

Resonances: An Introduction



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Introduction

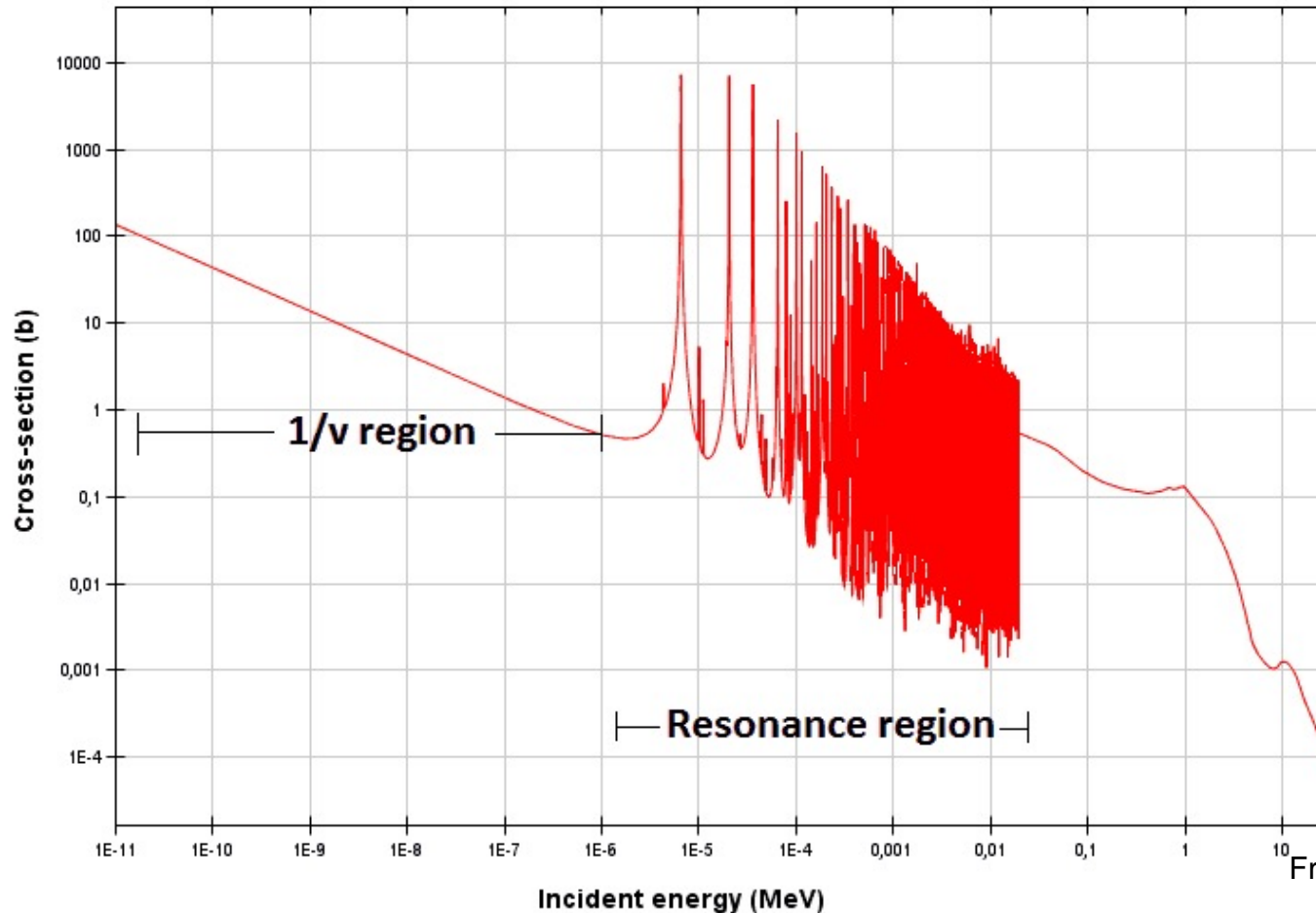
Will mainly concentrate on non-relativistic quantum mechanics

Ideas strongly influenced by atomic and nuclear physics

Introductory; shallow; some very good references at the end of the talk (and in the rest of the workshop)

Resonances: neutron scattering

Incident neutron data / ENDF/B-VII.1 / U238 / MT=102 : (z,y) / Cross section



From periodic-table.org

Content

1. Naive ideas

- Siegert BC

2. Short introduction to formal scattering:

- the S-matrix

3. Resolvent and spectrum: link to S matrix

4. Single channel:

- Complex energy plane: $S(E)$ as an analytic function
- Shape resonances

5. Rearrangement channels

- Complex energy plane: $S(E)$ as an analytic function
- Embedded (Fano) resonances
- Threshold effects

6. Summary and references

1. Naive ideas

What is a resonance? a ubiquitous phenomenon¹

- A (quasi-)particle state with finite lifetime
- A peak in a differential cross section



Not a normal square-integrable solution to a SE!
Let us investigate the idea of a decaying state (Siegert)²

1. I. Prigogine and S. Rice, *Resonances, Instability, and Irreversibility* Adv. Chem. Phys. **99** (1996)
2. A. J. F. Siegert, Phys. Rev. **56**, 750 (1939).

