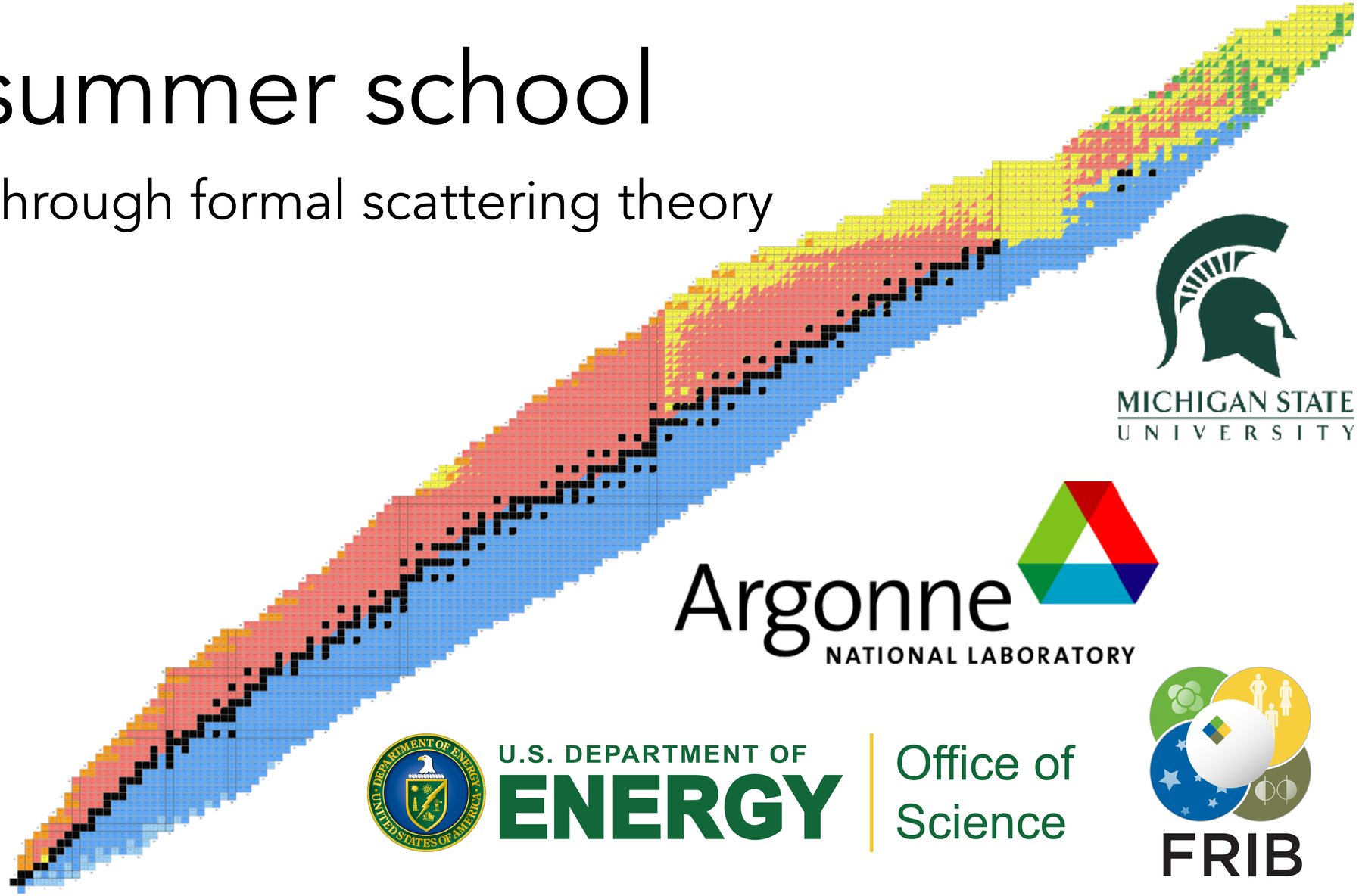
FRIB-TA summer school

A practical walk through formal scattering theory



Kévin Fossez

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Resonances

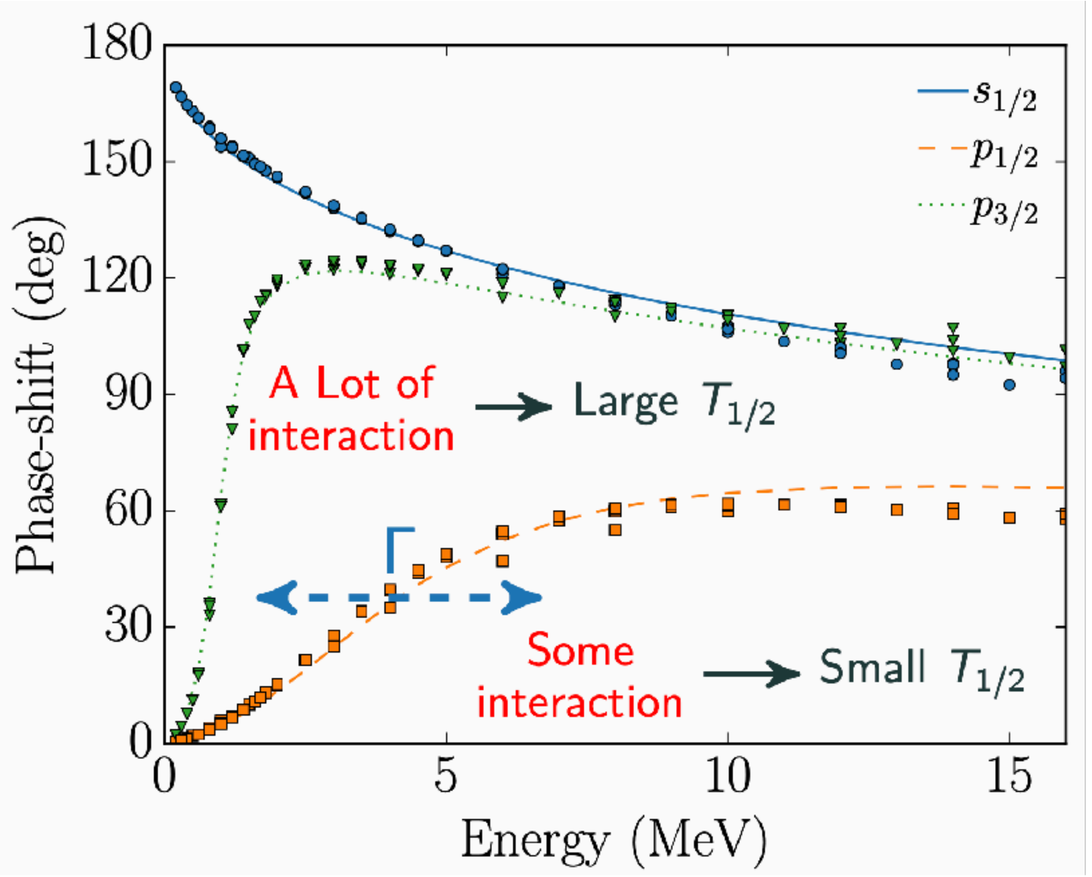
Decaying resonances have been known for a long time and are states characterized by their **energy position** E_r and their energy dispersion or **width** Γ.

The quantities E_r and Γ could be extracted from the phase shifts as shown on the figure.

Moreover, it was known that the **lifetime** $T_{1/2}$ of a resonance was directly related to its width by:

$$T_{1/2} = \frac{\hbar}{\Gamma} \ln 2$$

