Log-Analytic Uncertainty Relation

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Content

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  Journal of Physical Chemistry A, 107 (37), 7170 - 7174 (2003).

  [Los-Alamos Archives -quant-ph/0406197]

Quantum Mechanics

Time-dependent Schrödinger equation *(general)*

$$i\hbar\frac{\partial}{\partial t}\Psi = \hat{H}\Psi$$

Time-dependent Schrödinger equation *(single non-relativistic particle)*

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

Schrödinger, E. (1926).

"An Undulatory Theory of the Mechanics of Atoms and Molecules". Physical Review 28 (6): 1049–1070.

The Wave Function

$$\Psi(x,t) = |\Psi(x,t)| e^{i\phi(x,t)}$$

The Amplitude has an obvious meaning in terms of probability density:

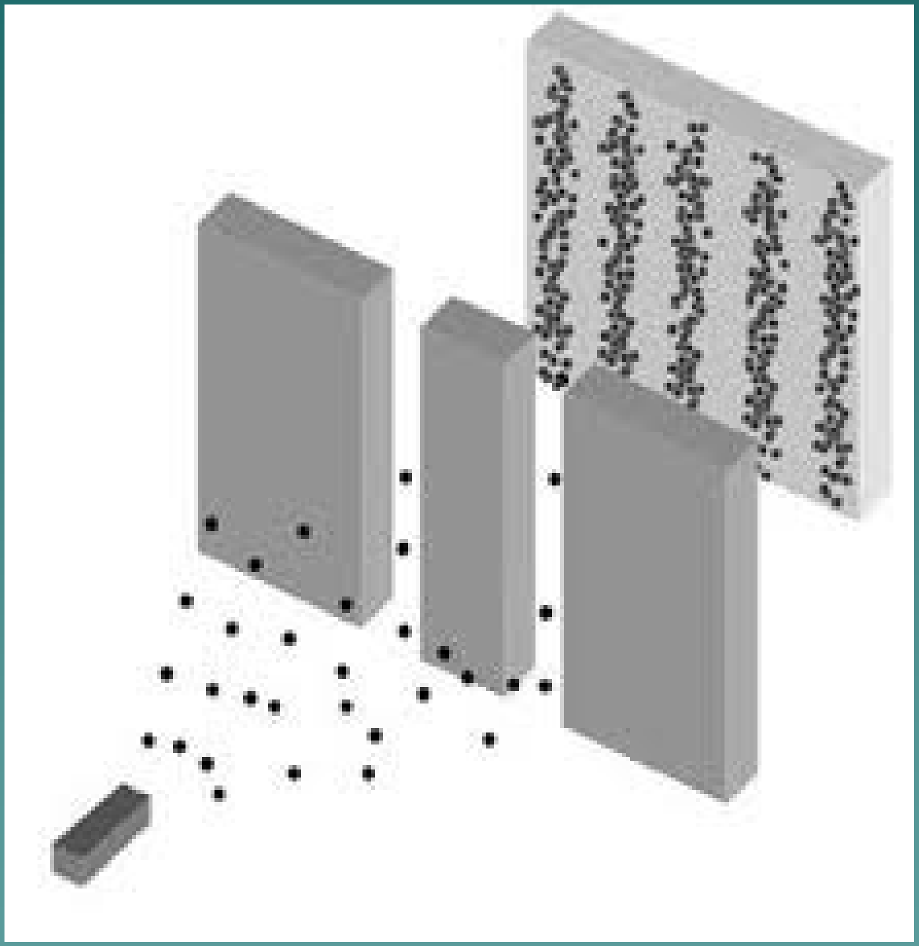
$$P_{a<x<b} = \int_a^b |\Psi(x,t)|^2 \, \mathrm{d}x$$

The Phase: Does It Have Any Physical Meaning at All?

- Relative phase in a superposition can be measured in interference experiments.

$$\Psi = \psi_1 + \psi_2 = |\psi_1| e^{i\phi_1} + |\psi_2| e^{i\phi_2} \Rightarrow$$

$$|\Psi| = \sqrt{|\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2| \cos(\phi_1 - \phi_2)}$$



What About the Absolute Phase?

