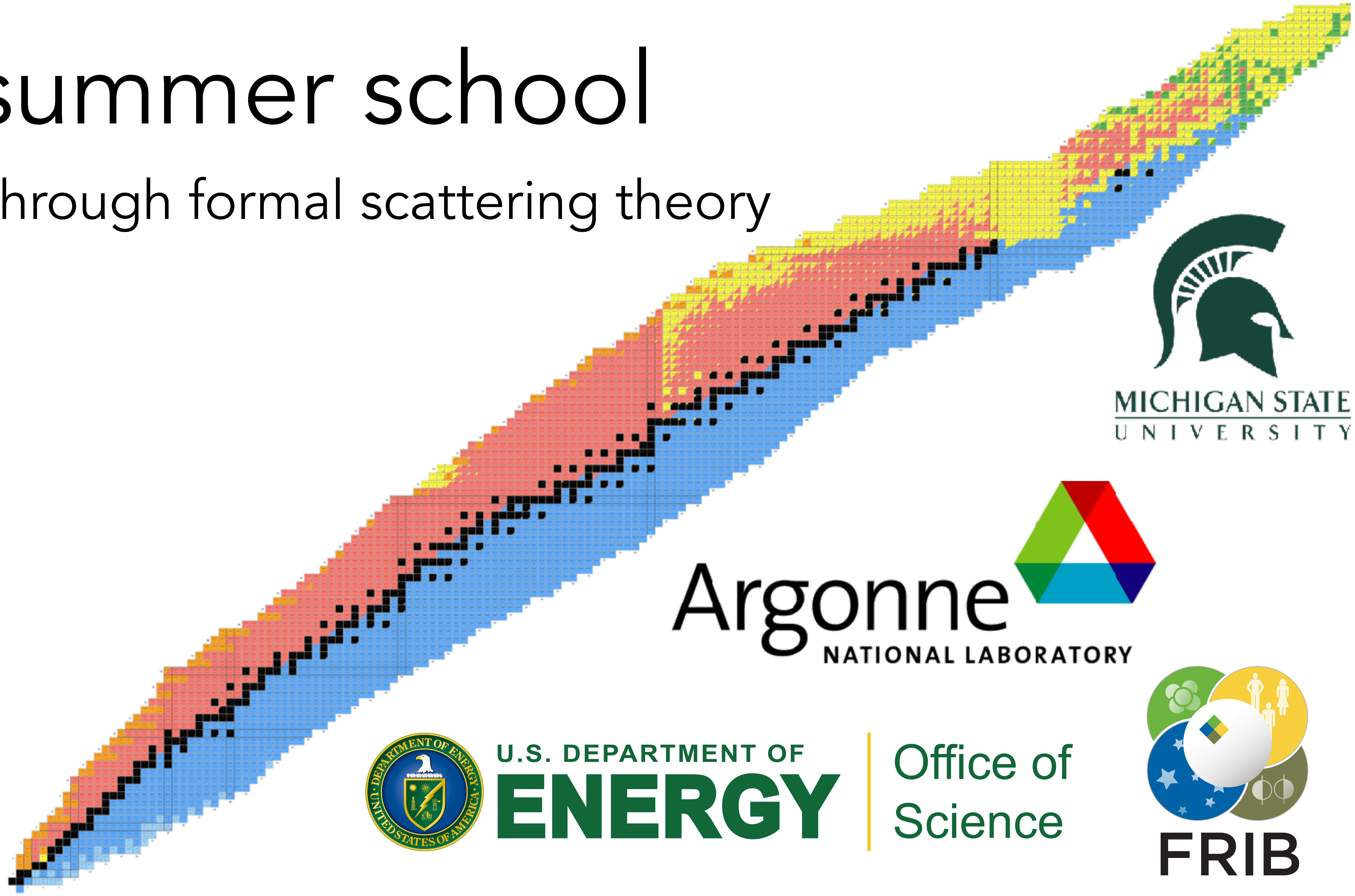
FRIB-TA summer school

A practical walk through formal scattering theory



Kévin Fossez

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Quasi-stationary formalism (D2-A1, 2h)

J. R. Taylor, *Scattering Theory: The Quantum Theory on Nonrelativistic Collisions, John Wiley and Sons, Inc., New York,* 1st ed. (1972)