since it has to do with how long the projectile interacts with the target.



Resonances

The intriguing finding came when both G. Gamow and A. Siegert (independently) realized that the stationary solutions of the reduced radial Schrödinger equation with outgoing boundary condition $C^{-}(k) = 0$ (like for bound states) and $k = \kappa - i\gamma$ and $\kappa, \gamma > 0$, had complex energies:

$$E = E_r - i\frac{\Gamma}{2}$$

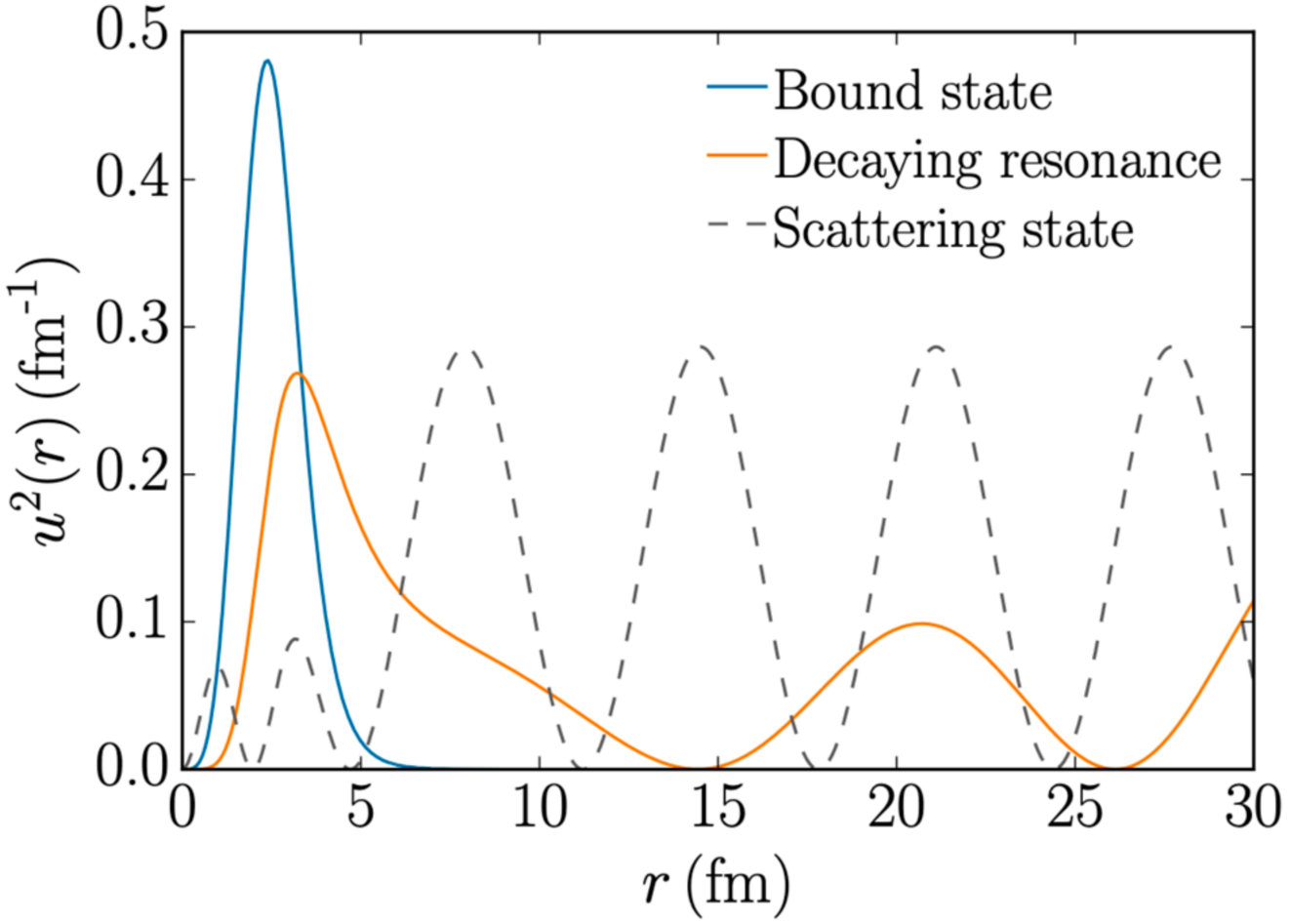
This finding opened some problem with, for instance, the asymptotic $e^{ikr} = e^{i\kappa r}e^{\gamma r}$ and the normalization.