- It seems not to have any physical significance, since it can be easily modified by a gauge transformation.

$$i\hbar\frac{\partial\Psi}{\partial t}=\frac{1}{2m}\left(-i\hbar\vec{\nabla}-q\vec{A}\right)^2\Psi+q\Phi\Psi$$

$$\Psi'=\Psi e^{i\frac{q\Lambda}{\hbar}}\Rightarrow$$

$$\vec{A}'=\vec{A}+\vec{\nabla}\Lambda,\ \Phi'=\Phi+\frac{\partial\Lambda}{\partial t}\Rightarrow$$

$$i\hbar\frac{\partial\Psi'}{\partial t}=\frac{1}{2m}\left(-i\hbar\vec{\nabla}-q\vec{A}'\right)^2\Psi'+q\Phi'\Psi'$$

- **Gauge Transformations do not change the physical system**
- **Nevertheless, the phase is changed (without consequence to the physical system):**

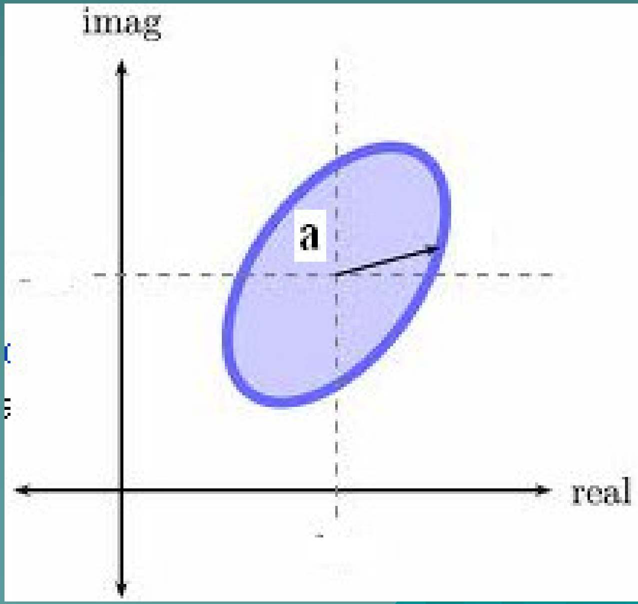
$$\phi' = \phi + \frac{q}{\hbar}\Lambda$$

Cauchy's Integral Formula (1831)

$$f(a) = \frac{1}{2\pi i} \oint_\gamma \frac{f(z)}{z-a}\, dz$$

f analytic and a inside the trajectory, if a is outside then the integral is null.