A. Messiah, *Quantum Mechanics,* Vol. 1, North Holland, Amsterdam, 1st ed. (1961)

R. G. Newton, *Scattering Theory of Waves and Particles,* Springer-Verlag, New York, 2nd ed. (1982)

N. Michel and M. Płoszajczak, *Gamow Shell Model: A Unified Theory of Nuclear Structure and Reactions,* Lecture Notes in Physics, Springer Vol. 983 (2021)

NIST Handbook of Mathematical Functions (https://dlmf.nist.gov/)

Free stationary scattering states

We saw in lecture D1-M1 that if one looks for stationary (time-independent) solutions of the Schrödinger equation for a spherical potential, one can treat the radial part separately by solving:

$$\left(-\frac{1}{2\mu}\frac{d^2}{dr^2}+\frac{l(l+1)}{2\mu r^2}+V(r)\right)u_l(r)=E_l u_l(r)$$

Let's consider first the non-interacting case $V(r)=0$. This is an important case as in many problems the potential vanishes at large distances ($r\rightarrow\infty$), and thus it will give us the asymptotic solution for such situations. Here, we just have two particles moving freely in space.

Note: Physical solutions must vanish at the origin: $u_l(r=0)=0$.

Free stationary scattering states

We reintroduce the factor "r" that we simplified earlier when we defined $u_l(r) = rR_l(r)$.

$$\left(-\frac{1}{2\mu}\frac{1}{r}\frac{d^2}{dr^2}(r\cdot) + \frac{l(l+1)}{2\mu r^2} - E_l \right) R_l(r) = 0 \qquad E = \frac{k^2}{2\mu}$$

Using the fact that:

$$\frac{1}{r}\frac{d^2}{dr^2}(r\cdot) = \frac{1}{r^2}\frac{d\,\cdot}{dr}\left(r^2 \frac{d\,\cdot}{dr} \right) = \frac{2}{r}\frac{d\,\cdot}{dr} + \frac{d^2}{dr^2}$$

we get:

$$\left(\frac{2}{r}\frac{d\,\cdot}{dr} + \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k_l^2 \right) R_l(r) = 0$$

Free stationary scattering states

It is now apparent that the change of variable $\rho = kr$ leads to the equation defining the spherical Bessel functions:

$$\left(\rho^2 \frac{d^2}{d\rho^2} + 2\rho \frac{d}{d\rho} + \rho^2 - l(l+1)\right)\Pi_l(\rho) = 0$$

$R_l(r) \to \Pi_l(\rho)$

This 2nd order differential equation has two analytically known solutions $j_l(\rho)$ and $y_l(\rho)$ (also written $-n_l(z)$ and called spherical Neumann function). We will see details later.

It follows that the solution must be a linear combination of the spherical Bessel functions:

$$\Pi_l(kr) = \alpha(k) j_l(kr) + \beta(k) y_l(kr)$$

Because $y_l(kr)$ is irregular when $r \to 0$, one must have: $\beta(k) = 0$.

Free stationary scattering states

It is usually more convenient to consider:

$$u_l(k, r) = r\Pi_l(kr) = r\alpha(k)j_l(kr) = \gamma(k)krj_l(kr)$$

$\gamma(k)$ to determine

When $r \to 0$, it can be shown that the proper behavior $u_l(k, r) \sim C_{l,0}(k)r^{l+1}$ is obtained since:

$$zj_l(z) \sim \frac{z^{l+1}}{(2l+1)!!}[1 + \mathcal{O}(z^2)]$$

Why $u_l(k, r) \sim C_{l,0}(k)r^{l+1}$? It has to do with having a wave function that behaves "nicely" and is regular at the origin (see next slide).

Condition at the origin

If we assume that, when $r \to 0$, $V(r)$ is analytical i.e can be expanded as a Taylor series):

$$V(r) = V(r=0) + \frac{1}{1!}\frac{dV(r)}{dr}\bigg|_{r=0}(r-0) + \frac{1}{2!}\frac{d^2V(r)}{dr^2}\bigg|_{r=0}(r-0)^2 + \dots$$

and the wave function can be written as:

$$u(r) = r^s(1 + a_1 r + a_2 r^2 + \dots)$$

By injecting these into the Schrödinger equation we are left with:

$$-s(s+1) + l(l+1) = 0$$

The solutions are $s = -l$ and $l+1$, and gives the **condition at the origin** $u(r,k) \sim C_{l,0}(k) r^{l+1}$ since the other one is irregular.

