Evidence of dispersion relations for the response of the Lorenz 63 system

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Motivation

- The analysis of how systems respond to external perturbations to their steady state constitutes one of the crucial subjects of investigation in physics and mathematics
- In particular, we are concerned with the response of chaotic systems:
  - How do their statistical properties change when (small) time dependent perturbations are applied?
  - Is it possible to develop a perturbation theory?
- Can we use the unforced fluctuations of the system for deducing its properties when perturbations are applied (FDT)?
- Can we find tools for decodifying a large class of dynamical systems?

Background

- In quasi-equilibrium statistical mechanics, the Kubo theory ('50s) allows for an accurate treatment of perturbations to the canonical equilibrium state
- When considering general dynamical systems (e.g. forced and dissipative), the situation is much worse $\longrightarrow$ FD relation does not apply
- Recent advances due mostly to Ruelle (late '90s) have lead to the idea that for SRB systems it is possible to define a perturbative theory of the response to small perturbations to the vector field. We follow this direction…

Perturbations to NESS Systems

Axiom A systems

- Axiom A dynamical systems are very special
  - Include Anosov flows (hyperbolic, struct. stable, dense)
  - Non-wandering set is hyperbolic & periodic points are dense
  - SRB invariant measure: time averages converge Lebesgue a.e. to the ensemble averages for measurable observables
    - For these systems all statistical properties are well-defined
- Often, when we perform numerical simulations, we more or less implicitly set ourselves in these hypotheses
  - Not generic systems, but, following the chaotic hypothesis by Gallavotti and Cohen (1995, 1996), systems with many d.o.f. can be treated as if they were Axiom A systems when macroscopic averages are considered.
  - These are good physical models!!!

SRB measure

- The invariant measure of the unperturbed system is not absolutely continuous w.r.t. Lebesgue; it is so only along the unstable (and neutral) manifold, whereas it is singular in the stable directions (effect of the contraction!)
  - Locally, “Cantor set times a smooth manifold”.
- Therefore, it is mathematically very different from the smooth measure of the canonical ensemble, the common framework for equilibrium (or quasi-equilibrium in the Kubo sense) thermodynamics.
- But…

Ruelle Response Theory

- If the Axiom A flow is perturbed as: $\dot{x} = F(x) + e(t)X(x)$

- We can express the expectation value of an observable Φ as: $\langle \Phi \rangle(t) = \langle \Phi \rangle_0 + \sum_{n=1}^{\infty} \langle \Phi \rangle^{(n)}(t)$

- where the n^{th} order perturbation can be expressed as:

$$\langle \Phi \rangle^{(n)}(t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \mathrm{d}\sigma_1 \mathrm{d}\sigma_2 \dots \mathrm{d}\sigma_n G^{(n)}(\sigma_1, \dots, \sigma_n) e(t-\sigma_1) e(t-\sigma_2) \dots e(t-\sigma_n).$$

Ruelle 1998

This is a perturbative theory…

- with a causal Green function:

$$G^{(n)}(\sigma_1,\ldots,\sigma_n) = \int \rho_{SRB}(\mathrm{d}x) \quad \Theta(\sigma_1)\Theta(\sigma_2-\sigma_1)\ldots\Theta(\sigma_n-\sigma_{n-1}) \times$$
$$\times\Lambda\Pi(\sigma_n-\sigma_{n-1})\ldots\Lambda\Pi(\sigma_2-\sigma_1)\Lambda\Pi(\sigma_1)\Phi(x)$$

  - Expectation value of an operator evaluated over the invariant measure $\rho_{SRB}(\mathrm{d}x)$ of the unperturbed flow!

- where: $\Lambda(\bullet) = X(x)\nabla(\bullet)$ and $\Pi(\tau)A(x) = A(x(\tau))$

  Projection on the perturbation flow — Unperturbed evolution operator

- Conventional Kubo theory is a special case

L. 2008

Linear Systems

- Let us consider a general linear system whose input *I*(*t*) and output *O*(*t*) are connected by the following linear relationship:

$$O(t) = \int_{-\infty}^{\infty} a(t-t')I(t')dt'$$

- By applying Fourier Transform to both members we obtain:

$$O(\omega) = a(\omega)I(\omega)$$

- Is there a connection between the properties of $a(t)$ and those of $a(\omega)$?

Titchmarsch Theorem

Theorem 1. (Titchmarsch)
The three statements 1., 2., and 3. are mathematically equivalent:

1. $a(t) = 0$ if $t \leq 0$ and $a(t) \in \mathrm{L}^2$.
2. $a(\omega) = \mathrm{F}\left[a\left(t\right)\right] \in \mathrm{L}^2$ if $\omega \in \mathbb{R}$ and if

$$a(\omega) = \lim_{\omega' \to 0} a(\omega + \mathrm{i}\omega'),$$

   then $a(\omega + \mathrm{i}\omega')$ is holomorphic if $\omega' > 0$.
3. Hilbert transforms [39] connect the real and imaginary part of $a(\omega)$ as follows:

$$\mathrm{Re}\{a(\omega)\} = \frac{1}{\pi}\mathrm{P}\int_{-\infty}^{\infty} \frac{\mathrm{Im}\{a(\omega')\}}{\omega' - \omega}\mathrm{d}\omega'$$

$$\mathrm{Im}\{a(\omega)\} = -\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{\infty} \frac{\mathrm{Re}\{a(\omega')\}}{\omega' - \omega}\mathrm{d}\omega'.$$

Kramers-Kronig relations

- Every causal linear model has to obey this constraint;
- The in-phase and out-of-phase responses of a causal system are connected by Kramers-Kronig relations:
  - If we have measurements of the real (imaginary) part of the susceptibility, we can derive via K-K the best estimate of the other consistently with the principle of causality

$$\Re\left\{\chi^{(1)}(\omega)\right\} = \frac{2}{\pi}\wp\int_0^\infty \frac{\omega'\Im\left\{\chi^{(1)}(\omega')\right\}}{\omega'^2-\omega^2}d\omega$$

$$\Im\left\{\chi^{(1)}(\omega)\right\} = -\frac{2\omega}{\pi}\wp\int_0^\infty \frac{\Re\left\{\chi^{(1)}(\omega')\right\}}{\omega'^2-\omega^2}d\omega'$$

with: $\chi^{(1)}(\omega) = [\chi^{(1)}(-\omega)]^*$

Kramers, 1926; Kronig, 1927

Other results

Theorem 2. (superconvergence)