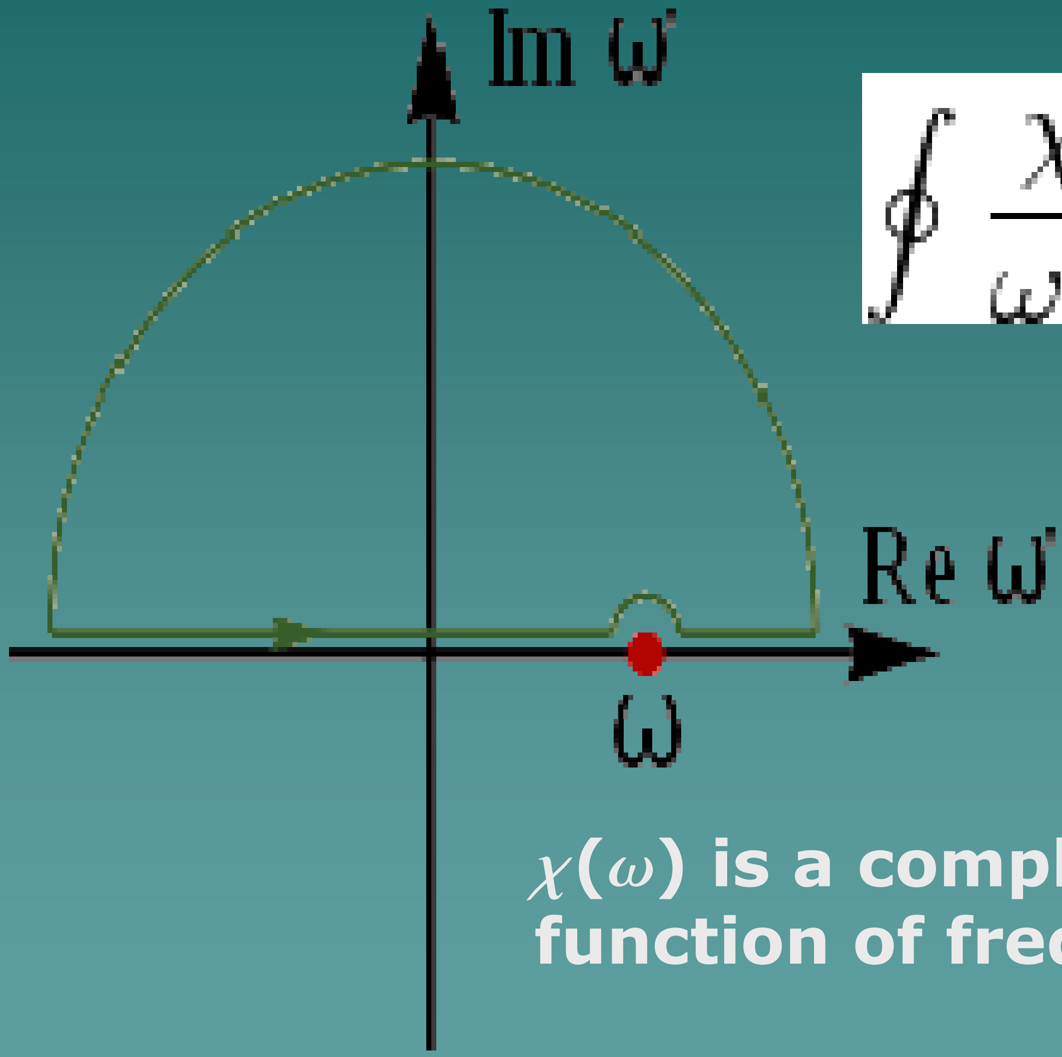
Complex Plane



Kramers - Kronig Relation

H. A. Kramers (1927). "La diffusion de la lumiere par les atomes". Atti Cong. Intern. Fisica, (Transactions of Volta Centenary Congress) Como 2: 545–557.

R. de L. Kronig (1926). "On the theory of the dispersion of X-rays". J. Opt. Soc. Am. 12: 547–557. doi:10.1364/JOSA.12.000547



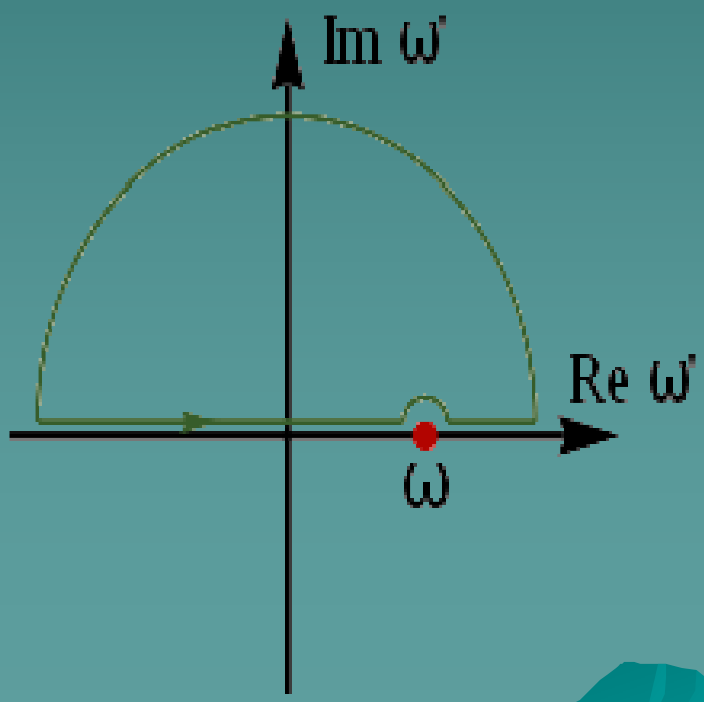
$$\oint \frac{\chi(\omega')}{\omega' - \omega} d\omega' = 0$$

$\chi(\omega)$ **is a complex dielectric function of frequency.**

Properties of $\chi(\omega)$

- $\chi(\omega)$ **is analytic in the upper complex frequency plane.**
- **If the response of the system is causal in the time domain (the output depends on past and current inputs but not future inputs), one can show that** $\chi(\omega)$ **must vanish on the infinite semicircle.**

$$\oint \frac{\chi(\omega')}{\omega'-\omega}\,d\omega' = \mathcal{P}\int_{-\infty}^{\infty} \frac{\chi(\omega')}{\omega'-\omega}\,d\omega' - i\pi\chi(\omega) = 0.$$



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

$$\chi(\omega) = \chi_1(\omega) + i\chi_2(\omega)$$

$$\chi_1(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi_2(\omega')}{\omega' - \omega}\, d\omega'$$

$$\chi_2(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} \frac{\chi_1(\omega')}{\omega' - \omega}\, d\omega'$$

Consider a Logarithm of the Wave Function in the Complex Time Domain

$$\ln \Psi = \ln|\Psi| + i\phi$$

Knowing the amplitude can we calculate the phase as in Kramers-Kronig relation?