These states are now known as Gamow or Siegert states and have been studied formally from many different approaches.

What is the nature of these solutions?

J.J. Thomson, Proc. London Math. Society, 197 (1884)
G. Gamow, Z. Physik 51, 204 (1928)
A. F. J. Siegert, Phys. Rev. 56, 750 (1939)

Resonances


Bound state
Decaying resonance
Scattering state
$u^2(r)$ (fm^{-1})
r (fm)
0.0
0.1
0.2
0.3
0.4
0.5
0
5
10
15
20
25
30

Resonances

From a more general perspective, the spectrum $\Sigma(H)$ of a Hamiltonian in a Hilbert space is defined as the set $\{\lambda\} \in \mathbb{C}$ such that the inverse of $\lambda - H$ is not defined. It is thus convenient to introduce the resolvent operator:

$$R(\lambda) = \frac{1}{\lambda - H}$$

and to find its singularities. It allows to divide $\Sigma(H)$ into three categories:

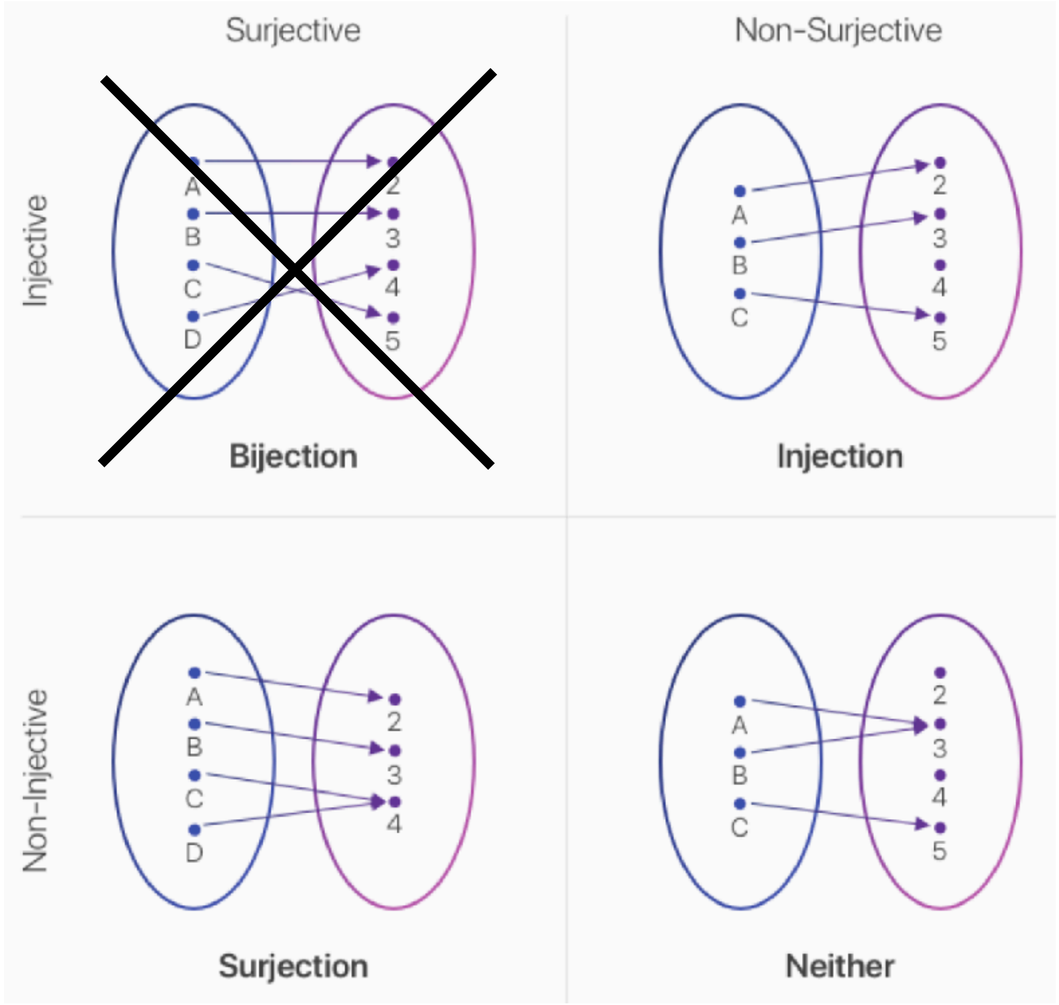
If $(\lambda - H)\,|\psi\rangle = |\phi\rangle$, how many $|\psi\rangle$ and $|\phi\rangle$ are there? How many are not connected?

