Week 7

PHY 304 Quantum Mechanics-II

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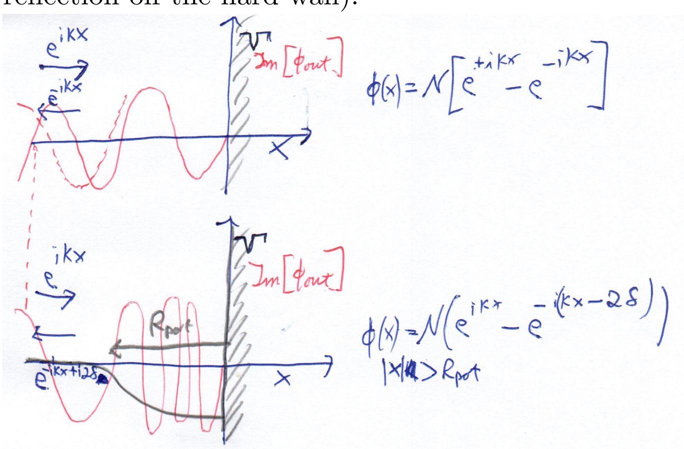
8.3.3 Scattering phase shifts

In the discussion so far, each partial wave amplitudes was one complex number. It turns out, we can use physical insight to reduce the required information further, into one real phase shift.

First consider the example sketched below, where we return to 1D scattering for simplicity, and probe a potential $V(x)$ bordered by a hard wall. The hard wall makes sure that the impinging quantum wave will be reflected with probability 1. However we can still learn something about the potential, if we can record the phase shift of the outgoing wave, compared to the case of $V(x)$ (just reflection off the hard wall).



left: Without any potential prior to the hard wall, we just have a scattering wavefunction $\phi(x) = \mathcal{N}(e^{ikx} - e^{-ikx}$, stating that wavenumber must be $k = \sqrt{2mE}/\hbar$ and we require $\phi(x = 0) = 0$ due to the hard wall boundary condition. With the potential, we still require the same boundary condition, and due to probability conservation the amplitudes of the incoming part ($\sim e^{ikx}$) and outgoing part ($\sim e^{-ikx}$) must be equal.

However in this case the wavelength of the incoming and outgoing waves varies nontrivially where $V(x) \neq 0$ (we could e.g. attempt to understand or calculate that wavelength using the WKB approximation in section 7.6). Because of that, the final outgoing wave will have a phase-shift δ (only), compared to the case without potential.

While it is less obvious, it turns out that also in 3D scattering, once we write the partial wave expansion, each partial wave can only suffer a phase-shift due to the potential $V(\mathbf{x})$, compared to no potential $V(\mathbf{x}) = 0$, but not be reduced in its amplitude. This is due to angular momentum conservation, enforced by the TISE for $\left[\hat{H}, \hat{\mathbf{L}}\right] = 0$ and thus already included in all our discussion so far.

Then identify the phase shift we write both scenarios as superpositions of spherical waves in the far field (large r).

Without scatterer, $V(\mathbf{x}) = 0$: In this case the incoming wavefunction e^{ikz} is unchanged, and we can start from Rayleigh's formula (8.13) which for large r can be written as

$$\mathcal{N}e^{ikz} = \mathcal{N}\sum_{\ell=0}^{\infty} i^\ell(2\ell+1)j_\ell(kr)P_\ell(\cos\theta) \overset{\text{large } r}{\approx} \mathcal{N}\frac{2\ell+1}{2ikr}\left(e^{ikr} - (-1)^\ell e^{-ikr}\right)P_\ell(\cos\theta), \tag{8.27}$$