Free stationary scattering states

At large distances $r \to \infty$, one should expect to have a plane-wave type of behavior $e^{\pm ikr}$. This can be seen by introducing the spherical Riccati-Hankel functions (see details later):

$$h^{\pm}(z) = y_l(z) \pm i j_l(z)$$

Sometimes denoted $h^{(1,2)}(z)$

It is easy to see that one has:

$$j_l(z) = \frac{h_l^+(z) - h_l^-(z)}{2i}$$

$$y_l(z) = \frac{h_l^+(z) + h_l^-(z)}{2}$$

and since: $h_l^{\pm}(kr) \sim e^{\pm ikr}/(kr)$ when $r \to \infty$, the proper behavior is obtained. In practice, we just say that at large distances (more later):

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

$$\hat{h}_l^{\pm}(z) = z h_l^{\pm}(z)$$

Free stationary scattering states

Finally, we can determine $\gamma(k)$ by normalizing the reduced radial wave function (and fix $C_{l,0}(k)$):

$$u_l(k,r) = \gamma(k) k r j_l(kr)$$

In spherical coordinates, one must have:

$$\int_0^\infty drr^2 \int_0^\pi d\theta \cos\theta \int_0^{2\pi} d\phi \, \Psi^*(\vec{r})\Psi(\vec{r}) = 1$$

With $\Psi(\vec{r})$ the total wave function:

$$\Psi(\vec{r}) = \langle r,\theta,\phi \,|\, \Psi \rangle = \frac{u_{n,l}(r)}{r} \times Y_{l,m}(\theta,\phi) = \gamma(k) k j_l(kr) Y_{l,m}(\theta,\phi)$$

Free stationary scattering states

Using the fact that:

$$\int_0^{\pi} d\theta \cos\theta \int_0^{2\pi} d\phi\, Y_{l',m'}(\theta,\phi) Y_{l,m}(\theta,\phi) = \delta_{l',l}\delta_{m',m}$$

Math-enthusiats: can you get the $\pi/(2k^2)$ result?

one is left with:

$$\gamma^*(k')\gamma(k)k^2\delta_{l',l}\delta_{m',m}\int_0^{\infty} drr^2\, j_l'(k'r)j_l(kr) = |\gamma(k)|^2 k^2 \delta_{l',l}\delta_{m',m}\frac{\pi}{2k^2}\delta_{k',k} = 1$$

We thus have: $|\gamma(k)|^2 = 2/\pi$. In the end, the normalized reduced radial wave function for a free particle is:

$$u_l(k,r) = \sqrt{\frac{2}{\pi}}krj_l(kr) \qquad \int_0^{\infty} dr\, u_{l'}^*(k',r)u_l(k,r) = \delta_{k',k}\delta_{l',l}$$

Quasi-stationary formalism

The result obtained, i.e. the (analytical) radial wave function of a "stationary scattering state” as a solution of the time-independent Schrödinger equation, has profound implications at a formal level.

- **Can we extract reaction observables (cross-section) and related quantities (phase-shifts, scattering amplitudes)?**

- If a scattering state ($k \in \mathbb{R}^+$) can be described from the time-independent Schrödinger equation, can we describe a resonance by analytical continuation of the wave function ($k \in \mathbb{C}$)?

- What is the integral formulation of this formalism and how does it connects with the time-dependent formalism?

Quasi-stationary formalism

We showed previously that the free wave function had the form: $$u_l(k,r) = \sqrt{\frac{2}{\pi}} kr j_l(kr)$$

Now, we switch on the potential $V(r) \neq 0$, still look for a scattering state, and assume that:

$$\lim_{r \to \infty} |V(r)| r^2 = 0$$

This condition ensures that the potential vanishes faster than the centrifugal term when $r \to \infty$, so we can recover the free solution asymptotically (spherical Bessel functions). One notes that it excludes, for example, the deceptively simple Coulomb potential:

$$V_C(r) = \frac{2\eta(k)k}{r}$$

$$\eta(k) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0} \frac{m}{\hbar^2 k}$$

Sommerfeld parameter

What happens at large distances?

Stationary scattering states

The asymptotic form of $j_l(kr)$ (free particle) is simply:

$$j_l(kr) \sim \frac{1}{kr}\sin\left(kr - \frac{\pi}{2}l\right) = -\frac{1}{2ik}\left(\frac{e^{-i\left(kr-\frac{\pi}{2}l\right)}}{r} - \frac{e^{+i\left(kr-\frac{\pi}{2}l\right)}}{r}\right)$$

but if $V(r) \to 0$ when $r \to \infty$, the asymptotic solution of a scattering state must have the same form as the free solution, and since the incoming part $\propto e^{-ikr}$ cannot change because of the potential, the only thing that can differ due to the scattering process is the phase of the outgoing part.