The idea of a Siegert BC:

Use $H = \frac{1}{2}p^2 + V(r)$, with $V(\infty) = 0$

(suitably quick decay of V for r to infinity)

Assume a time-decaying separable solution,

$$\psi(r)e^{iE_R t - (\Gamma/2)t} = \psi(r)e^{iEt}.$$

For large r , $\psi(r) \sim e^{ikr}$ (outgoing wave) with $\hbar k = \sqrt{2mE}$ (complex).

Since $\text{Im}(k) < 0$, this state grows exponentially, so there is something fishy with this (even worse non-normalisable than a continuum state), but we have a definite problem to solve.

Example

Borrowed from Klaiman and Gilary

Look at modified Pöschl-Teller potential

$$V(x) = \left(1 - \frac{1}{\cosh^2 x}\right) e^{-\alpha x^2}$$

Exactly solvable if $\alpha = 0$: one eigenstate at $E = \frac{1}{2}$.

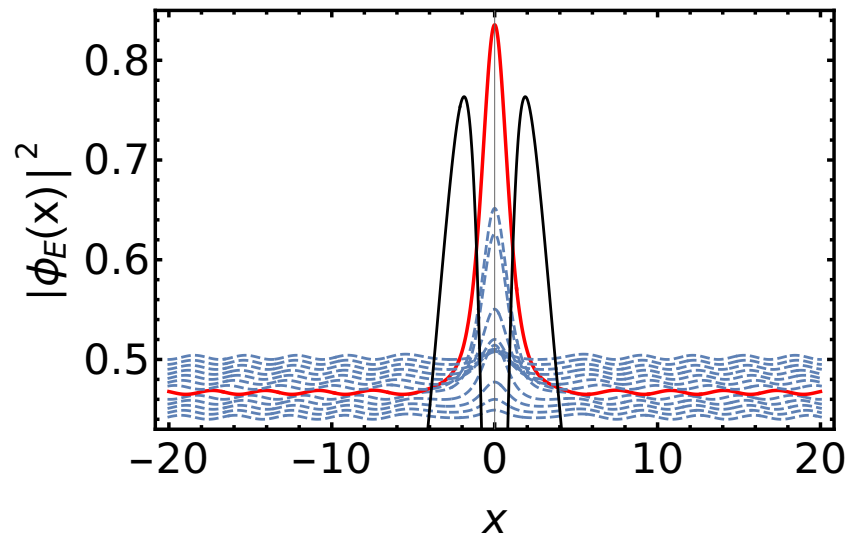
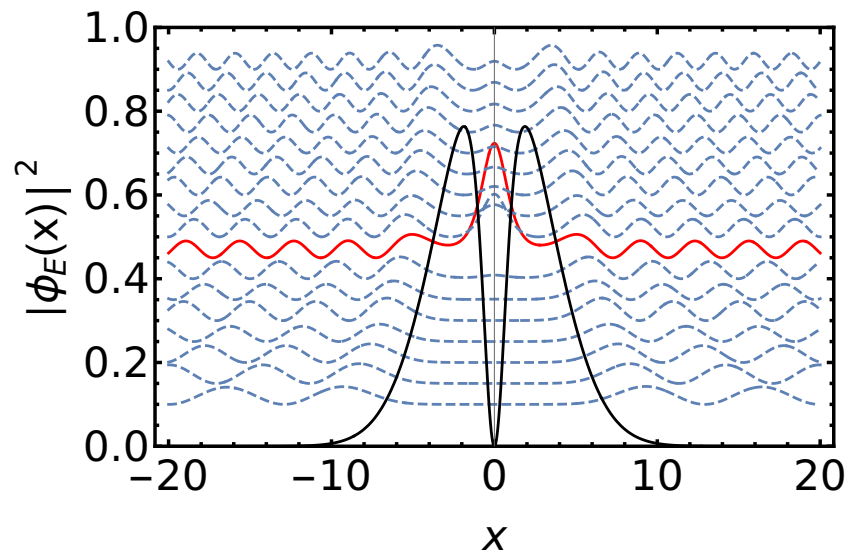
For $\alpha > 0$ state becomes a shape resonance