- The point spectrum where $\lambda - H$ is not injective (bound states).

- The continuous spectrum where $\lambda - H$ is injective but not surjective, and its image is dense in the Hilbert space (scattering states).

- The residual spectrum where $\lambda - H$ is injective but not surjective, and its image is **not** dense in the Hilbert space (capturing, decaying, and antibound states).

Resonances

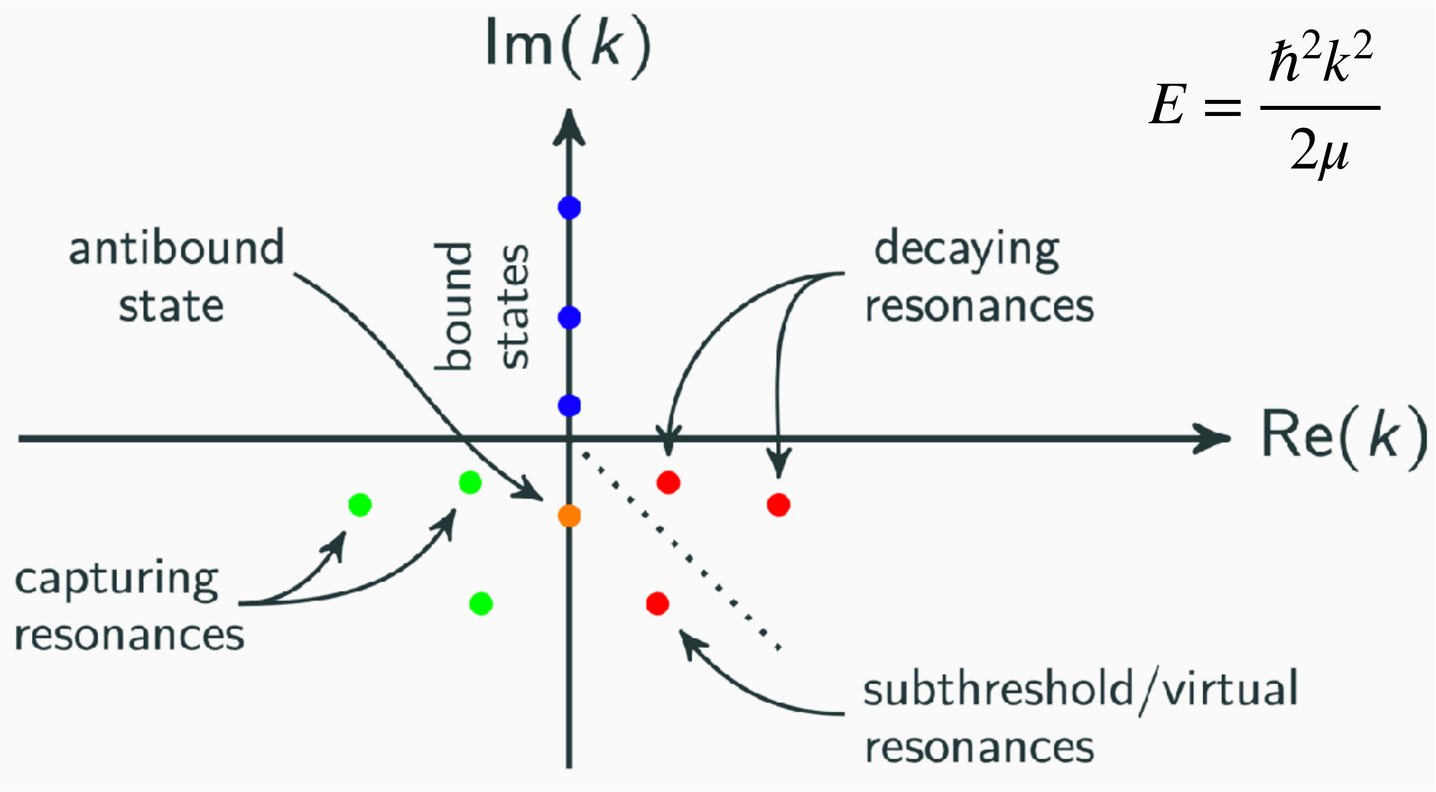


Scattering states are dense (continuum) and resonances are discrete, but both are not invariant by time reversal: $|\psi(-t)\rangle \neq |\psi(t)\rangle$, only one state can satisfy $(\lambda - H)|\psi\rangle = |\phi\rangle$.

Bound states are discrete and invariant by time reversal: $|\psi(-t)\rangle = |\psi(t)\rangle$, so "two" states can give the same $|\phi\rangle$.

Resonances

What is a time-reversed decaying resonance? A capturing resonance!



The complex-momentum plane is the appropriate way to visualize outgoing solutions ($C_l^-(k) = 0$) of the stationary Schrödinger equation.

What about antibound states and subthreshold resonances?

Here, we reach the limits of the quasi-stationary formalism.