Nussenzweig, 1972

If

$$g(y) = \mathrm{P} \int_0^\infty \frac{f(x)}{y^2 - x^2} \mathrm{d}x,$$

where

1. $f(x)$ is continuously differentiable,
2. $f(x) = O\left[(x \ln x)^{-1}\right]$,

then for $y \gg x$ the following asymptotic expansion holds

$$g(y) = \frac{1}{y^2} \int_0^\infty f(x)\, \mathrm{d}x + O\left(y^{-2}\right).$$

By applying this theorem to the **K-K**, and considering the asymptotic behaviour, we obtain the **sum rules**

Nonlinear susceptibilities

- If my input has one or more monochromatic components, the n^{th} order response will be nonzero for all the sums of n-combinations of the input frequencies.
- Example: input has a monochromatic component at $\omega=\pm\omega_0$
- Linear response at $\omega=\pm\omega_0$
- Second order response at $\omega=\pm 2\omega_{0;}\ \omega=0$
- Third order response at $\omega=\pm 3\omega_0$; $\omega=\pm\omega_0$
- Can we write KK relations for the corresponding susceptibilities?

Scandolo's Theorem

- Specific classes of nonlinear susceptibilities obey KK;
- Basically, in the case of monochromatic input, only the nth order susceptibility responsible for the nth order harmonic generation process obeys KK

- Linear response: $\chi^{(1)}(\omega)$ → KK rels. apply
- 3rd order HG: $\chi^{(3)}(3\omega;\omega,\omega,\omega)$ → KK rels. apply
- Kerr susceptibility $\chi^{(3)}(\omega;\omega,\omega,-\omega)$ → KK rels. don't apply
  - KK don't apply for nonlinear correction to linear

- This is a formal, model-independent result (developed for optics)

Scandolo and Bassani, 1991
L. et al 2005

Dispersion Relations for NESS systems

Asymptotic Behavior

- If $G^{(n)}(t) \sim t^{\beta}$ for $t \to 0$, we have that:

$$\lim_{\omega_0 \to \infty} \omega_0^{\beta+n} \chi^{(n)}(\omega_0, \ldots, \omega_0) = \alpha \in \mathbb{C} \setminus \{0\}$$

- and: $\beta + n = 2\gamma$ and $\alpha = \alpha_R \in \mathbb{R}$, otherwise $\beta + n = 2\gamma - 1$ and $\alpha = i\alpha_I$, $\alpha_I \in \mathbb{R}$.
  - because the real part and the imaginary part of the susceptibility have opposite parity.

Therefore:

- Kramers Kronig relations:

$$-\frac{\pi}{2}{\omega_0}^{2p-1}\mathrm{Im}\left\{\left[\chi^{(n)}\left(\omega_0,\ldots,\omega_0\right)\right]^m\right\} = \mathrm{P}\int_0^\infty d\omega_0' \frac{{\omega_0'}^{2p}\mathrm{Re}\left\{\left[\chi^{(n)}\left(\omega_0',\ldots,{\omega'}_0\right)\right]^m\right\}}{\left(\left({\omega_0'}^2-\omega_0^2\right)\right.}, \qquad (26)$$

$$\frac{\pi}{2}{\omega_0}^{2p}\mathrm{Re}\left\{\left[\chi^{(n)}\left(\omega_0,\ldots,\omega_0\right)\right]^m\right\} = \mathrm{P}\int_0^\infty d\omega_0' \frac{{\omega_0'}^{2p+1}\mathrm{Im}\left\{\left[\chi^{(n)}\left(\omega_0',\ldots,{\omega'}_0\right)\right]^m\right\}}{\left({\omega_0'}^2-\omega_0^2\right)}. \qquad (27)$$

with $p = 0,\ldots,m\gamma-1$ if $\beta+n=2\gamma$, and $p=0,\ldots,\mathrm{int}(m\gamma-(m+1)/2)$ (with $\mathrm{int}(x)$ indicating the integer part of x) if $\beta+n=2\gamma-1$.

- This, plus the ensuing sum rules, is the end of the story
- But, let's see an application…

L. 2008, 2009

Lorenz 63 system

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = rx - y - xz$$
$$\dot{z} = xy - bz$$

- With the classical values $\sigma = 10; r = 28; b = 8/3$
- Actually, in principle this is a bad model:
  - Not Axiom -A
  - Not Uniformly Hyperbolic
    - Singular hyperbolic (Bonatti et al., 2005)
- We add the perturbation flow:

$$e(t)X = \begin{pmatrix} 0 \\ x \cdot 2\varepsilon \cos(\omega' t) \\ 0 \end{pmatrix}$$

Linear Response

- We consider the observable $\Phi(x, y, z) = z$
- Background (noise) :

$$\left\langle z(\omega)\right\rangle_0 = \frac{1}{T}\int_0^T dt f_o^t(z)\exp[-i\omega t] = \frac{1}{N\tau}\sum_{j=1}^{N} f_0^{j\tau}(z)\exp[-i\omega j\tau]$$

- Perturbed signals:

$$\left\langle z(\omega)\right\rangle_{\varepsilon,\omega'} = \frac{1}{T}\int_0^T dt f_{\varepsilon,\omega'}^t(z)\exp[-i\omega t] = \frac{1}{N\tau}\sum_{j=1}^{N} f_{\varepsilon,\omega'}^{j\tau}(z)\exp[-i\omega j\tau]$$

Our signal:

$$\delta\left\langle z(\omega)\right\rangle_{\varepsilon,\omega'} = \left\langle z(\omega)\right\rangle_{\varepsilon,\omega'} - \delta\left\langle z(\omega)\right\rangle_0$$