We use the convention:

$$e^{+i\left(kr-\frac{\pi}{2}l\right)} \to e^{2i\delta_l(k)}e^{+i\left(kr-\frac{\pi}{2}l\right)} = S_l(k)e^{+i\left(kr-\frac{\pi}{2}l\right)}$$

where $S_l(k)$ is the so-called **scattering matrix** with $|S_l(k)| = 1$ and $\delta_l(k)$ the scattering **phase-shift**.

Stationary scattering states

The free solution we found is uniquely defined by its angular momentum l, m and its momentum k (which could correspond to different momenta $\mathbf{k}$). The ensemble of these spherical waves form a complete ensemble.

However, the plane waves $e^{i\mathbf{k}.\mathbf{r}}$ form another complete set of solutions, which do not have a defined angular momentum l, m but a well defined $\mathbf{k}$. This is another valid free solution (in Cartesian coordinates $\mathbf{k} = (k_x, k_y, k_z)$).

It can be shown that by taking the momentum $\mathbf{k}$ along the z axis, the plane wave can be expanded using the free solutions as:

$$e^{i\mathbf{k}.\mathbf{r}} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta)$$

Math-enthusiats: good luck.

This is an important formula because in practice, plane waves are used to model the incoming target in scattering experiments.

Stationary scattering states

We can now nicely connect the asymptotic free solution with the plane wave representation, and extract scattering information in relation to experiments, without ever solving the time-dependent Schrödinger equation! (Wait for the next chapter)

The usual ansatz for the asymptotic wave function when $V(r) \neq 0$ is simply the sum of the incident plane wave $e^{i\mathbf{k}.\mathbf{r}}$ (which is a free solution of defined $\mathbf{k}$ but not l, m) and the scattered spherical wave e^{ikr}/r times an angular factor $f_k(\theta, \phi)$ called scattering amplitude.

$$u_l(k, r) \sim e^{i\mathbf{k}.\mathbf{r}} + f_k(\theta, \phi)\frac{e^{ikr}}{r}$$

This is of course an approximation since in real experiments one does not have a perfect plane wave (but a packet), there are interferences between the incident and scattered waves, etc. but it is useful to model experiments.

Stationary scattering states

Of course, the ansatz for the asymptotic wave function must equal the free asymptotic modified by the scattering phase-shift introduced before with the S-matrix notation:

$$e^{i\mathbf{k}.\mathbf{r}} + f_k(\theta,\phi)\frac{e^{ikr}}{r} = \sum_{l=0}^{\infty}(2l+1)i^l\left[-\frac{1}{2ik}\left(\frac{e^{-i\left(kr-\frac{\pi}{2}l\right)}}{r} - S_l(k)\frac{e^{+i\left(kr-\frac{\pi}{2}l\right)}}{r}\right)\right]P_l(\cos\theta)$$

If we introduce the expansion of the plane wave $e^{i\mathbf{k}.\mathbf{r}}$, the incoming parts cancel and we obtain:

$$f_k(\theta,\phi)\frac{e^{ikr}}{r} + \sum_{l=0}^{\infty}(2l+1)i^l\left(-\frac{1}{2ik}\right)(S_l(k)-1)\frac{e^{+i\left(kr-\frac{\pi}{2}l\right)}}{r}P_l(\cos\theta) = 0$$

Math-enthusiats:
$i^l e^{i\frac{\pi}{2}l} = 1.$

which finally gives:

$$f_k(\theta,\phi) = \sum_{l=0}^{\infty}(2l+1)\frac{S_l(k)-1}{2ik}P_l(\cos\theta)$$

Stationary scattering states

We immediately see that with our choice of having $\mathbf{k}$ along the z axis: $f_k(\theta, \phi) = f_k(\theta)$. This quantity represents the fraction of the incident plane wave which is scattered. Usually, we also define the partial wave amplitude:

$$f_l(k) = \frac{S_l(k) - 1}{2ik} = \frac{1}{k} e^{i\delta_l(k)} \sin(\delta_l(k)) = \frac{1}{k(\cot \delta_l(k) - i)}$$

Math-enthusiats: show the last identity.