Resonances

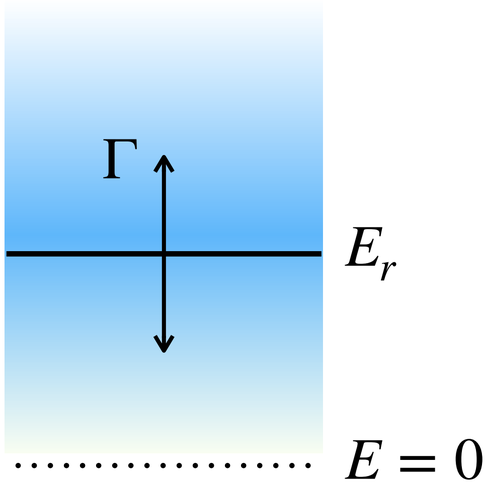
Let's take a step back and think about the physical meaning of Gamow/Siegert's finding. If the complex energy of a resonance can be written using the energy position (energy above the particle emission threshold) and width:

$$E = E_r - i\frac{\Gamma}{2}$$

and the width (dispersion around the energy position), to be safe one could impose:

$$E_r > \frac{\Gamma}{2}$$

If we pose $k = |k|e^{i\theta}$, since $E \propto k^2 = |k|^2 e^{2i\theta}$, to satisfy the condition on E_r and Γ one must have: $0 \geq \theta > -\pi/8$. However, it might be too restrictive, but one certainly must have $E_r, \Gamma > 0$, and this imposes: $0 \geq \theta > -\pi/4$.



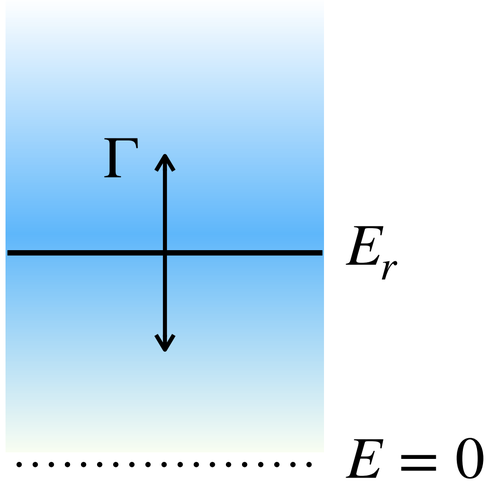
Math-enthusiats: show it.

Resonances

One can see that there is something “fishy” about the quasi-stationary description of resonances because there is some arbitrariness in what is a “physical” or “proper” resonance.

Fundamentally, we are trying to describe a time-dependent phenomenon as a stationary state. It is a representation which is appropriate for narrow resonances ($\Gamma/2 << E_r$), but less so for broad resonances ($\Gamma/2 \geq E_r$).

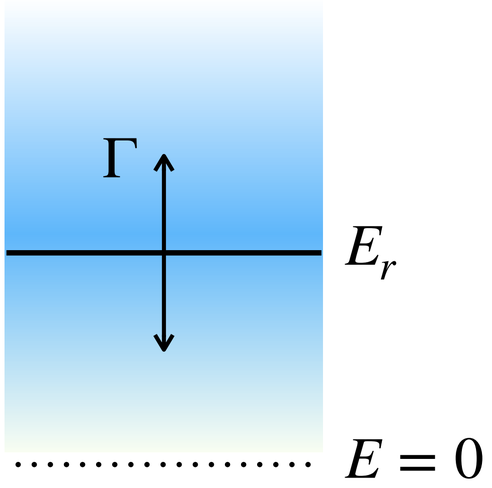
For this reason, we often call physical states those for which $k = |k| e^{i\theta}$ with $0 \geq \theta > -\pi/4$, but the problem is deeper than it seems.



Resonances

For instance, what if $\Gamma/2 < E_r$, but Γ is so large that it corresponds to a lifetime $T_{1/2} = (\hbar \ln 2)/\Gamma$ too short for all the particles of the system to interact with each other? Do we have one system or more?

Another way to think about resonances is as bound states with $E > 0$ **coupled to the continuum** of scattering states. The system stays in a given state for some time (stays a system) and then decays through continuum couplings (breaks apart).



This is a useful picture for many-body resonances (see later), but once again, it breaks down for broad resonances.

From here, we will only consider narrow resonances.

Jost functions

To study Gamow states, we need to introduce the Jost functions $J_l^{\pm}(k)$ defined using the Wronskian:

$$J_l^{\pm}(k) = W[u_l(k,r), u_l^{\pm}(k,r)] = u_l(k,r)\frac{du_l^{\pm}(k,r)}{dr} - \frac{du_l(k,r)}{dr}u_l^{\pm}(k,r)$$

and which is independent of r (easy to prove).

The wave functions $u_l^{\pm}(k,r)$ are just the outgoing and incoming components before matching with the known asymptotic form:

$$C_l^+(k)u_l^+(k,r) + C_l^-(k)u_l^-(k,r) \rightarrow u_l^{(out)}(k, r \geq r_m) = C_l^+(k)\hat{h}_l^+(kr) + C_l^-(k)\hat{h}_l^-(kr)$$

We will now connect the outgoing solutions (bound states and resonances) with the poles of the scattering matrix!

Jost functions

First, we need to remark that since at $r = r_m$ one must have:

$$C_l^+(k)u^+(k,r) + C_l^-(k)u^-(k,r) = C_l^+(k)\hat{h}_l^+(kr) + C_l^-(k)\hat{h}_l^-(kr)$$

It follows that the following Wronskians (which are independent of r) must satisfy:

$$W[u^+(k,r), u^-(k,r)] = W[\hat{h}_l^+(kr), \hat{h}_l^-(kr)]$$

but we also know that when $r \to \infty$, one has:

$$H_{l,\eta}^{\pm}(kr) \sim i^{\mp l} e^{\pm\sigma_l} e^{\pm i\left(kr - \eta \ln(2kr)\right)}$$

The Hankel functions $H_{l,\eta}^{\pm}(kr)$ are the generalization of the $\hat{h}_l(kr)$ when Coulomb is included.