Bad example since no resonances above threshold

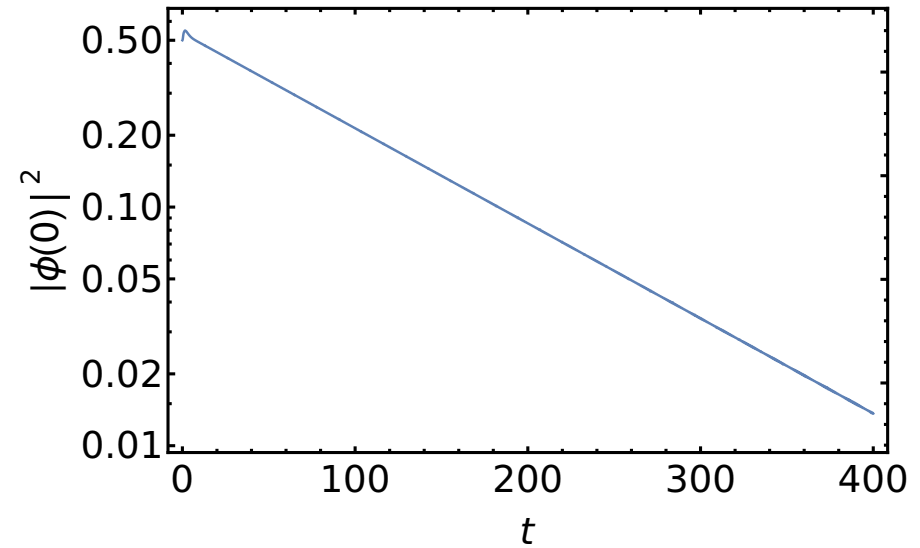
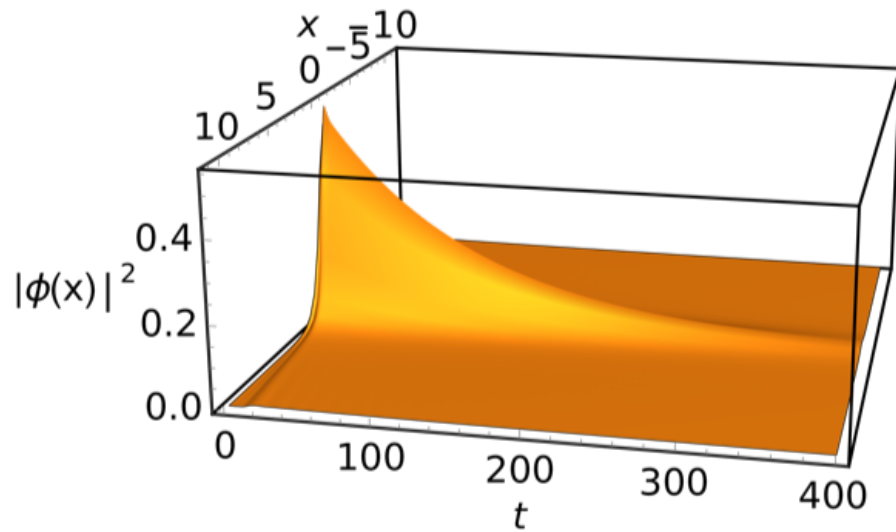
Will use $\alpha = 0.05$ below.

Shape resonance

We look at the scattering wave functions (normalized to flux and offset by energy) and see a remnant of the bound state wave function at $E = 0.465$. Characterised by a strong change in behaviour and lots of probability near the origin. Corresponds to a long time-delay in the scattering.

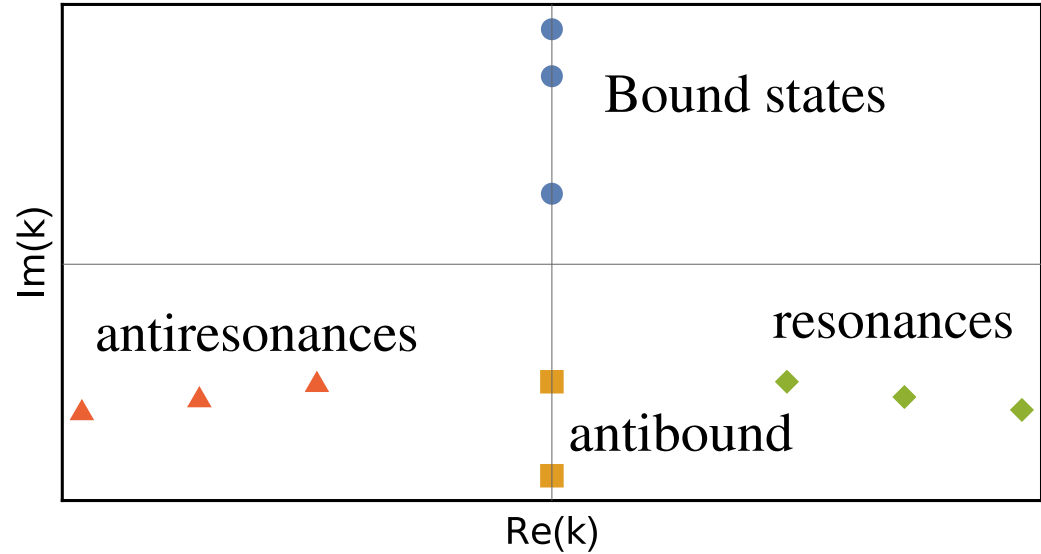
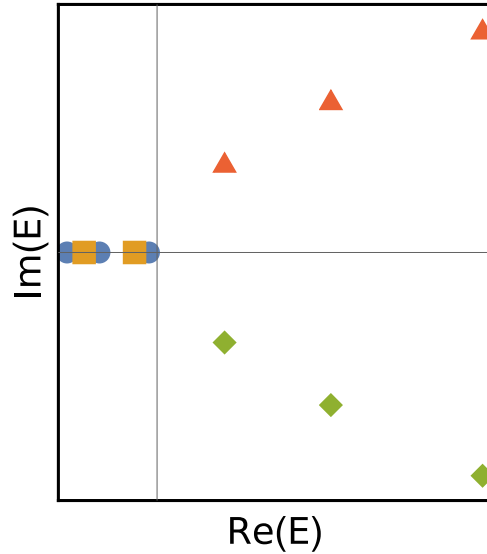