With scatterer, $V(\mathbf{x}) \neq 0$: we instead start from (8.23) and do the same expansion of special functions to find

$$\begin{aligned}\phi(r,\theta,\varphi) &= \mathcal{N}\left(\sum_{\ell=0}^{\infty} i^\ell(2\ell+1)\left[j_\ell(kr) + ika_\ell h^{(1)}(kr)\right]P_\ell(\cos\theta)\right) \\ &\overset{\text{large } r}{\approx} \mathcal{N}\left[\frac{2\ell+1}{2ikr}\left(e^{ikr} - (-1)^\ell e^{-ikr}\right) + \frac{2\ell+1}{r}a_\ell e^{ikr}\right]P_\ell(\cos\theta),\end{aligned} \tag{8.28}$$

We want to write this as

$$\phi(r,\theta,\varphi) \approx \mathcal{N}\frac{2\ell+1}{2ikr}\left(e^{i(kr+2\delta_\ell)} - (-1)^\ell e^{-ikr}\right)P_\ell(\cos\theta), \tag{8.29}$$

where δ_ℓ controls the relative phase shift of the outgoing wave part compared to (8.27). Through direct comparison of (8.28) and (8.29), we read off that the

Partial wave scattering phase shifts δ_ℓ, are related to partial wave amplitudes a_ℓ via

$$a_\ell = \frac{1}{2ik}\left(e^{2i\delta_\ell} - 1\right) = \frac{1}{k}e^{i\delta_\ell}\sin\delta_\ell. \tag{8.30}$$

What we have seen, is thus that the scattering process is completely described by the set of all the real numbers δ_ℓ, which is simpler than unspecified complex numbers a_ℓ.

8.4 Born approximation

For a complementary way of (approximately) solving the TISE for the scattering problem to the partial wave expansion, we want to first reformulate the TISE in a different manner.

8.5 Integral form of Schrödinger's equation and Green's functions

Starting from the 3D TISE:

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\phi(\mathbf{r}) + V(\mathbf{r})\phi(\mathbf{r}) = E\phi(\mathbf{r}), \qquad \text{we can write this as}$$

$$(\boldsymbol{\nabla}^2 + k^2)\phi(\mathbf{r}) = Q(\mathbf{r}), \tag{8.31}$$

where we have used the definitions $k = \sqrt{2mE}/\hbar$ and $Q(\mathbf{r}) = 2mV(\mathbf{r})\phi(\mathbf{r})/\hbar^2$. The TISE has now taken the form of the Helmholtz equation[20], with an inhomogenous source term $Q(\mathbf{r})\phi(\mathbf{r})$ on the

[20] That is the mathematical name, in physics you have seen this as the wave-equation or diffusion equation.

RHS. As is usually done, let us define its solution in the presence of a delta function source first, for which we use the

Definition of Green's function of the scattering TISE as $G(\mathbf{r})$ solving

$$(\boldsymbol{\nabla}^2 + k^2)G(\mathbf{r}) = \delta^{(3)}(\mathbf{r}), \tag{8.32}$$

- If we know the Green's function, we can use it to express the solution for the inhomogeneous equation (8.31) as

$$\phi(\mathbf{r}) = \int d^3\mathbf{r}\,'G(\mathbf{r} - \mathbf{r}')Q(\mathbf{r}'). \tag{8.33}$$

  Proof: We can see this by simple substitution into (8.31)

$$(\boldsymbol{\nabla}^2 + k^2)\int d^3\mathbf{r}\,'G(\mathbf{r} - \mathbf{r}')Q(\mathbf{r}') = \int d^3\mathbf{r}\,'\underbrace{\left[(\boldsymbol{\nabla}^2 + k^2)G(\mathbf{r} - \mathbf{r}')\right]}_{=\delta^{(3)}(\mathbf{r}-\mathbf{r}')}Q(\mathbf{r}') = Q(\mathbf{r}) \tag{8.34}$$

  In the first equality we used that we can interchange derivatives wrt to $\mathbf{r}$ and an integration over $\mathbf{r}'$, and in the braces we then applied Eq. (8.33).