This gives $H_{l,\eta}^{\pm}(kr)H_{l,\eta}^{\mp}(kr) = 1$ and:

$$\frac{dH_{l,\eta}^{\pm}(kr)}{dr} \sim \pm i\left(k - \frac{\eta}{r}\right) H_{l,\eta}^{\pm}(kr)$$

Jost functions

We can now evaluate one of the Wronskians. We will drop indices and arguments for simplicity:

$$
\begin{aligned}
W[H_l^+(kr), H_l^-(kr)] &= H^+ \frac{dH^-}{dr} - H^- \frac{dH^+}{dr} \\
&= H^+ H^- (-i)\left(k - \frac{\eta}{r}\right) - H^- H^+ (+i)\left(k - \frac{\eta}{r}\right) \\
&= -2i\left(k - \frac{\eta}{r}\right) \\
&\to -2ik
\end{aligned}
$$

At the end we just took the limit $r \to \infty$. This simple result will be very useful to express the wave function using the Jost functions.

Jost functions

We can now use a few tricks to re-express the wave function:

$$
\begin{aligned}
2iku &= -W[H^+, H^-]u \\
&= -W[u^+, u^-]u \\
&= \left(u^- \frac{du^+}{dr} - u^+ \frac{du^-}{dr}\right) u \\
&= \left(u^- \frac{du}{dr} u^+ - u \frac{du^-}{dr} u^+\right) - \left(u^+ \frac{du}{dr} u^- - u \frac{du^+}{dr} u^-\right) \\
&= J^- u^+ - J^+ u^-
\end{aligned}
$$

We thus have for the asymptotic wave function:

$$
u_l(k, r) = \frac{1}{2ik}[J_l^-(k) u_l^+(k, r) - J_l^+(k) u_l^-(k, r)]
$$

Jost functions

Here is the magic. We also know that at large distances the wave function can be written as:

$$u_l(k,r) = C_l^+(k)u_l^+(k,r) + C_l^-(k)u_l^-(k,r)$$

But also, using the S-matrix as defined before $S_l(k) = e^{2i\delta_l(k)}$:

$$u_l(k,r) = A_l(k)[u_l^-(k,r) - S_l^-(k)u_l^+(k,r)]$$

Remember, the S-matrix is the term we added in front of the outgoing part to account for the… scattering.

It follows immediately that:

$$J_l^{\pm}(k) = \mp 2ikC_l^{\mp}(k) \qquad S_l(k) = -\frac{C_l^+(k)}{C_l^-(k)} = \frac{J_l^-(k)}{J_l^+(k)} \qquad \delta_l(k) = \frac{1}{2i}\ln\left(\frac{J_l^-(k)}{J_l^+(k)}\right)$$

Finding the Jost functions (or $C_l^{\pm}(k)$) can give us scattering information for any type of solution (bound, scattering, and resonance state).

Jost functions

We note that for bound states and resonances, $C_l^-(k) = 0$, and the scattering matrix and the phase-shift diverge (there is no scattering after all). We say that these states are poles of the S-matrix.

Another use of the Jost functions is to find the discrete solutions or poles of the S-matrix. Indeed, since for such states $C_l^-(k) = 0$, and we showed that $J_l^{\pm}(k) = \mp 2ikC_l^{\mp}(k)$, we can look for values of k where $J_l^+(k) = 0$. We will denote the momentum of a pole k_p.

To do that, we first need the derivative of $J_l^+(k)$ with respect to k (the proof is rather long):

$$\left.\frac{dJ_l^+(k)}{dk}\right|_{k=k_n} = 2k_p \int_0^\infty dr\, u_l(k_p, r) u_l^+(k_p, r) = iJ_l^-(k_p) \int_0^\infty dr\, [u_l^+(k_p, r)]^2$$

Jost functions

It is then possible to express the outgoing Jost function $J_l^+(k)$ as a Taylor series and to vary the value of k until one gets $J_l^+(k = k_p) = 0$:

$$J_l^+(k) \approx (k - k_p) \frac{dJ_l^+(k)}{dk}\bigg|_{k=k_n}$$

In practice, it means that the wave function must be calculated from $r = 0$ up to $r = r_m$ and matched with the asymptotic form to fix $C_l^{\pm}(k)$ (and thus $J_l^{\pm}(k)$) for several values of k until the desired result is obtained. A simple bisection method can help converge on k_p.

Normalization

So far, we have carefully avoided the problem of the normalization of scattering states and decaying resonances.

In fact, it can be shown with some effort that for scattering states (with and without Coulomb potential) that the "normalization":

$$\int_0^\infty dr\, u_{l'}(k', r) u_l(k, r) = \delta_{k',k}\delta_{l',l}$$

See later for the missing complex conjugate.

is equivalent to:

$$C_l^+(k)C_l^-(k) = \frac{1}{2\pi}$$

The case of resonances requires an additional mathematical tool.

Normalization

For decaying resonances, $C_l^-(k) = 0$ and the main problem comes from the exponentially increasing asymptotic $e^{ikr} = e^{i\kappa r}e^{\gamma r}$ with $k = \kappa - i\gamma$ and $\kappa, \gamma > 0$.