Exponential decay from bound state



Structure of spectrum

- Integrable states: bound states
- States that only grow exponentially (no oscillation): antibound
- Resonances, solution at complex energy, negative imaginary part
- Since H is Hermitian, antiresonances corresponding to incoming waves
- Note the second Riemann sheet of the square root



$$\psi \sim e^{ikr}$$

2. Formal scattering

Resonances need preparation: can really only be seen in scattering

unless the lifetime is very long, in which case the preparation is temporally separated from the decay: e.g., natural radioactive decay

Experimentally that requires the measurement of the (differential) cross section

Theoretically, that is approached through the S matrix

The idea is to describe the evolution from a non-interacting initial state in the far past to a non-interacting final state in the far future, interacting in the middle. [Normally allows “compound states”]

Formal definition in terms of Møller operators, but slightly less formally

$$S_{fi} = \langle f | U(\infty, -\infty) | i \rangle$$

The S matrix and scattering

S contains a trivial part; scattering uses $S = 1 + iT$, and then T gives the transition probability,

$$P_{i \rightarrow f}/V^{(4)} = (2\pi)^4 \delta^{(4)}(p_f - p_i) |T_{fi}|^2$$

Some trivial phase space factors turn this into the cross section.

So that raises lots of interesting questions: What is the structure of S and T ? What happens in the complex energy plane? How does that link to the Hamiltonian?

Resolvent and spectrum: link to S

The analytical properties of S and T can be encoded in the resolvent $(z - H)^{-1}$ (where we have replaced E by z to show it is complex). For a generic operator H , we can have multiple options (Reid and Simon) for a given z

1. The operator $(z - H)$ maps the whole Hilbert space \mathcal{H} onto itself: z is not part of the spectrum
2. There is an eigenvector $\Phi \in \mathcal{H}$, $(z - H)\Phi = 0$: z is part of the point spectrum. Resolvent not defined
3. There is a sequence $\Phi_n \in \mathcal{H}$ so that $\lim (z - H)\Phi_n = 0$, but $\lim \Phi_n$ is not in \mathcal{H} : z is part of the continuous or essential spectrum
4. $(z - H)$ maps \mathcal{H} onto a subset (not one to one) In this case $(z^* - H^\dagger)\Phi = 0$: residual spectrum, not for self-adjoint operators (If Hamiltonian is well behaved)

Consequences

The spectrum of H is only the point spectrum; continuous spectrum is not part of the Hilbert space

For a “normal” Hamiltonian, the continuous spectrum is only dominated by the kinetic energy (i.e., if a potential is smooth and decays fast at infinity).

So we find that the resolvent has poles at discrete energy corresponding to bound states, and is not defined along the positive real axis. As an analytic function, that is just a branch cut.

Branch cut as $\left(z - \frac{k^2}{2}\right)^{-1}$: that is a square root type behaviour.

Suggests that we have a double Riemann sheet cover of the complex plane: $k = \sqrt{2E}$.

We know that the choice of branch cut is arbitrary; in this case determined by the boundary conditions

Phase shifts

Of course we often define a resonance by a change in the phase shift of 180°

Why so?

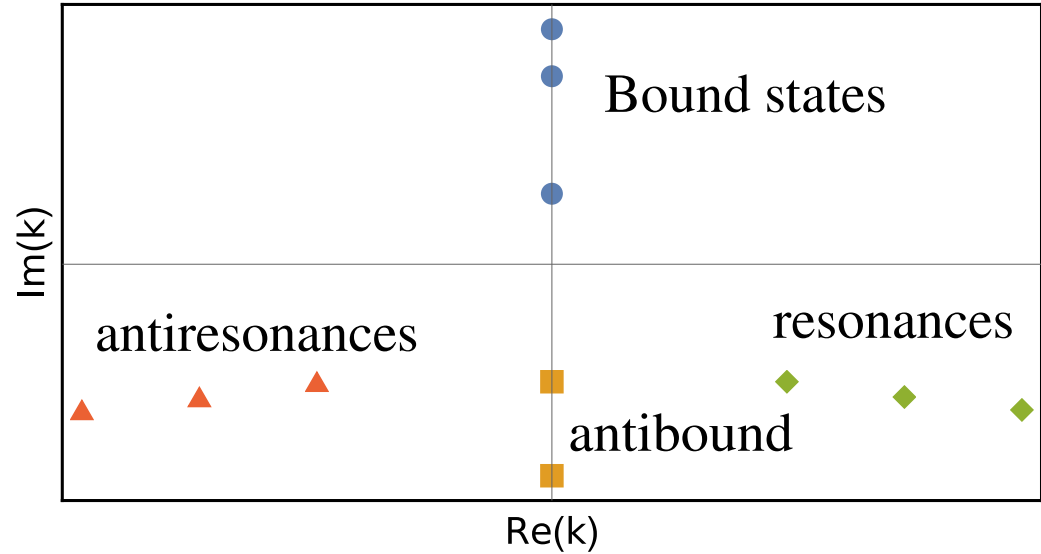
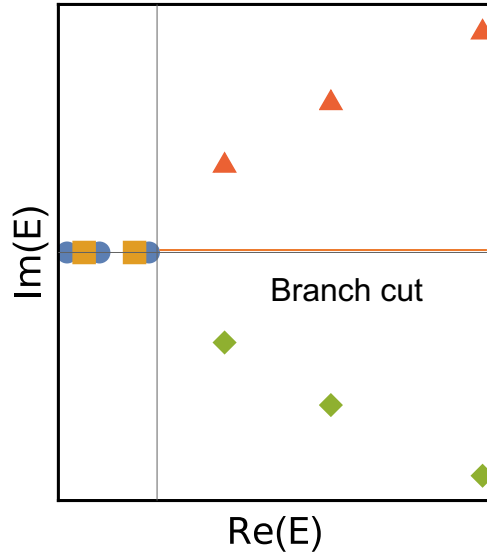
1. $S \propto e^{2i\delta(E)}$ (equals if elastic)
2. If we have a pole near (but just below) the real axis, we find that from