To proceed further, we need to actually find the Green's function, which means solving Eq. (8.33) for $G(\mathbf{r})$. This calculation requires complex contour integrals (residue theorem, see (2.81)) and is given in full length in Griffith. Please go through it there if you did encounter the residue theorem in your math courses. Otherwise we shall directly jump to the result, which is the

Solution for Green's function of the scattering TISE as ($r = |\mathbf{r}|$)

$$G(\mathbf{r}) = -\frac{e^{ikr}}{4\pi r}. \tag{8.35}$$

- In terms of a wave, this function represents an outgoing spherical wave, the denominator $1/r$ takes care of intensity conservation (see discussion in section 8.3). This seems an appropriate response to a delta-function source at the origin.
- This is in fact <u>not</u> a unique solution of (8.32) but a special solution, since we can now add any solution $G_0(\mathbf{r})$ of the <u>homogenous Helmholtz equation</u> $(\boldsymbol{\nabla}^2 + k^2)G_0(\mathbf{r})$. In our quantum mechanical context, that means any solution $\Psi_0(\mathbf{r})$ of the free particle TISE (2.2).

Backtracing our steps so far, we can now write the general solution of Schrödinger's equation for the scattering problem (8.31) through the

Integral form of Schrödinger's equation

$$\Psi(\mathbf{r}) = \Psi_0(\mathbf{r}) - \frac{m}{2\pi\hbar^2}\int d^3\mathbf{r}' \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(\mathbf{r}')\Psi(\mathbf{r}'). \tag{8.36}$$

- This looks like a solution for $\Psi(\mathbf{r})$, but it is not, since there also is a $\Psi(\mathbf{r}')$ in the integral. Really we just rewrote the TISE into a form into which we can insert approximations more easily shortly.
- Since we are interested in a scattering problem, we shall later use the part $\Psi_0(\mathbf{r}) = e^{ikr}$ to represent the incoming wave, recall section 8.3.

8.6 The first Born-approximation

As we did in section 8.3 let us again assume the potential has a finite range R_{pot}, such that $V(\mathbf{r}') \approx 0$ in the integration (8.36), for $|\mathbf{r}'| \geq R_{pot}$. Additionally, we are only interested in the scattering wavefunction $\Psi(\mathbf{r})$ at some faraway detector, such that we can assume $|\mathbf{r}| \gg R_{pot}$. This means that $|\mathbf{r}| \gg |\mathbf{r}'|$ for all non-vanishing contributions to the integral, which allows us to simplify $|\mathbf{r}-\mathbf{r}'|$ by writing

$$|\mathbf{r}-\mathbf{r}'| = \sqrt{(\mathbf{r}-\mathbf{r}')^2} = \sqrt{r^2 + r'^2 - 2\mathbf{r}\cdot\mathbf{r}'} \approx \sqrt{r^2\left(1 - 2\frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}\right)} = r\left(1 - \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}\right) = r - \mathbf{e}_r\cdot\mathbf{r}', \tag{8.37}$$

where we have used the Taylor expansion $\sqrt{1+x} \approx 1 + x/2$ for small x, and defined a unit vector in the radial direction $\mathbf{e}_r = \mathbf{r}/r$.

We now apply this result to the relevant part of the integrand:

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \overset{Eq.\ (8.37)}{\approx} \frac{e^{ik(r-\mathbf{e}_r\cdot\mathbf{r}')}}{r} = \frac{e^{ikr - i\mathbf{k}_f\cdot\mathbf{r}')}}{r} = \frac{e^{ikr}}{r}e^{i\mathbf{k}_f\cdot\mathbf{r}'}. \tag{8.38}$$

See Shankar for the reason we could be more brutal in our approximation of the denominator. In the last step we defined the final wavevector of the scattered particle $\mathbf{k}_f = k\mathbf{e}_r$, which has the same magnitude as the incoming wavevector in $\Psi_0(\mathbf{r}) = e^{ikr}$, but now point in the direction of the part of the outgoing wave of interest. With the approximations above and the form of Ψ_0, we can write (8.36) as

$$\Psi(\mathbf{r}) = e^{ikz} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3\mathbf{r}' e^{-i\mathbf{k}_f\cdot\mathbf{r}'} V(\mathbf{r}')\Psi(\mathbf{r}'). \tag{8.39}$$