One versatile way to deal with this problem is the exterior complex-scaling method. The idea is to break the integral into four terms to isolate the troublesome ones, and to rotate the integral path in the complex plane so that the exponentially increasing oscillations die-off.

We will consider a norm integral of the form:

$$\int_0^\infty dr\, u(k_p', r)u(k_p, r)$$

where k_p and k_p' are two poles of the same system.

Normalization

To illustrate the method, we will replace the wave functions by representative functions for simplicity. We will simply use $u(k,r) \rightarrow e^{ikr}$.

We first split the integral into an inner part $[0,R]$, and an outer part $]R,\infty[$. The first integral is necessarily finite since the wave function is regular in the interval. Then, for the second integral we rotate the integral path using the following change of variable:

$$r \rightarrow R + xe^{i\theta}$$

with $x \geq 0$ and θ a fixed parameter. The integral then writes:

$$\int_R^\infty dr\, e^{ik'_p r} e^{ik_p r} = \int_0^\infty dx\, e^{i\theta} e^{ik'_p(R+xe^{i\theta})} e^{ik_p(R+xe^{i\theta})} = e^{i\theta} e^{i(k'_p+k_p)R} \int_0^\infty dx\, e^{i(k'_p+k_p)xe^{i\theta}}$$

Normalization

Moreover, we can write $k_p = |k_p| e^{-i\theta_p}$ and $k'_p = |k'_p| e^{-i\theta'_p}$ with θ_p, $\theta'_p > 0$, and thus we have:

$$\int_R^\infty dr\, e^{ik'_p r} e^{ik_p r} = e^{i\theta} e^{i(k'_p + k_p)R} \int_0^\infty dx\, e^{i(k'_p + k_p)x e^{i\theta}}$$
$$= e^{i\theta} e^{i(k'_p + k_p)R} \int_0^\infty dx\, e^{ix(|k'_p| e^{i(\theta - \theta'_p)} + |k_p| e^{i(\theta - \theta_p)})}$$

In the exponential under the integral we have terms of the form:

$$ix|k'_p| e^{i(\theta - \theta'_p)} = x|k'_p|[-\sin(\theta - \theta'_p) + i\cos(\theta - \theta'_p)]$$

To ensure the convergence, one wants at least $\sin(\theta - \theta'_p) > 0$ or $\theta \in]\theta'_p, \theta'_p + \pi[$ (idem for θ_p).

Normalization

Using the exterior complex scaling it is thus possible to regularize a priori non-convergent integrals involving resonance states.

In the previous derivations, instead of using the usual norm in the Hilbert space, we used:

$$\int_0^\infty dr\, u(k_p', r) u(k_p, r)$$

In fact, the complete notation was:

$$\int_0^\infty dr\, \tilde{u}^*(k_p', r) u(k_p, r)$$

where the tilde means “time-reversal” and cancels the usual complex conjugate except for bound states where there is no time reversal.

Rigged Hilbert space

The presence of a time-reversed “bra” comes from the rigged Hilbert space (RHS).

As we saw in the first lecture, the Hilbert space is a vectorial space with a scalar product and in which any Cauchy series (sequence) converges. In short, Dirac distributions used everywhere in quantum mechanics and are resonances are not part of it.

This point was already noted at the foundation of quantum mechanics by P. Dirac himself and J. von Neumann, but it took several years before K. Maurin, I. Gel’fand, and N. Vilenkin formulated the RHS, also called Gel’fand triplet.

To make it simple, the RHS is the Hilbert space extended to distribution theory. In fact, the word “rigged” in RHS comes from a bad translation of a Russian word meaning “equipped” or “enriched”.

The concept is too formal to be presented here, but you should know that it exists.

Jost function method

H. Masui *et al.*, Prog. Theor. Exp. Phys. **2013**, 123A02 (2013)

Before we continue, let's review a method for the numerical project based on everything we saw before.

The principle of this method is to express the Schrödinger equation, which is a homogeneous 2nd order differential equation, as a system of two homogeneous 1st order differential equation where the unknowns are "r-dependent Jost functions".

First, we note that in the articles where this method was introduced and used, a different set of conventions was used:

$$H^{\pm}_{l,\eta}(z) = \begin{cases} F_{l,\eta}(z) \mp iG_{l,\eta}(z) & \eta \neq 0 \\ z[j_l(z) \mp iy_l(z)] & \eta = 0 \end{cases}$$

Instead of the NIST standard:

$$H^{\pm}_{l,\eta}(z) = \begin{cases} G_{l,\eta}(z) \pm iF_{l,\eta}(z) & \eta \neq 0 \\ z[y_l(z) \pm ij_l(z)] & \eta = 0 \end{cases}$$

and there is a typo: $H^{\pm}_{l,\eta=0}(z) = z[j_l(z) \pm iy_l(z)]$

Jost function method

H. Masui *et al.*, Prog. Theor. Exp. Phys. **2013**, 123A02 (2013)

We will derive the equations using the conventions of the articles, and then switch to the more conventional ones using:

$$H_l^{\pm}(z) \rightarrow \pm i H_l^{\mp}(z)$$

We start from the reduced radial wave function (including the Coulomb potential):

$$\frac{\partial^2}{\partial r^2} u_l(r,k) = \left(\frac{\ell(l+1)}{r^2} + 2mV(r) - \frac{2\eta k}{r} + k^2 \right) u_l(r,k) = \left(2mV(r) - q(r) \right) u_l(r,k)$$

and note, as we have seen, that the asymptotic solutions are of the form:

$$u_l(r,k) = \frac{1}{2} \left(F_{l,\eta}^{+}(k,r) H_{l,\eta}^{+}(k,r) + F_{l,\eta}^{-}(k,r) H_{l,\eta}^{-}(k,r) \right)$$