$$S \sim 1 + \frac{1}{2\pi} \frac{1}{E - E_r + i\Gamma/2},$$
$$\delta \approx \tan^{-1} \frac{\Gamma/2}{E_r - E}$$

3. So for an isolated pole, phase shift goes through 180 degrees

Structure of spectrum

- Integrable states: bound states
- States that only grow exponentially (no oscillation): antibound
- Resonances, solution at complex energy, negative imaginary part
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$$\psi \sim e^{ikr}$$

Breit Wigner form

So why does an (isolated!) pole give a Breit Wigner form:

Simple: $S(E) \sim T(E) = \frac{r}{E - E_R + \frac{i\Gamma}{2}}$. Contribution to Cross section

goes as the square:

$$\sigma \propto \frac{r^2}{(E - E_R)^2 + \frac{\Gamma^2}{4}}$$

Of course that fails for substantial smooth background.

Complex scaling

One of the very neat tricks to deal with the branch cut, is to change the Hilbert space

Complex scaling is one technique, where $r \rightarrow re^{i\theta}$ (and thus $p \rightarrow pe^{-i\theta}$).

It is immediately clear what happens: wherever the potential energy is irrelevant, we see $E \rightarrow Ee^{-2i\theta}$, i.e., the continuous spectrum rotates in the lower half plane

Poles in the lower part of the 2nd Riemann sheet (resonances) are now uncovered and become real eigenvalues of the non-Hermitian Hamiltonian

This can easily be applied numerically

Procedure goes back quite far, popularized in atomic and molecular physics.

Example

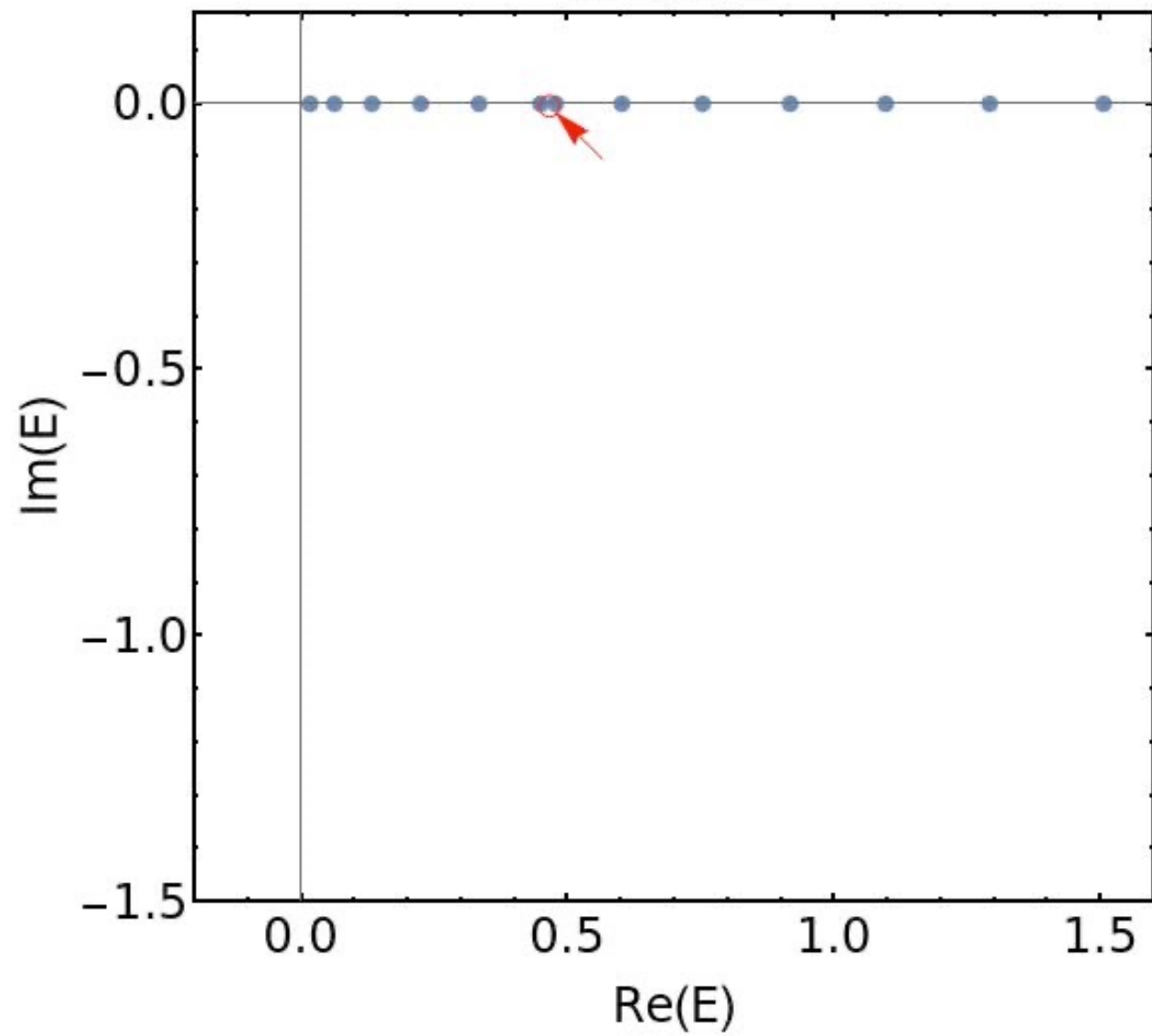
Let us return to the problem studied before, of the modified Pöschl-Teller potential,