The Born-approximation now amounts to assume the potential $V(\mathbf{r}')$ is "weak enough", such that the scattering wavefunction $\Psi(\mathbf{r})$ is not that dramatically changed from the incoming plane wave e^{ikr}, so that we can replace $\Psi(\mathbf{r}') \approx e^{ikz'} = e^{i\mathbf{k}\cdot\mathbf{r}'}$ with the incoming wavevector $\mathbf{k}_{in} = k\mathbf{e}_z$ in the integral. We will see in section 8.48 a somewhat more formal approach to this.

After that replacement we are getting somewhere, because the integral no longer contains the unknown function $\Psi(\mathbf{r}')$. We also see that the second term depends like $\frac{e^{ikr}}{r}$ on r, thus comparing (8.39) after $\Psi(\mathbf{r}') \to e^{i\mathbf{k}\cdot\mathbf{r}'}$ with (8.8), we can extract the

Scattering amplitude in the Born-approximation as

$$f(\theta, \varphi) = -\frac{m}{2\pi\hbar^2} \int d^3\mathbf{r}' e^{i(\mathbf{k}_{in} - \mathbf{k}_f)\cdot\mathbf{r}'} V(\mathbf{r}'). \tag{8.40}$$

- We recognize the RHS as related to the 3D Fourier transform of the potential, see (2.74).
- The dependence on angles θ, φ on the RHS is somewhat hidden: Recall that $\mathbf{k}_f = k\mathbf{e}_r$, and the unit vector $\mathbf{e}_r$ does depend on those angles, see Eq. (4.30).
- The argument of the Fourier-transform $\hbar(\mathbf{k}_{in} - \mathbf{k}_f)$ is the momentum transfer onto the target.

Example 66, Yukawa scattering: Let's take as the scattering potential the Yukawa potential

$$V(\mathbf{r}) = V_0 \frac{e^{-\lambda r}}{r}, \tag{8.41}$$

which provides for example a useful approximation for the interactions of nucleons mediated by pi-mesons.
Assuming the Born approximations is valid, we can calculate the scattering amplitude as

$$f(\theta, \varphi) = -\frac{mV_0}{2\pi\hbar^2} \int d^3\mathbf{r}' e^{i(\mathbf{k}_{in} - \mathbf{k}_f)\cdot\mathbf{r}'} \frac{e^{-\lambda|\mathbf{r}'|}}{|\mathbf{r}'|}, \tag{8.42}$$

Since $\mathbf{q} = \mathbf{k}_{in} - \mathbf{k}_f$ is just a constant vector during the integration, we chose spherical polar coordinates for $\mathbf{r}'$, with z-axis parallel to $\mathbf{q}$, then

$$\begin{aligned} f(\theta) &= -\frac{mV_0}{\hbar^2} \int_0^\infty dr'\, r'^2 \frac{e^{-\lambda r'}}{r'} \underbrace{\int_0^\pi d\theta \sin\theta \;\, e^{iqr'\cos\theta}}_{=[-e^{qr'\cos\theta}/(iqr')]_0^\pi}, \\ &= -\frac{2mV_0}{q\hbar^2} \underbrace{\int_0^\infty dr' e^{-\lambda r'} \frac{1}{2i} \left(e^{iqr'} - e^{-iqr'} \right)}_{=q/(q^2+\lambda^2)} = \frac{2mV_0}{\hbar^2(q^2+\lambda^2)}. \end{aligned} \tag{8.43}$$

The differential cross section is $d\sigma/d\Omega = |f(\theta)|^2$, it depends on θ via $q^2 = 2k^2(1-\cos\theta) = 2k^2 = 4k^2\sin^2(\theta/2)$. For $k \ll \lambda$ (low energy scattering), it thus becomes isotropic as it has to (see example 65). For high-energy scattering $k \gg \lambda$, the cross section goes like $\sin^{-4}(\theta/2)$, such that forward scattering is much more likely than backwards scattering. Also the total cross sections keeps decreasing with energy as E^{-2} in this case.