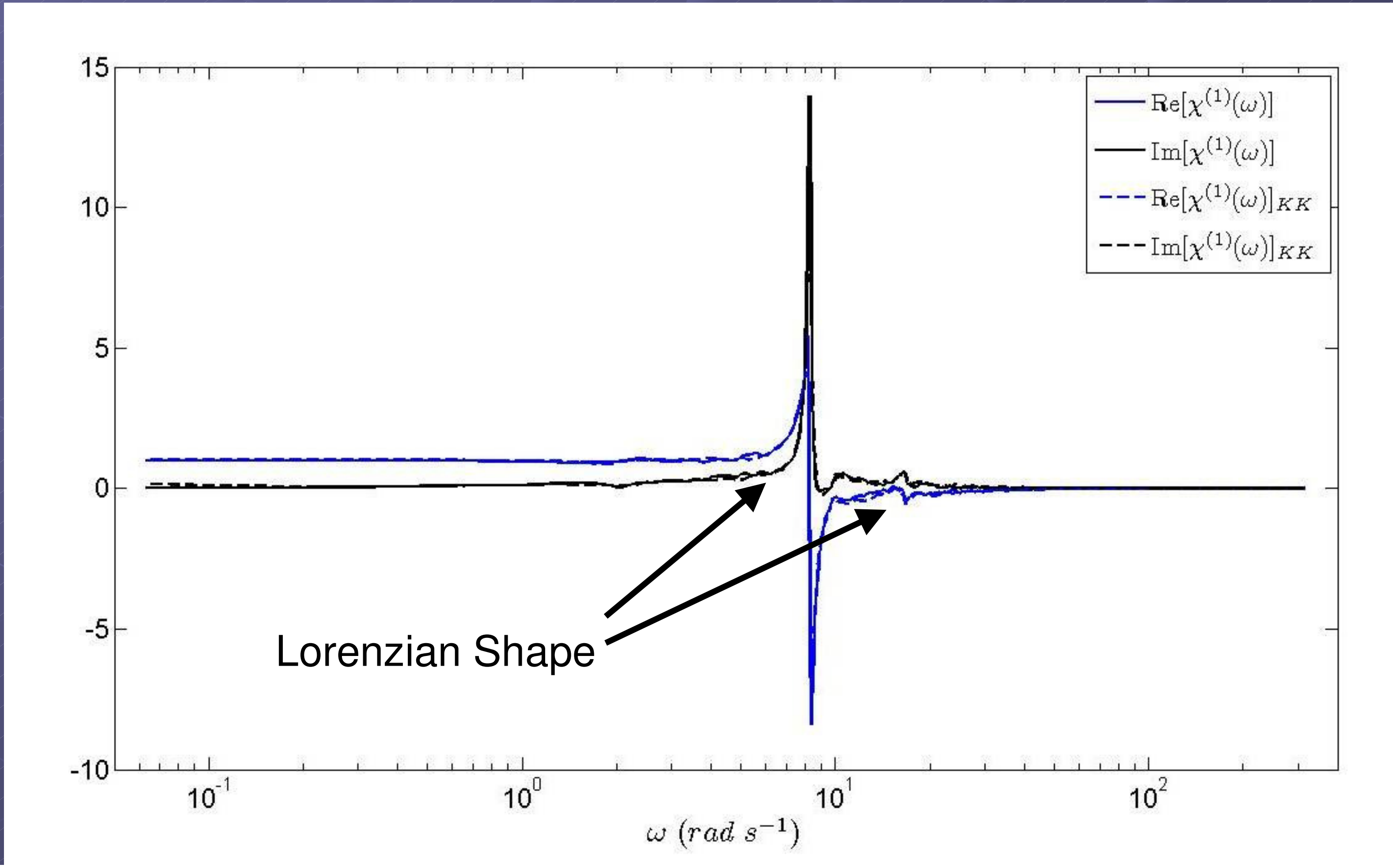
Reich 2002

Attention!!

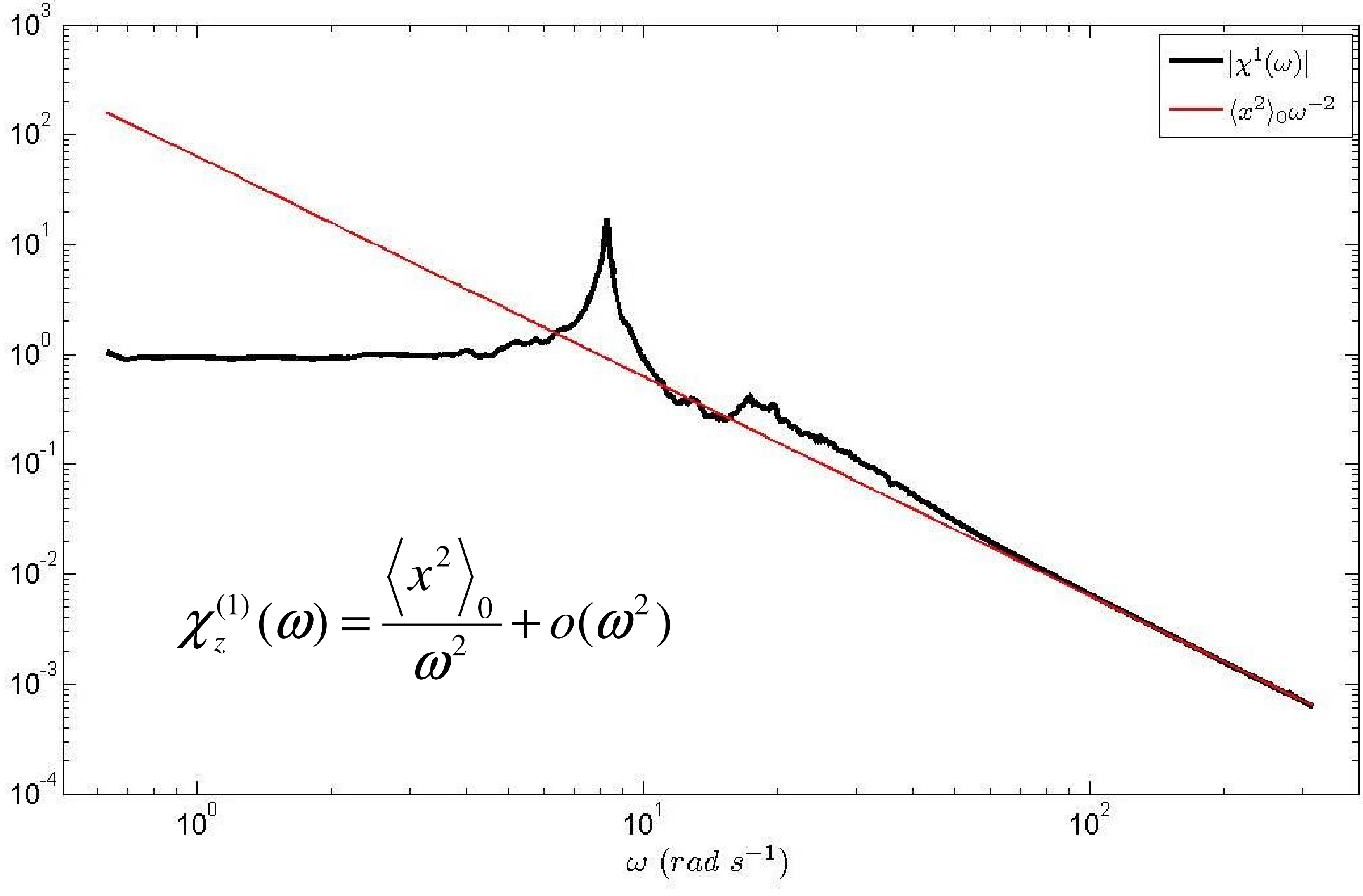
- As opposed to the quasi-equilibrium case, the background flow has a component with frequency ω – due to noise [but with random phase], since the system has naturally a continuous spectrum.
- So, in order to detect the signal, we need to distinguish it from noise.
  - Long Integrations (the peaks become more pronounced
  - Ensemble of simulations in order to average out the phase of the background signal

