon_\nu + i\gamma_\nu) + a_\nu^* \tanh \frac{\beta}{4N}(z - \epsilon_\nu - i\gamma_\nu)]$$

Spectral weight conservation: $\frac{1}{2}\sum_\nu (a_\nu + a_\nu^*) = 1$

Single Poles from conformal mapping:

$$z' = \coth(\frac{\beta}{4N} z - i\frac{\pi}{4})$$



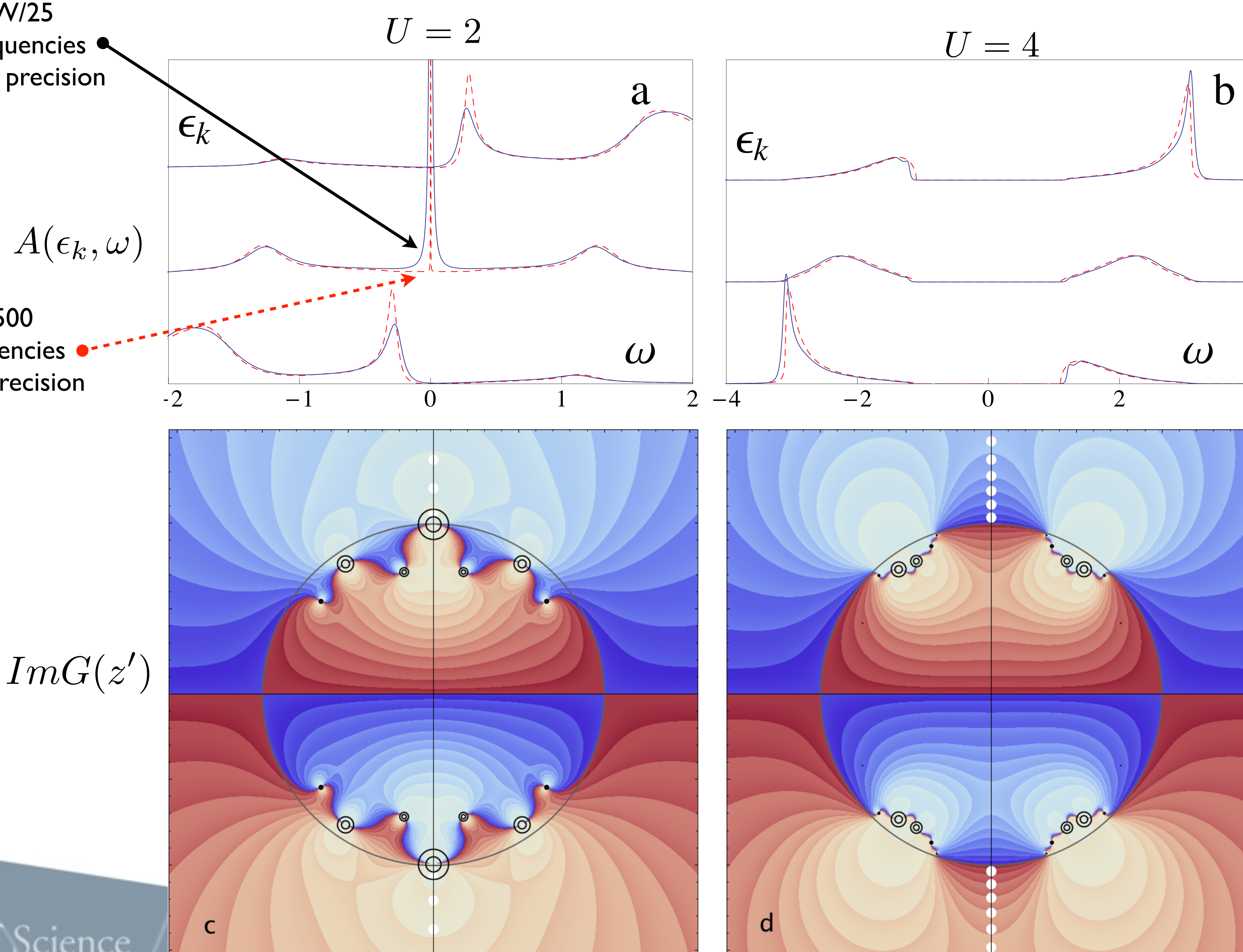


$$\text{Fit } G(z'(i\omega_n)) \text{ to } P(z')/Q(z')$$

Applied to DMFT (Iterated perturbation theory) on Hubbard model

T=W/25
25 frequencies
40 digits precision

T=W/500
501 frequencies
700 digits precision



1. Do calculations to high precision at finite N
2. Make "numerically exact" analytic continuation
3. Take N to infinity to find full analytic Green's function and spectral function

M.Granath, A. Sabashvili, H.U.R. Strand, S. Östlund, arXiv: 1103.3516

H.U.R. Strand, A. Sabshvili, M. Granath, B. Hellsing, S. Östlund, PRB 2011

Formalism looking for more applications...

There is also a consistent functional formulation

$$\Gamma = \Phi(\{G\}) - Tr(G^{+}\Sigma) + Tr\log\left(-G^{-}/(2\eta)\right) \approx \beta\Omega$$
$$\Sigma_k(i\omega_n) = \frac{\delta\Phi}{\delta G_k(i\omega_n)}$$

Gives exact free energy in the non-interacting limit for any N