Example 67, S-wave scattering of ultracold atoms II: In example 65 we had seen that very low energy scattering between atoms is governed by just one single real number, the s-wave scattering length a_s. In the Born-approximation we just learnt that the scattering amplitude is given by (8.40). For $\lambda = 2\pi/k \gg R_{\text{pot}}$, we can ignore the exponential factor in the region where the potential is nonzero, and reach.

$$f = -\frac{m}{2\pi\hbar^2} \int d^3\mathbf{r}' V(\mathbf{r}'). \tag{8.44}$$

This contains almost no details of the shape of the potential. We can thus replace the latter by a pseudo potential $V(\mathbf{r}) = V_0 \delta^{(3)}(\mathbf{r})$, insert this into (8.44) and use $f = -a_s$ from example 65.

Further recall that our discussion so far assumes an infinitely heavy target, but can be adapted to two equal mass scattering partners by replacing the mass by the reduced mass $m \to \mu = m/2$ everywhere.

We now see that a pseudo potential strength

$$V_0 = \frac{4\pi\hbar^2 a_s}{m}, \tag{8.45}$$

will give rise to exactly the same low energy scattering behaviour as the real finite range potential, but is theoretically much easier to handle.

8.7 Born series

The Born approximation in the previous section is just the first step of a more systematic expansion. Let us rewrite Eq. (8.36) as

$$\Psi(\mathbf{r}) = \Psi_0(\mathbf{r}) + \int d^3\mathbf{r}' g(\mathbf{r} - \mathbf{r}') V(\mathbf{r}') \Psi(\mathbf{r}'). \tag{8.46}$$

using the shortcut $g(\mathbf{r} - \mathbf{r}') = -\frac{m}{2\pi\hbar^2} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$ and then schematically (dropping all dependencies), as $\Psi = \Psi_0 + \int gV\Psi$. We can now just insert this equation itself for Ψ on the right hand side, to reach

$$\Psi = \Psi_0 + \int gV(\Psi_0 + \int gV\Psi) = \Psi_0 + \int gV\Psi_0 + \int\int gVgV\Psi. \tag{8.47}$$

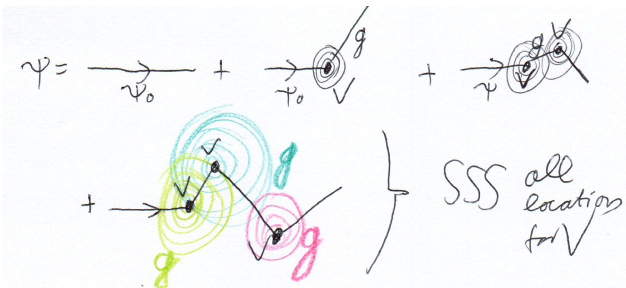
Doing this repeatedly provides the

Born series

$$\Psi = \Psi_0 + \int gV\Psi_0 + \int\int gVgV\Psi_0 + + \int\int\int gVgVgV\Psi_0 + \cdots \tag{8.48}$$

- This iterative expansion method is known in the mathematics of solving differential equations (converted to an integral equation) as Picard iteration. It is helpful whenever there is reason to believe that only a few iterations are needed.

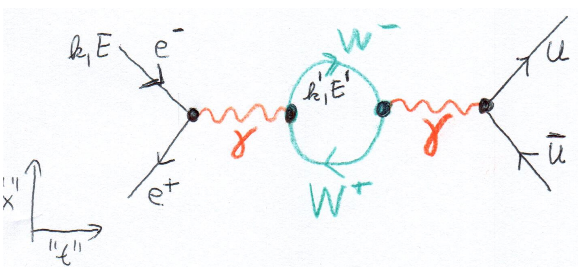
- Since this requires some smallness of $V(\mathbf{r}')$, this amounts to perturbation theory applied to the scattering problem. Our earlier result (8.40) represents the first order in this expansion.
- One can associate an intuitive interpretation with the series, that we attempt to sketch below, following Griffith:



left: Drawing correspond term by term to (8.48). Ψ_0 represents unperturbed propagation of the incoming particle. It then can receive a localized kick from the potential V at some point, and afterwards propagate out via the propagator g. The actual wavefunction will be the sum of all orders and within each all possible locations of the kick and subsequent propagation directions.