Linear Susceptibility

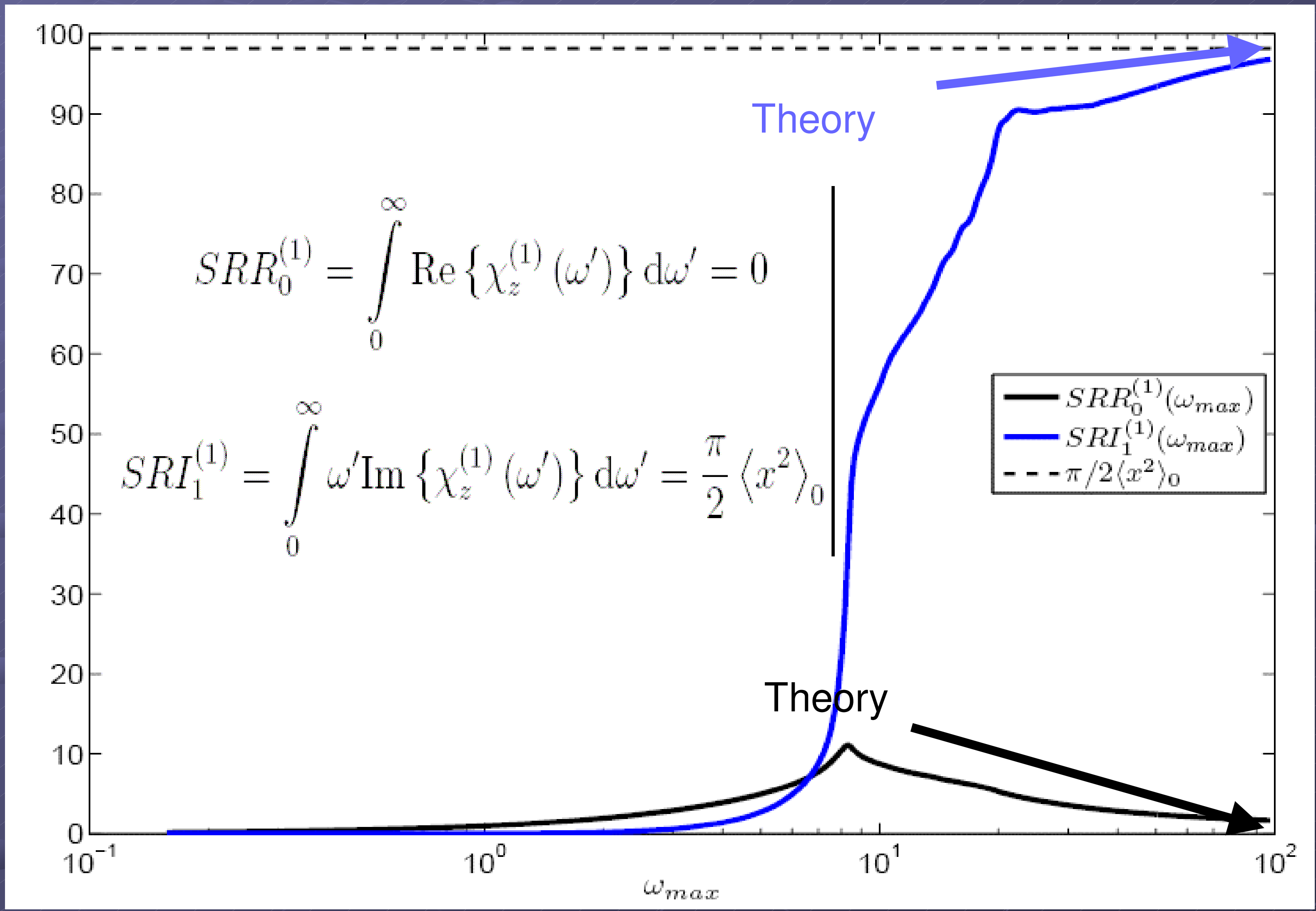
- Definition: $\chi_z^{(1)}(\omega) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \delta \langle z(\omega) \rangle_{\varepsilon,\omega}$



Asymptotic behavior



Sum rules



Theory
Theory
$SRR_0^{(1)} = \int_0^\infty \mathrm{Re}\{\chi_z^{(1)}(\omega')\}\,d\omega' = 0$
$SRI_1^{(1)} = \int_0^\infty \omega' \mathrm{Im}\{\chi_z^{(1)}(\omega')\}\,d\omega' = \frac{\pi}{2}\langle x^2\rangle_0$
$SRR_0^{(1)}(\omega_{max})$
$SRI_1^{(1)}(\omega_{max})$
$\pi/2\langle x^2\rangle_0$
ω_{max}

Second Harmonic Susceptibility

- Signal: $$\delta\langle z(2\omega)\rangle_{\varepsilon,\omega} = \langle z(2\omega)\rangle_{\varepsilon,\omega} - \delta\langle z(2\omega)\rangle_{0}$$

- Definition: $$\chi_z^{(2)}(2\omega;\omega,\omega) = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon^2}\delta\langle z(2\omega)\rangle_{\varepsilon,\omega}$$