- Can we claim that the logarithm of the wave function is analytic in any part of the complex time plane?
- If so can we claim that it vanishes on the infinite semicircle?
- We shall try to answer using a concrete example.

A Free Propagating Wave-Packet

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m_{physical}} \vec{\nabla}^2 \psi$$

Initial condition =
Gaussian wave packet

$$\psi(x,a,0) = \frac{1}{\sqrt{\Delta}} \exp\left[-\frac{(x-a)^2}{4\Delta^2}\right] \exp\left[iK(x-a)\right]$$

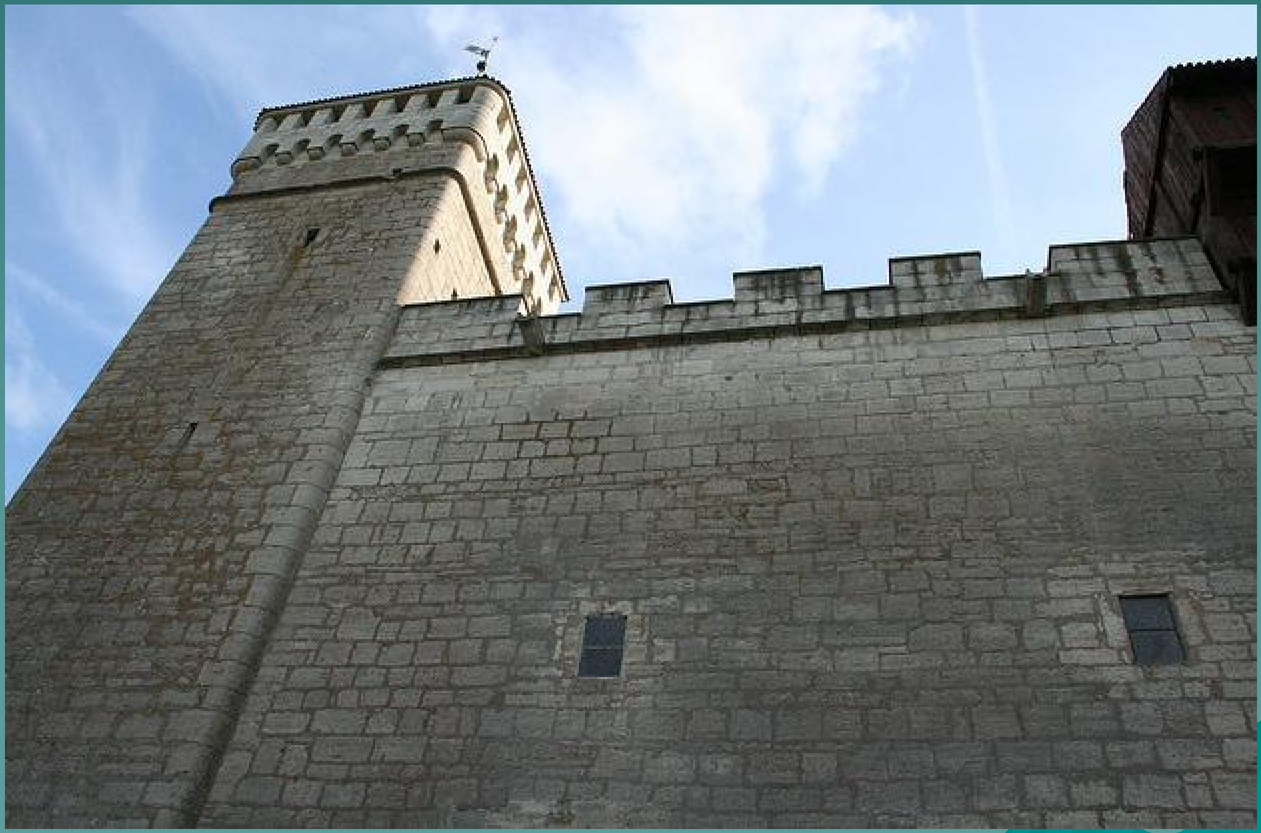
Solution:

$$\psi(x,a,t) = \frac{1}{\sqrt{(\Delta + \frac{it}{2m\Delta})}} exp[-\frac{(x-a)^2 - 4i\Delta^2 K(x-a-\frac{Kt}{2m})}{4\Delta^2 + \frac{2it}{m}}]$$