$$V(x) = \left(1 - \frac{1}{\cosh^2 x}\right) e^{-\alpha x^2}$$

We know there is a narrow resonance at $E_R \approx 0.465$

Let us see what happens

$\theta=0.00$



Message part 1

Resonances are a scattering phenomenon

Can be studied without studying the full scattering problem

Analytic structure of the resolvent is key (since resolvent drives the structure of scattering)

Usually dominated by the “free Hamiltonian”

We can coax out the resonances by using a different branch cut.

But have only looked at “shape resonances”

Multi Channel

Many problems in physics are multi-channel

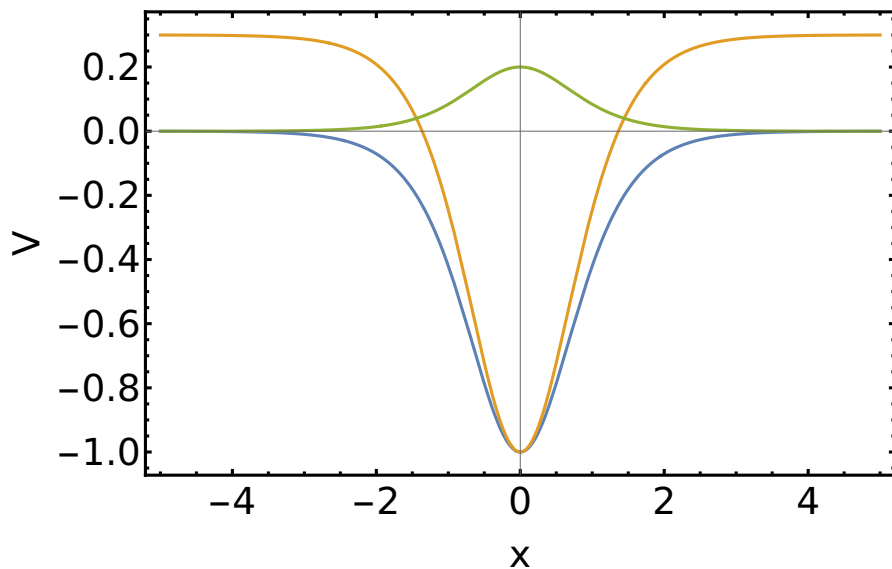
- Angular momentum coupling for non-central potentials
- Rearrangement channels
- Multi-particle break-up channels
- Multiple open decay channels

And even closed channels play a role

Analyticity of S matrix

Let us make a generic model of a two channel problem.

1D problem, with two $1/\cosh^2 x$ potentials, with similar coupling:



Blue, Yellow: potentials

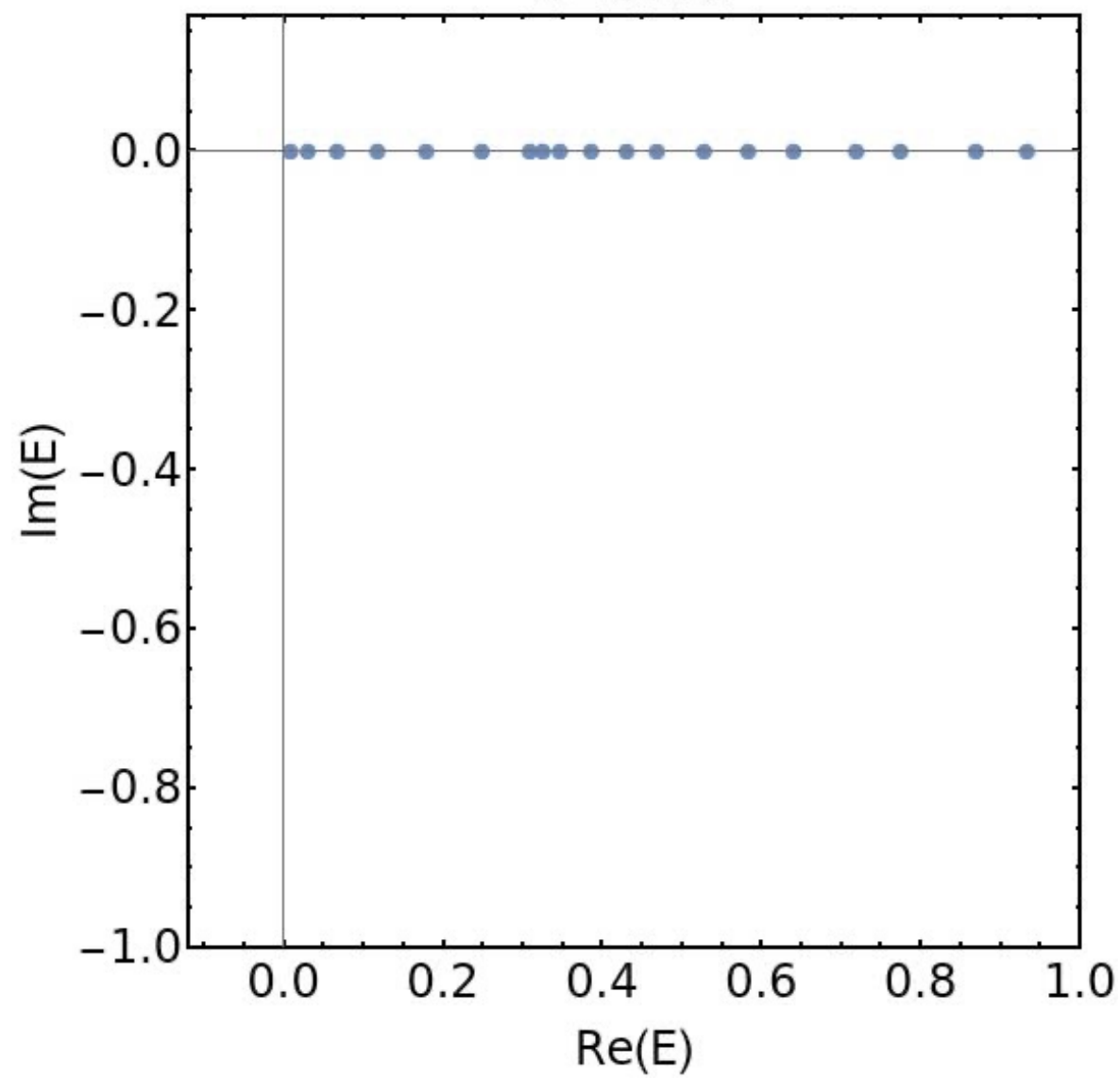
Green: coupling

No coupling, two bound states

Coupling: one deeply bound state

What happened?

$\theta=0.00$



Structure

We now have multiple Riemann sheets.

Poles uncovered and recovered

May want to find ways to move different continua at different rates (some control in atoms and molecules, little in nuclei)

Very tough when the thresholds coincide.

But possible

The channel coupling turned two bound states into one deeply bound state and a second state embedded in the continuum.

This is the Fano or Feshbach mechanism for resonances

Alternative Understanding of Resonances

Partition Hilbert space in a channel α and the rest (β)

$$P_\alpha + P_\beta = 1.$$

Project Hamiltonian on those channels

$$H = \begin{pmatrix} H_\alpha & V_{\alpha\beta} \\ V_{\beta\alpha} & H_\beta \end{pmatrix}$$

And calculate the full Green's function (with outgoing wave BCs)

$$P_\alpha \frac{1}{E - H + i0^+} P_\alpha = \frac{P_\alpha}{E - \mathcal{H}_\alpha(E)},$$
$$\mathcal{H}_\alpha(E) = H_\alpha + V_{\alpha\beta} \frac{1}{E - H_\beta + i0^+} V_{\beta\alpha}$$

There is a big differences between open (E above threshold for β) or closed channels

- Closed channel:
 - Interaction is always attractive: bound state moves down, as we have seen
- Open channel,
 - things are complicated, since we now have to be above the branch-cut,

$$\mathcal{H}_\alpha(E) = H_\alpha + V_{\alpha\beta} \mathcal{P}(E - H_\beta)^{-1} V_{\beta\alpha} - i\pi V_{\alpha\beta} \delta(E - H_\beta) V_{\beta\alpha}$$
 - Non-Hermitian Hamiltonian. First correction repulsive, and second term pushes any bound state to the second Riemann sheet (negative imaginary part): a resonance
 - See Newton for discussion how that leads to Bright-Wigner