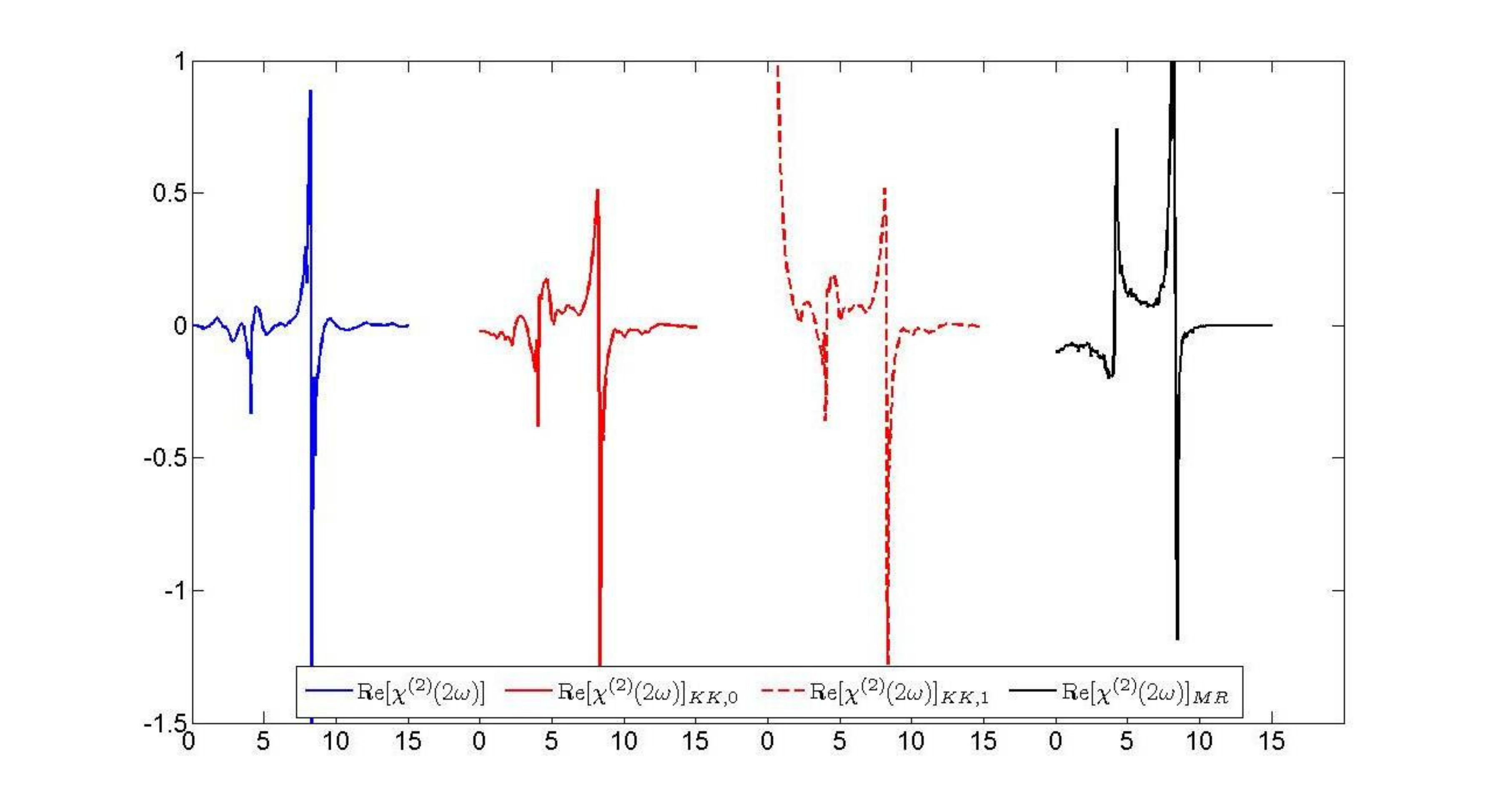
  - The limit is far from being trivial …

- An old tale of solid state physicists:

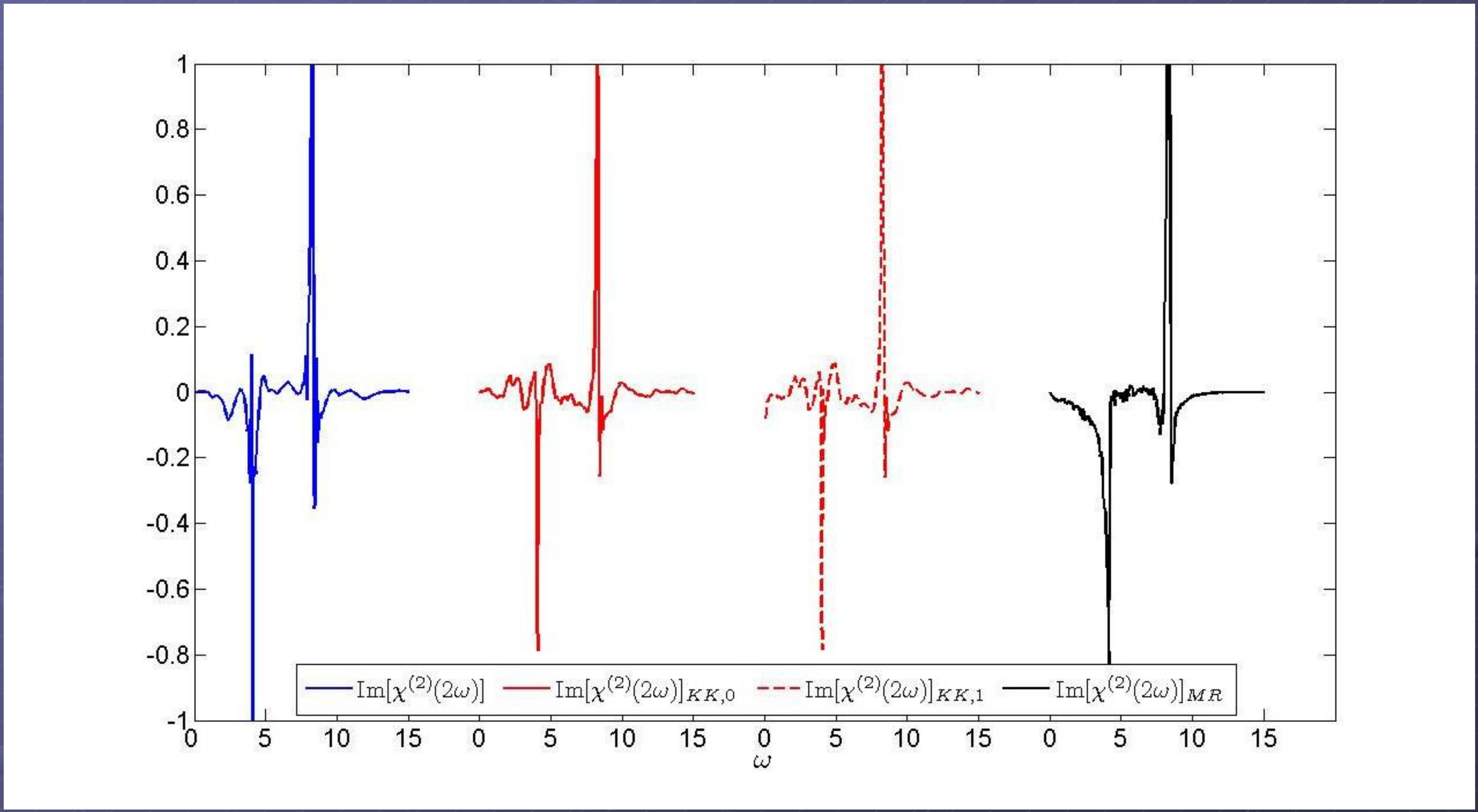
Miller's rule: $\chi_z^{(2)}(2\omega;\omega,\omega) \propto \chi_z^{(1)}(2\omega)\chi_z^{(1)}(\omega)\chi_z^{(1)}(\omega)$