Tomonaga, S.I. Quantum Mechanics Vol. II (North Holland, Amsterdam, 1966) Sections 41 and 61.

$$m = \frac{m_{phsical}}{\hbar}$$

Insert an Infinite Potential Barrier with no Tunneling



Insert an Infinite Potential Barrier at x=0

$$\Psi(x,t) = 0 \quad for \ x \geq 0$$

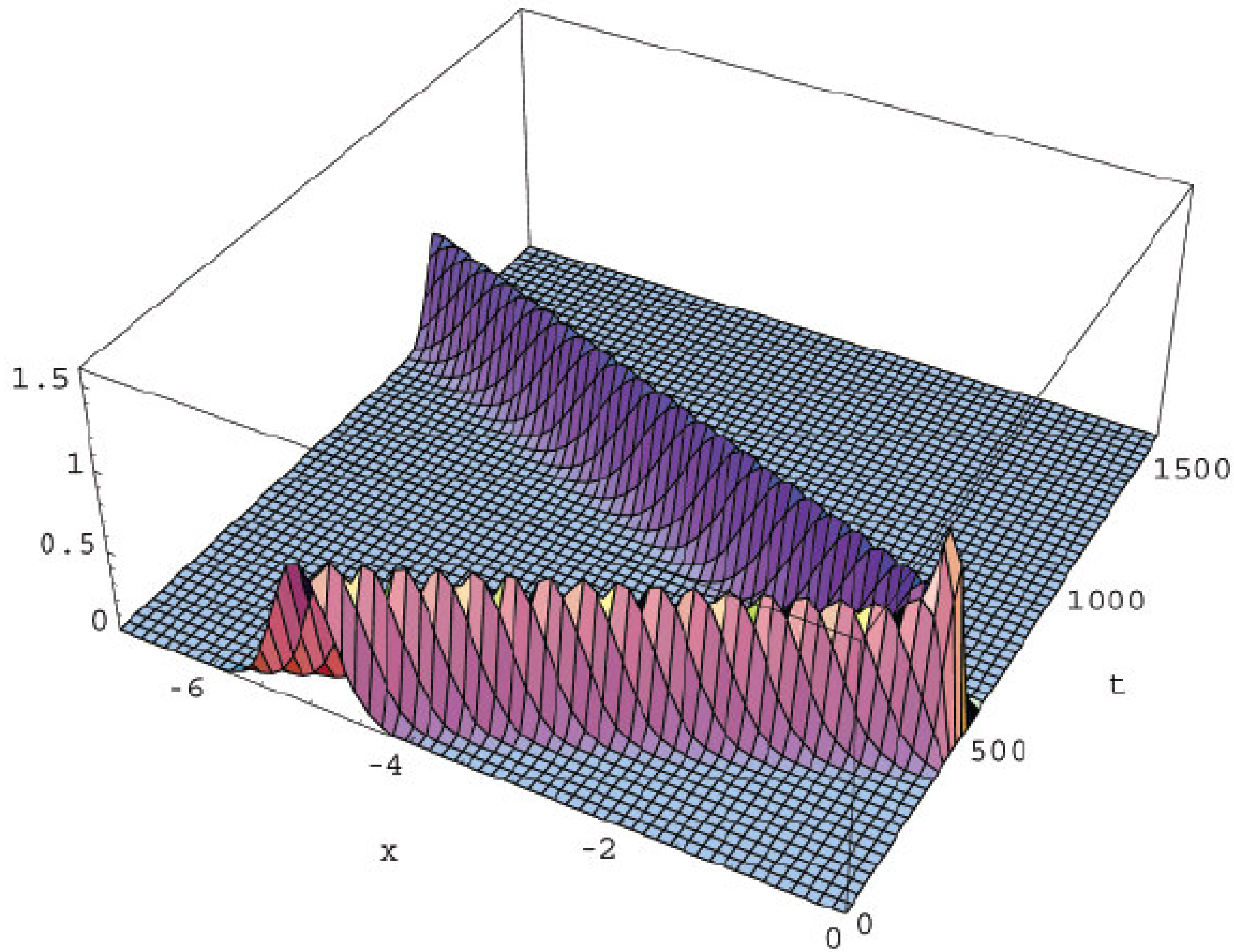
$$\Psi(x,t) = 0 \quad for \ x = 0$$

By the method of images:

$$\Psi(x,t) = N[\psi(x,a,t) - \psi(-x,a,t)] \ \ for\ x < 0$$

$$N^{-2} = \int_{-\infty}^{0} dx |\Psi(x,t)|^2$$

$|\Psi|$



Consider the Following Quantity:

$$\chi'(x,t) = 1 - \frac{\psi(-x,t)}{\psi(x,t)}$$

A multiplicative correction to the free wave function due to the potential barrier.

$$\Psi(x,t) = N\psi(x,t)\chi'(x,t)$$

Explicitly:

$$\chi'(x,t) = 1 - e^{\frac{-4x(2iK\Delta^2+a)}{4\Delta^2+\frac{2it}{m}}}$$

Question:

- If we measure the amplitude of χ' can we calculate its phase?
- More specifically can we use a Kramers-Kronig type relation to calculate the phase from the amplitude?

$$\frac{1}{\pi} P \int_{-\infty}^{\infty} dt' [\ln |\chi(t')|] / (t - t') = - \arg \chi(t)$$

$$\frac{1}{\pi} P \int_{-\infty}^{\infty} dt' [\arg \chi(t')] / (t - t') = \ln |\chi(t)|$$

The answer, it depends:

- We should check if the function is analytic either in the upper complex t plane or the lower t plane.
- Since we use the function logarithm we should avoid zeros as well as infinities of the wave function.
- We should check if the logarithm of the function disappears at infinity in other words we require that the function be unity at infinity.

$$\chi'(x,t) = 1 - e^{\frac{-4x(2iK\Delta^2 + a)}{4\Delta^2 + \frac{2it}{m}}}$$

$$t = t' + it"$$

Obviously there are singularities in the upper t plane, so we better look at the lower t plane.

However, in the lower t plane there are null points:

$$\chi'(x,t) = 1 - e^{\frac{-4x(2iK\Delta^2+a)}{4\Delta^2+\frac{2it}{m}}}$$

$$\frac{4|x|(2iK\Delta^2 - |a|)}{4\Delta^2 + \frac{2it}{m}} = 2i\pi n$$

$$\frac{4|x|(2iK\Delta^2 - |a|)}{4\Delta^2 + \frac{2it}{m}} = 2i\pi n$$

n integer.

$$\begin{aligned} t_n &= t'_n + it"_n \\ t'_n &= m\frac{|x||a|}{n\pi}, \quad t"_n = 2\Delta^2 m(1 - \frac{K|x|}{n\pi}) \end{aligned}$$

Let us define:

$$t_r = \frac{m|a|}{K}$$

t_r time for a classical particle to reach the barrier.

$$t_d = 2m\Delta^2$$

t_d wave packet broadening typical time.

$$n_r(x) = \frac{|x|K}{\pi}$$

Null Points:

$$t_n = t'_n + i t''_n$$

$$t'_n = m\frac{|x||a|}{n\pi}, \quad t''_n = 2\Delta^2 m\left(1 - \frac{K|x|}{n\pi}\right)$$

$$t'_n = t_r \frac{n_r(x)}{n}, \quad t''_n = t_d\left(1 - \frac{n_r(x)}{n}\right)$$

$$t'_n = t_r \frac{n_r(x)}{n}, \quad t"_n = t_d(1 - \frac{n_r(x)}{n})$$

For n negative we have many null points above the axis ($n_r(x) > 0$).

However, for n positive we may have either null points above or below the real axis.