Analytic structure of S matrix

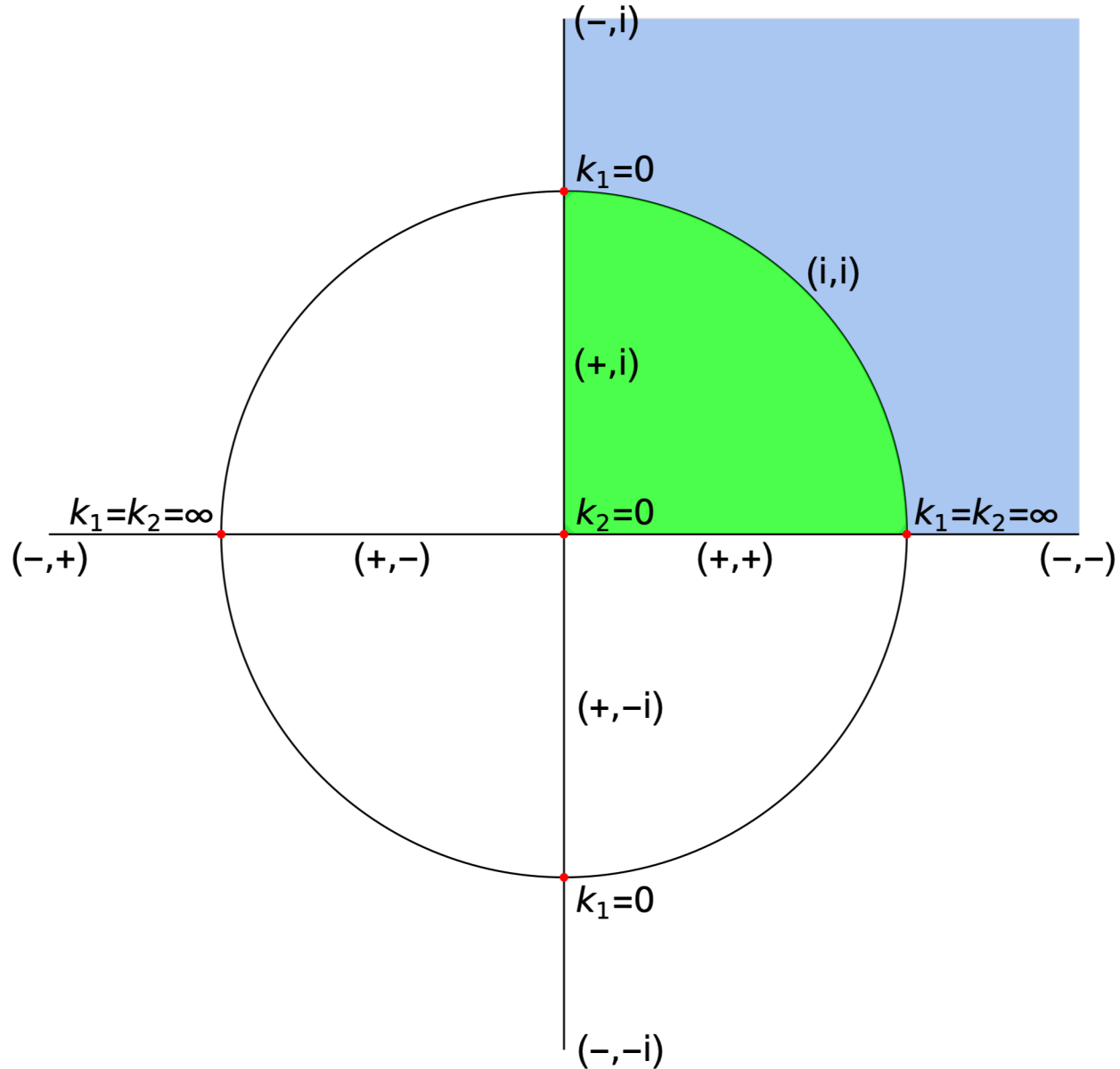
E is not the best variable to understand analyticity: for single channels it is k ($E = \hbar^2 k^2 / 2m$). S is a meromorphic function of k .

How about for two channels (let assume same mass, that doesn't have to be the case). We have two k 's encoding the energy, which are mapped as

$$k_1 + k_2 = \Delta \frac{1 + t}{1 - t}$$

$$k_1 - k_2 = \Delta \frac{1 - t}{1 + t}$$

Δ is the threshold in channel 2 relative to 1



Why

Useful to describe motion of poles on strengthening interactions
Can be continued to more channels: plane (or surface of sphere)
for two channel, torus for three channels, genus $[(n + 1)/2] - 1$
for n channels
Would like to show all of that

Channel opening

What happens if the energy is high enough to allow for new channels to open?

Most important for $l = 0$. Flux factor gives cross section linear in the channel momentum: so the slope of the “new” cross section is infinite as a function of E .

Also influences the old cross section: one flux!

So typically infinite slope of all cross sections: Threshold anomalies, and not resonances

To conclude

We have looked a little bit at resonances as poles of the S matrix
Complex scaling (and friends) are a good way to see what is happening
Much more complex in multichannel situations
Analytic structure of the energy plane will have many branch cuts
Can be mapped to a single plane with holes?
Look at Newton for a few examples.

References

RG Newton, Scattering Theory of Waves and Particles
(2nd ed, Springer, New York, 1982)

Adv. in Q. Chem 63 (2012) (CA Nicolides, E Brändas,
JR Sabin, eds)

Especially chapter 1: S Klaiman and I Gilary, on
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Unstable states

M Reid and B Simon, Methods of Modern
Mathematical Physics, Scattering Theory, Vol 3
(Elsevier, 1979)