Bassani and Scandolo 1995

Real Part of the susceptibility

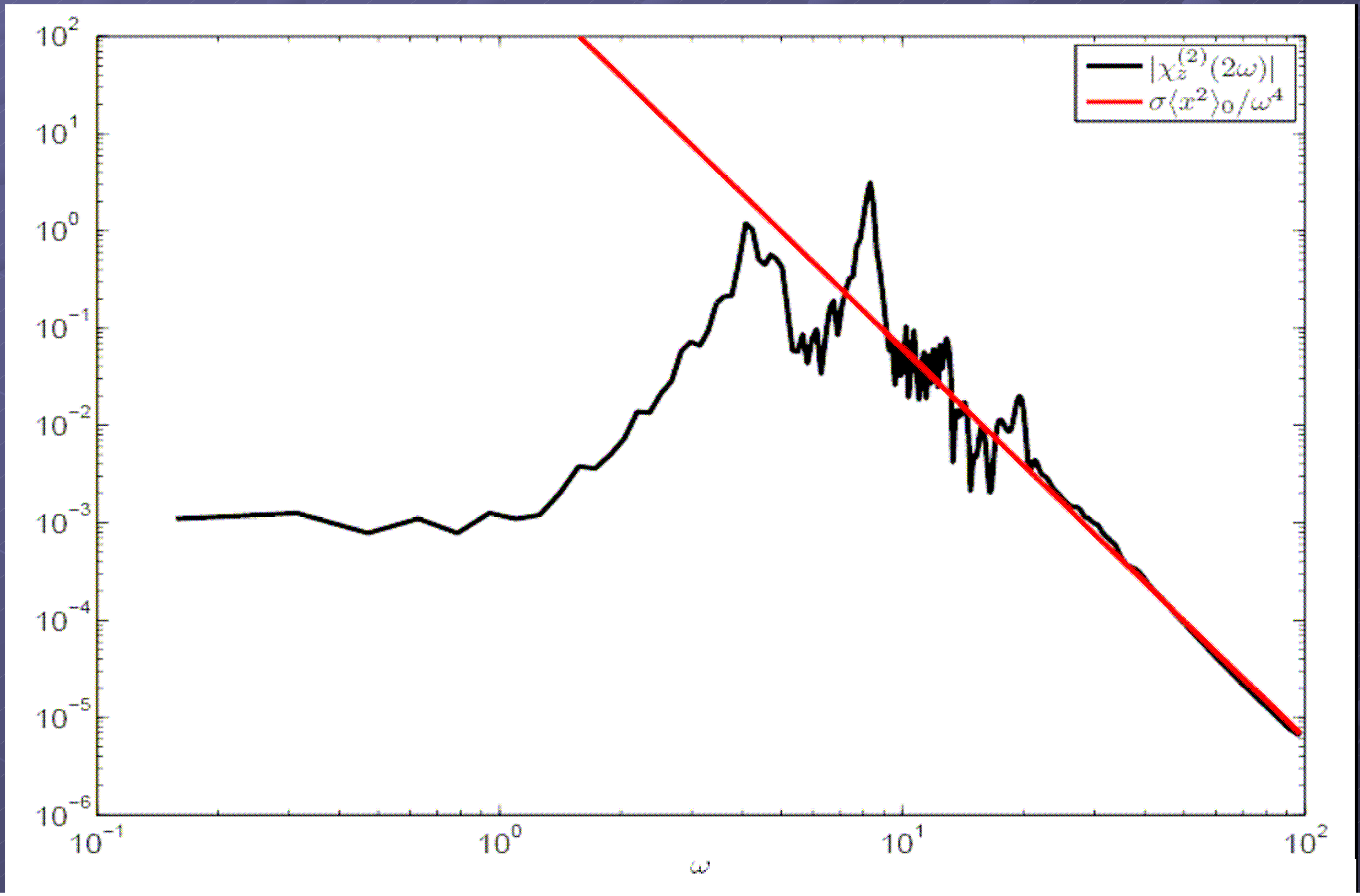


Imaginary Part of the susceptibility

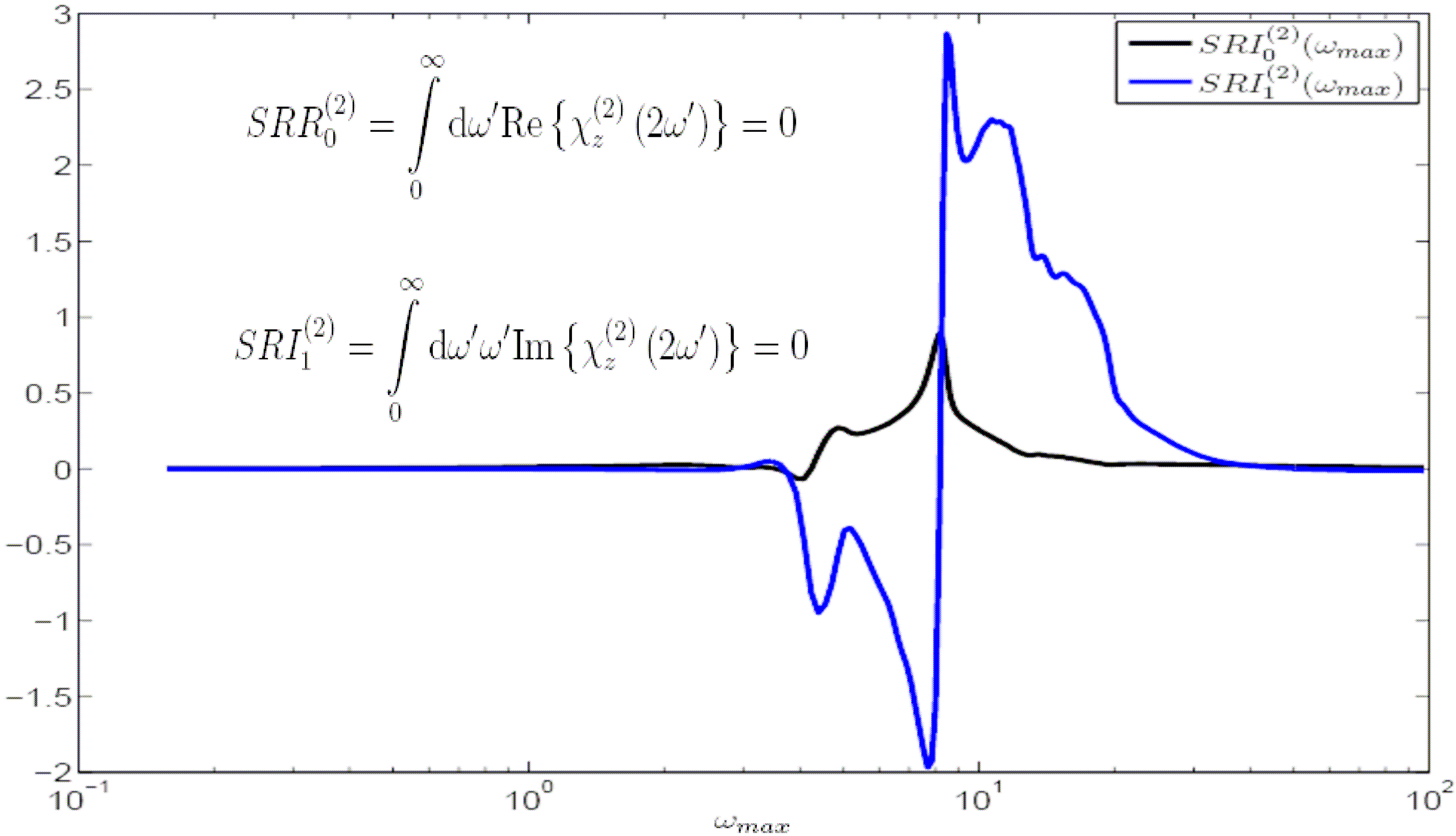


Asymptotic behavior

- Since: $\chi_z^{(2)}(2\omega;\omega,\omega) = \dfrac{\sigma\left\langle x^2 \right\rangle_0}{\omega^4} + o(\omega^4)$