The Condition for Null Points Below the Real Axis:

$$n_r(x) > n$$

Hence we arrive at the necessary condition:

$$n_r(x) \geq 1$$

The condition for log-analyticity below the real axis is therefore:

$$n_r(x) < 1$$

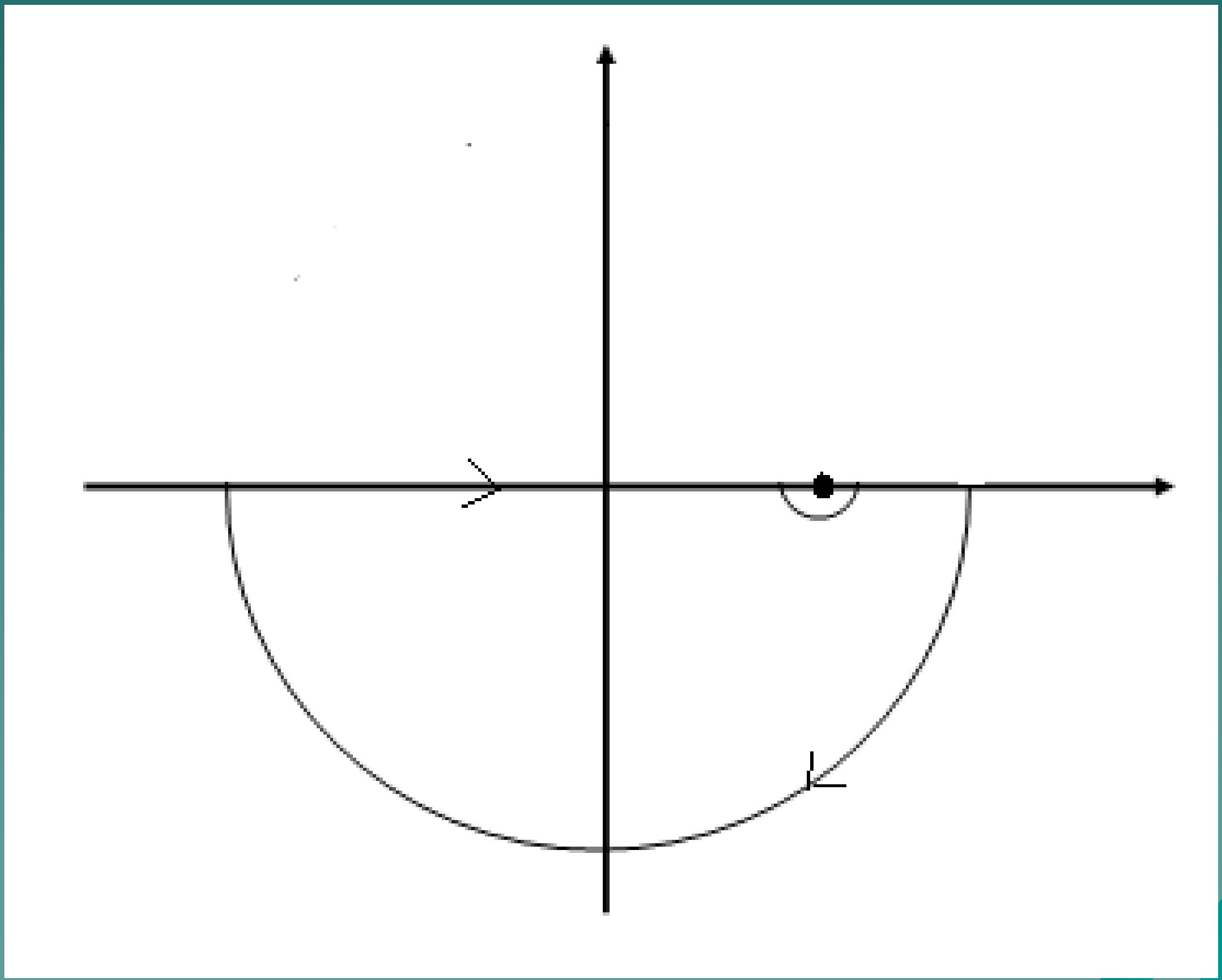
$$n_r(x) = \frac{|x|K}{\pi}$$

+

$$p = \hbar K$$

→

$$|x|p \;<\; \pi\hbar$$



The phase cannot be calculated (and is thus uncertain) if:

$$|x|p > \frac{h}{2}$$

Which is the log-analytic uncertainty relation.

Compare to the Heisenberg (1927) Uncertainty Relation:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

The principles look similar but are actually quite different. σ_x and σ_p are the standard deviations for the displacement and momentum of a particle.

In the log-analytic case what is considered is the distance from the potential barrier and the momentum of a classical particle (which the average momentum of a quantum particle).