Jost function method

Of course, we already know that the functions $F^{\pm}_{l,\eta}(k,r)$ must be the Jost functions when $r \to \infty$ and become independent of r. If we take the first derivative of the wave function and use one of the two conditions from the *variation of parameter method:*

$$\frac{\partial}{\partial r}F^{+}_{l,\eta}(k,r)H^{+}_{l,\eta}(k,r) + \frac{\partial}{\partial r}F^{-}_{l,\eta}(k,r)H^{-}_{l,\eta}(k,r) = 0$$

We obtain (the prime means derivative w.r.t. r:

$$u'_l(r,k) = \frac{1}{2}\left(F^{+}_{l,\eta}(k,r)\frac{\partial}{\partial r}H^{+}_{l,\eta}(k,r) + F^{-}_{l,\eta}(k,r)\frac{\partial}{\partial r}H^{-}_{l,\eta}(k,r)\right)$$

Jost function method

Then, we calculate the second derivative of the wave function:

$$u_l''(r,k) = \frac{1}{2}\left(\frac{\partial}{\partial r} F^+_{l,\eta}(k,r) \frac{\partial}{\partial r} H^+_{l,\eta}(k,r) + F^+_{l,\eta}(k,r) \frac{\partial^2}{\partial r^2} H^+_{l,\eta}(k,r) \right.$$

$$\left. = + \frac{\partial}{\partial r} F^-_{l,\eta}(k,r) \frac{\partial}{\partial r} H^-_{l,\eta}(k,r) + F^-_{l,\eta}(k,r) \frac{\partial^2}{\partial r^2} H^-_{l,\eta}(k,r) \right)$$

and insert it into the Schrödinger equation:

$$\frac{1}{2}\left(\frac{\partial}{\partial r} F^+_{l,\eta}(k,r) \frac{\partial}{\partial r} H^+_{l,\eta}(k,r) + \frac{\partial}{\partial r} F^-_{l,\eta}(k,r) \frac{\partial}{\partial r} H^-_{l,\eta}(k,r) \right)$$

$$+ F^+_{l,\eta}(k,r)\left(\frac{\partial^2}{\partial r^2} H^+_{l,\eta}(k,r) + q(r) H^+_{l,\eta}(k,r) \right) + F^-_{l,\eta}(k,r)\left(\frac{\partial^2}{\partial r^2} H^-_{l,\eta}(k,r) + q(r) H^-_{l,\eta}(k,r) \right) = \frac{2m}{\hbar^2} V(r) u_l(r,k)$$

Jost function method

The second and third terms vanish because $H^{\pm}_{l,\eta}$ are solutions of the homogeneous Schrödinger equation ($V(r) = 0$). We are left with:

$$\frac{1}{2}\left(\frac{\partial}{\partial r}F^{+}_{l,\eta}(k,r)\frac{\partial}{\partial r}H^{+}_{l,\eta}(k,r) + \frac{\partial}{\partial r}F^{-}_{l,\eta}(k,r)\frac{\partial}{\partial r}H^{-}_{l,\eta}(k,r)\right) = \frac{2m}{\hbar^2}V(r)u_l(r,k)$$

We can then use the second condition of the variation of parameter method:

$$H^{-}_{l,\eta}(k,r)\frac{\partial}{\partial r}F^{-}_{l,\eta}(k,r) = -H^{+}_{l,\eta}(k,r)\frac{\partial}{\partial r}F^{+}_{l,\eta}(k,r)$$

which gives:

$$\frac{1}{2}\frac{\partial}{\partial r}F^{+}_{l,\eta}(k,r)\left(H^{-}_{l,\eta}(k,r)\frac{\partial}{\partial r}H^{+}_{l,\eta}(k,r) - H^{+}_{l,\eta}(k,r)\frac{\partial}{\partial r}H^{-}_{l,\eta}(k,r)\right) = H^{-}_{l,\eta}(k,r)\frac{2m}{\hbar^2}V(r)u_l(r,k)$$

Jost function method

We immediately recognize the Wronskian:

$$W[H^{-}_{l,\eta}(k,r), H^{+}_{l,\eta}(k,r)] = 2ik$$

In the end we have the two 1st order equations to solve:

$$\frac{\partial}{\partial r} F^{\pm}_{l,\eta}(k,r) = \pm \frac{1}{ik} \frac{2m}{\hbar^2} V(r) H^{\mp}_{l,\eta}(k,r) u_l(r,k)$$

Jost function method

For the programming project, we go back to the more conventional notations and get:

$$u_l(r,k) = \frac{i}{2}\left(F^+_{l,\eta}(k,r)H^-_{l,\eta}(k,r) - F^-_{l,\eta}(k,r)H^+_{l,\eta}(k,r)\right)$$

And:

$$\frac{\partial}{\partial r}F^\pm_{l,\eta}(k,r) = \pm\frac{1}{ik}2mV(r)(\mp i)H^\pm_{l,\eta}(k,r)u_l(r,k)$$

Moreover, we will not consider the Coulomb potential ($\eta = 0$), so we can use:

$$H^\pm_{l,\eta=0}(z) = \hat{h}^\pm_l(z) = z[y_l(z) \pm ij_l(z)]$$