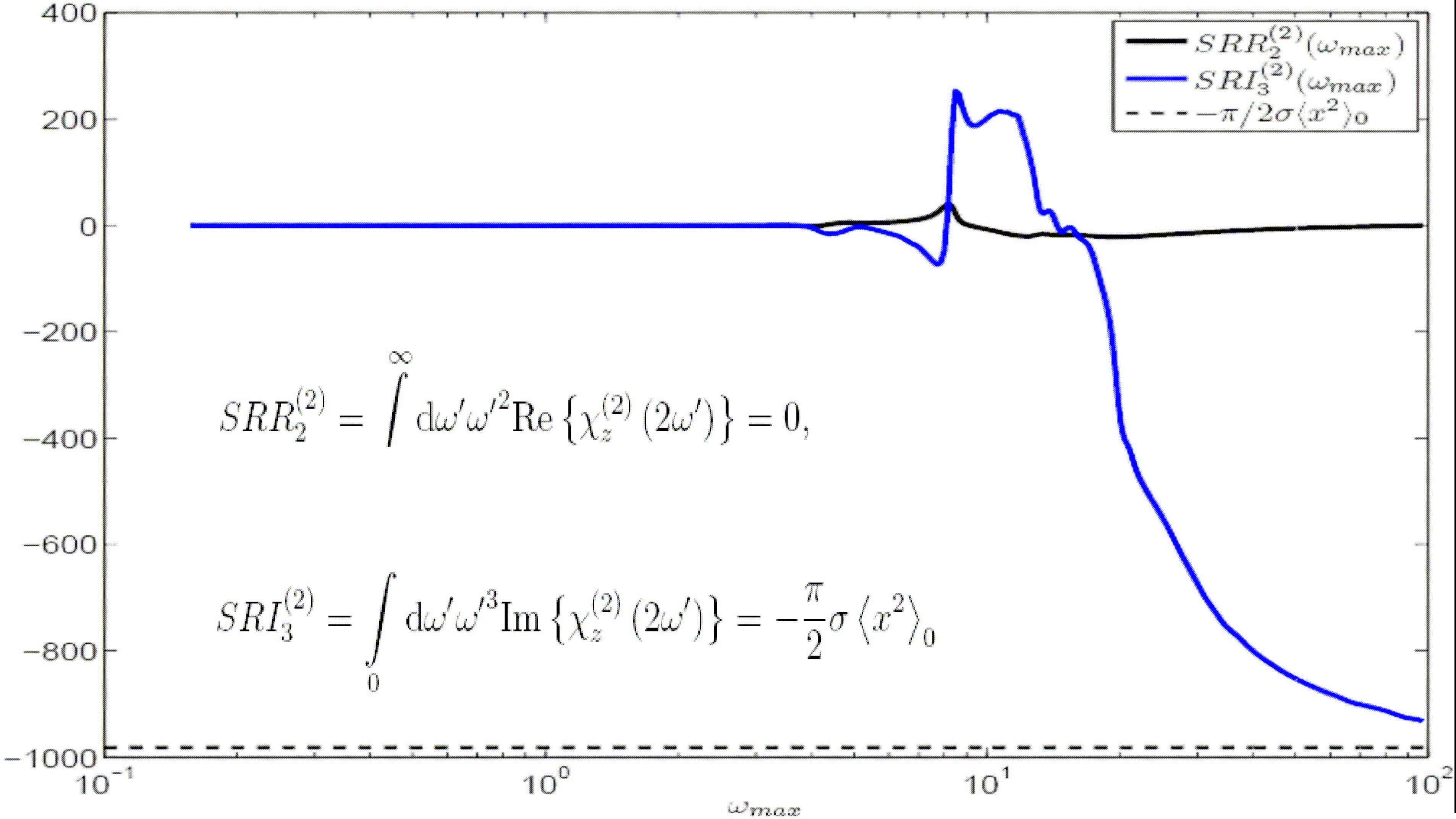


Sum Rules - a



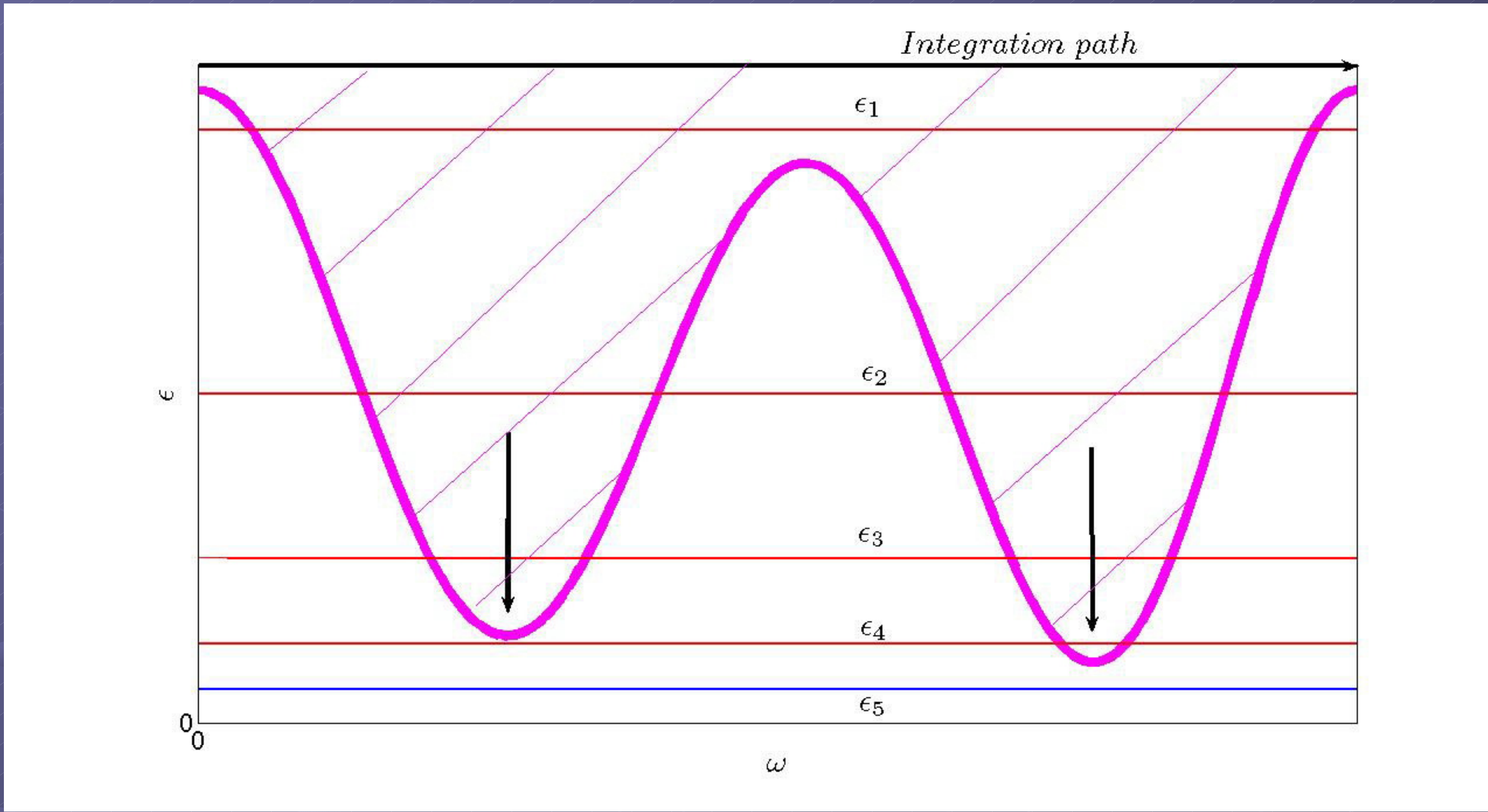
$SRR_0^{(2)} = \int_0^\infty d\omega' \mathrm{Re}\{\chi_z^{(2)}(2\omega')\} = 0$
$SRI_1^{(2)} = \int_0^\infty d\omega' \omega' \mathrm{Im}\{\chi_z^{(2)}(2\omega')\} = 0$
$SRI_0^{(2)}(\omega_{max})$
$SRI_1^{(2)}(\omega_{max})$
ω_{max}

Sum Rules - b



400
200
0
−200
−400
−600
−800
−1000
10^{-1}
10^{0}
10^{1}
10^{2}
ω_{max}
$SRR_2^{(2)}(\omega_{max})$
$SRI_3^{(2)}(\omega_{max})$
$-\pi/2\sigma\langle x^2\rangle_0$
$SRR_2^{(2)} = \int^{\infty} d\omega' \omega'^2 \mathrm{Re}\left\{\chi_z^{(2)}(2\omega')\right\} = 0,$
$SRI_3^{(2)} = \int_0 d\omega' \omega'^3 \mathrm{Im}\left\{\chi_z^{(2)}(2\omega')\right\} = -\frac{\pi}{2}\sigma\left\langle x^2\right\rangle_0$

Finite-size ϵ-perturbations



- Large values of epsilon, regions where motion is periodic (purple) $\Longrightarrow$ theory K.O.

Windows of periodicity..

- Using finite size ϵ-perturbations we may encounter WoP for some ω_j (usually resonances of the system)
- If Axiom A, the extent of WoP should vanish as perturbation strength $\longrightarrow 0$
- The values of susceptibility $\chi_\epsilon(\omega_j)$ are "wrong"
  - We are out of the validity of the Ruelle expansion, SRB measure is not smoothly deformed
- KK relations do not work properly anymore
- We can nevertheless cure these points
  - We use KK of the "measured" real part evaluated at point ω_j as *first guess of the imaginary part* of the "correct" value
  - We do the same for imaginary part $\longrightarrow$ real part
  - After just one iteration the agreement is excellent
  - Analytic continuation of (a well defined) χ? Multistability?
- Preparing a new paper on that (not using Lorenz 63!).

Conclusions

- We have extended the Ruelle response theory and have clarified its relationship with the Kubo approach
  - We have defined a new theory of linear and nonlinear dispersion relations for chaotic systems. The theory is based on the principle of causality – and that's all.
  - If a model does not obey K-K, it is not a good model
- We have proved its precision and applicability in a specific (and problematic) low-dimensional case
- … but what if we add stochastic perturbations? Will the FD relation be again in place (Lacorata and Vulpiani, 2007)?
- Dispersion relations connect the system's response at all forcing frequencies. This sounds like a good way of conceptualizing climate change (on all time scales)
- Let's perform experiments on "reasonable" systems

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