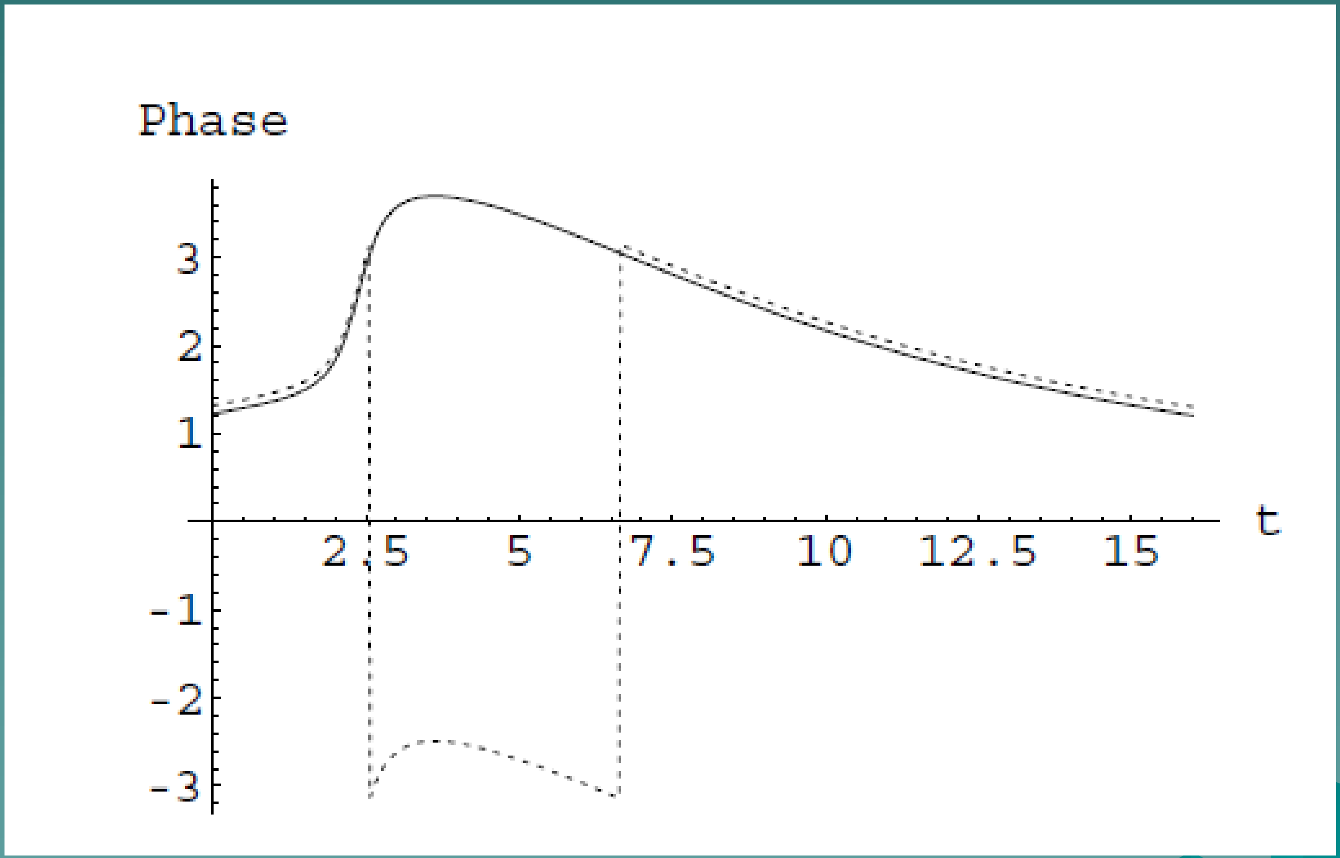
Is log-analyticity below the axis enough to calculate the phase?

No!

We need to know how the function behave on the infinite semi-circle. However, by factoring asymptotic behavior the limitation can be overcome:

$$\chi(t) = \frac{\chi'(t)}{\lim\limits_{|t|\to\infty} \chi'(t)} \Rightarrow \lim_{|t|\to\infty} \chi(t) = 1 \Rightarrow \lim_{|t|\to\infty} \ln \chi(t) = 0$$

Now the phase can be calculated:



Conclusion

1. Topology is important not only in space but also in space-time.
2. This is true for real time but also for complex time in which the topological structures (null points or infinities) determine if a phase carries additional information to the amplitude or can simply be derived from it.
3. Provided that the log-analytic uncertainty relation is not satisfied some aspects of the phase can be calculated from the amplitude.
4. Notice that the entire phase cannot be derived but only a partial phase.