In the end, we simply have:

$$f_k(\theta) = \sum_{l=0}^{\infty} (2l+1) f_l(k) P_l(\cos\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l(k)} \sin(\delta_l(k)) P_l(\cos\theta)$$

The final step is to calculate the total scattering cross section as:

$$\sigma = \int_0^{\pi} d\theta \cos\theta \int_0^{2\pi} d\phi \, |f_k(\theta)|^2 = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2(\delta_l(k))$$

Quasi-stationary formalism (D3-M1, 1h30)

- Can we extract reaction observables (cross-section) and related quantities (phase-shifts, scattering amplitudes)?

- **If a scattering state ($k \in \mathbb{R}^+$) can be described from the time-independent Schrödinger equation, can we describe a resonance by analytical continuation of the wave function ($k \in \mathbb{C}$)?**

- What is the integral formulation of this formalism and how does it connects with the time-dependent formalism?

Bound states

Previously, we looked at the effect of having $V(r) \neq 0$ on a scattering state with $E > 0$. Now, let's look at the case of bound state with $E < 0$. One recalls the radial equation:

$$\left(-\frac{1}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)}{2\mu r^2} + V(r) \right) u_l(r) = E_l u_l(r) \qquad \lim_{r\to\infty} |V(r)| r^2 = 0$$

We will assume that the potential is attractive enough to support a bound state and that we already know the momentum k of the considered bound state. Finding this momentum k is an interesting problem in itself.

As mentioned previously, when there is a potential barrier, it might be possible to have bound states but also decaying resonances, which in some ways look like "temporary bound states".

Bound states

We have already used one of the three conditions necessary to uniquely define a solution: the **regularity at the origin** $u(r, k) \sim C_{l,0}(k) r^{l+1}$. This was enough for the free particle problem since there were only two mathematically possible solutions $j_l(kr)$ and $y_l(kr)$ valid at any distance, and only one physically acceptable, but this is not true in the general case.

In practice, if $V(r) \neq 0$ vanishes at large distances, we need to fix the asymptotic behavior of the wave function as well to uniquely determine the solution, and, of course, to normalize the wave function.

This is where one of the most useful “trick” in scattering theory comes in. The idea is to divide a problem into inner and outer regions defined by a distance $r = r_m > 0$ after which the potential can be neglected.

Bound states

Let's assume that in practice $V(r \geq r_m) = 0$. We already know from the free particle problem that in this case, spherical Bessel functions are both solutions and since the origin is not included one must consider both contributions in the outer region:

$$u_l^{(out)}(k, r \geq r_m) = \alpha(k)krj_l(kr) + \beta(k)kry_l(kr)$$

To prepare for the next lectures, we introduce (again) the Riccati-Hankel functions ($\eta = 0$ means no Coulomb potential):

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

It is easy to see that the wave function in the outer region can be expressed equivalently as:

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

Continuity conditions

Now, all we need to do is to impose that whatever regular-at-the-origin wave function $u_l^{(in)}(r,k)$ we have in the inner region matches the wave function $u_l^{(out)}(k,r)$ in the outer region at $r = r_m$:

$$u_l^{(in)}(k, r_m) = u_l^{(out)}(k, r_m)$$

and that the same is true for their derivatives:

$$\frac{d}{dr} u_l^{(in)}(k,r)\bigg|_{r=r_m} = \frac{d}{dr} u_l^{(out)}(k,r)\bigg|_{r=r_m}$$

These are the **two continuity conditions** and they determine the asymptotic constants $C_l^{\pm}(k)$.

Bound states

If the potential has a bound state, by definition the wave function must vanish when $r \to \infty$ and there cannot be any incoming wave. Since the asymptotic behavior of Hankel functions is:

$$\hat{h}_l^{\pm}(kr) \propto e^{\pm ikr}$$

we must have: $C_l^{-}(k) = 0$ and $k = +i|k|$ for the wave function to behave like $u_l(k, r) \propto e^{-|k|r}$. It follows that for a bound state one must have:

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

One note that $k = -i|k|$ gives a negative energy too, but it corresponds to a virtual bound state or antibound state and is not a physically acceptable solution (exponential divergence).

Bound states

Of course, bound states must be normalized by satisfying:

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

which is easily done since the wave function is analytical everywhere and falls off exponentially when $r \to \infty$.

One notes that for a scattering state, one would have had $C_l^\pm(k) \neq 0$, and the main issue would have been the normalization (more later).

At that point, one can look at another known type of solution: decaying resonances, but this will require a little detour to the origins of the quasi-stationary formalism.