In a more complicated context, diagrams like the above have become very common for both, communication between physicists and an actual first step for complex quantum scattering calculations:

Example 68, Feynman diagrams: You may have seen on occasion a drawing like the one below in a particle physics context



left: Feynman diagram for electron-positron annihilation with one virtual W-Boson loop and quark-anti-quark pair production as final state. Also here, lines represent propagators (like g in our Born series, but now different ones for different particles), and dots/vertices interaction potentials V (which depend on the type of interaction, here electro-magnetic).

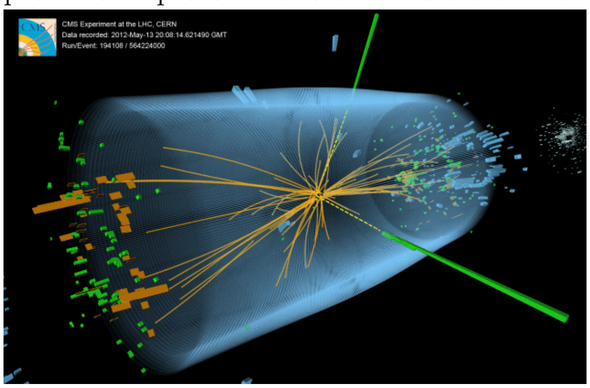
These are called Feynman diagrams. Essentially the lines represent g in (8.48) and are called propagator, the line-style tells you which particle is propagating. Nodes V are called vertices, and represent certain interactions (potentials), like V in (8.48). Unlike what we have done, for particle physics the entire formalism has to be relativistic, thus interactions typically are capable of converting different types of particles into each other. The open legs of the diagram are the incoming and outgoing particles of the scattering event in the collider. More in courses on nuclear/particle physics or quantum field theory.

8.8 Outlook

We have but scratched the surface of quantum scattering theory, as already evident from the previous example. Whenever you collide microscopic particles with one another, the kinematics of the scattering process will give you insight into their properties, even if they themselves are way too small to see. You had seen an example in PHY106 (Rutherford scattering), or example 64, where the total cross section contained information on the size of the hard-sphere.

Even when non-relativistic, these scattering processes typically depend on the spin. We then see the concept of multi-channel scattering [e.g. channel=different spin states of the outgoing particles]. Already when doing chemistry, the scattering particles can change their character. I.e. a chemical reaction is a quantum scattering process, whereby two molecules (see section 7.5.2) collide, to form a new molecule (channel). Once we go to relativistic energies, even fundamental (non-compound) particles can be created, destroyed and converted, thanks to $E = mc^2$.

Example 69, Scattering event at the Large Hadron Collider (LHC): Much of what we know about the fundamental workings of the universe has been unravelled with the help of quantum scattering theory. The image below represents one measurement of a proton-anti-proton heads on collisions at the LHC (take from the CERN webpage).



left: The p-$\bar{p}$ collide at the centre and produce a large set of collision fragments. Their trajectories are tracked as yellow lines (i.e. θ, φ in our discussion). Unlike our discussion, there are lots of different final states which hence can all have different energies (displayed in the orange green and blue bar diagrams).

By averaging over many such events, one tries to deduce cross sections $d\sigma/d\Omega$, and by comparing those with theoretical calculations gains some inside, for example into yet undiscoverd particles within virtual loops as shown in example 68. We had only looked at elastic scattering of identical particles, fully described by θ, φ. In contast for inelastic events such as the one above, there are many more variables describing it, such as energies E_k, final state charges q_k, final state spins etc,