Notes for Lecture 16

Scattering

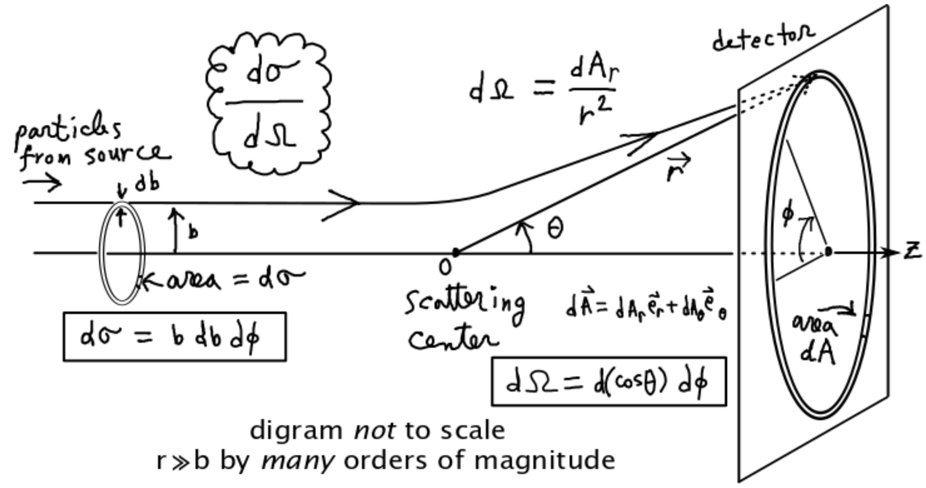
As we approach the finale of this course, we turn to the topic of scattering. This is quite an essential topic, since it is a major method of investigating properties of matter.

Before we discuss this topic, let us remember one thing that distinguishes the physics of waves from the physics of particles: the interference phenomenon. The interference phenomenon is described mathematically in terms of the phase. So, it is not surprising that the phase plays a central role in quantum mechanics. For instance, the time evolution operation, the rotation operation, and the translation operation—all of them can be thought of as a phase shifting operator since that is what they do, if they operate on appropriate eigenstates—energy, angular momentum, and translation, respectively.

So, it should not surprise you too much to be told at this point that **the physics of scattering is all in the phase**. Please remember this point. And this other point as well: the physics of the topics that we will discuss after scattering (adiabatic theorem, Berry's phase, Aharanov-Bohm effect, topological effect) is also *all in the phase*!

16.1 Cross section

Let us consider the following schematic diagram. It depicts an experiment in which a stream of particles come from the left side (sent by an experimenter) and then emerge on the right side, deflected by some sort of interaction, to be captured by a detector[1]. These deflected particles will be referred to as **probing particles**. We shall assume that the interaction that deflects the probing particle is described by a potential energy for the incident particle[2] $V(\vec{r})$. The origin of $\vec{r}$ is referred to as the "scattering center" in the diagram. We assume that the scattering center is fixed in space. Therefore, in general, the scattering center corresponds to the center of mass of the entire system[3], the probing particle plus the probed system, whose interaction with the probing particle gives rise to the deflection of the incoming beam of probing particles.



The above diagram depicts the effect of a repulsive interaction, while it can be modified, trivially, to be applicable to the case of an attractive interaction. Here, b is the so-called **impact parameter**. We will explore the meaning of this parameter as

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[1] Here, we assume is a planar shape detector, but this is just an example. A spherical-shell shaped detector will do equally well in this diagram.

[2] This assumption is not always valid and is generally an unnecessary one to make. However, this assumption does make the problem an easy one to deal with, to aid the construction of the formalism, which can remain useful even for general cases. In general, the scattering must be described by a many-body initial state, an interaction Hamiltonian, and a many-body final state. If the probing particle and the/some scattering particle(s) are identical, then it is not possible to reduce the interaction Hamiltonian to a *one particle* potential energy of the form $V(\vec{r})$.

[3] In some cases, the system probed is heavy (e.g. a solid) compared to the probing particle (e.g. photon/electron/neutron) and so the *center of mass frame* will be identical with the *lab frame*. In such a case, what we calculate can be used without modification to compare with data recorded in the lab frame. In some cases, however, the system probed may not be heavy compared to the probing particle. For example, if an atomic scattering is performed on an atom vapor, then the probed system, as well as the probing particle, is an atom. And so, the calculation that we carry out will have to be converted to the *lab frame* before it can be compared with the data recorded in the lab frame. The conversion formulae between the center of mass frame to the lab frame (e.g. LN 15 of `https://griffin.ucsc.edu/ph105-11/Lecture%2B` or any standard classical mechanics textbooks) can be used in such a case.

we go on. At this point, it suffices to note that b must be on the order of the range of the interaction to be important. Below, we will discuss some more about this simple statement. For the most part, we will assume that the range of the interaction to be finite. In such a case, note that the assumption of a scattering theory is that r (the distance between the scattering center to the detector) is much greater than the interaction range.

The measured quantity in the above setup is the number of particles detected at solid angle angle $d\Omega$ per unit time, given the incoming particles sent per unit time and per unit area. This is called the **differential cross section** $d\sigma/d\Omega$:

$$\frac{d\sigma}{d\Omega} = \frac{I_{out}}{I_{in}} \tag{16.1}$$

where I_{in} (**flux density**) is the number of particles entering from left per unit time *per unit area*, while I_{out} is the number of particles emerging to right per unit time *per unit solid angle*. It makes sense that I_{in} is defined as per unit area, while I_{out} is defined as per unit solid angle, if one gives some thoughts to the experimental set-up.

Note that Eq. 16.1 is the definition of the differential cross section for any scattering experiment, in purely experimental terms, and thus is valid no matter what theory we use to explain the experimental data.

Eq. 16.1 is a bit odd one: it is half definition and half result. On one hand, it *defines* the differential cross section as I_{out}/I_{in}. On the other hand, it also states that this can be *computed* as $d\sigma/d\Omega$, where $d\sigma$ is the area element on the left and $d\Omega$ is the solid angle element on the right in the above diagram. Where does this latter *result* come from? It can be seen as follows. $I_{in} \cdot d\sigma$ is the number of particles that emerge on the right within $d\Omega$ per unit time, and so I_{out}, which is the number of particles that emerge on the right per unit time per solid angle, is given by $I_{in} \cdot d\sigma/d\Omega$. So, the ratio I_{out}/I_{in} is indeed equal to $d\sigma/d\Omega$, justifying Eq. 16.1.

For this reason, it is both customary and practical to simply define/write the differential cross section as $d\sigma/d\Omega$ without any extra symbol to invent for it[4]!

Let us discuss the **symmetry** of this problem. First of all, note that the interaction between the scattered particle and the scattering particle must have the full rotational symmetry[5]. This is because, we assume, they form a closed system. Assuming then that the incident beam is uniform in intensity, the scattered intensity must be independent of ϕ. In other words, the full rotational symmetry of the problem and the boundary condition on the left end makes this problem a **cylindrically**

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[4] So, here we forgo with the symbol such as $D(\theta)$ as used in the textbook.

[5] This means that the position dependent potential energy, if applicable, is of the form $V(r)$. This is what we will assume in this and the next lecture.

symmetric one. Therefore, *$d\sigma/d\Omega$ must be independent of ϕ*: it can be a function of θ and the attributes of the incident particle, such as its energy, but not of ϕ.

The **total cross section**, σ, is defined as the integrated cross section.

$$\sigma \equiv \int d\Omega \frac{d\sigma}{d\Omega} = \int d\sigma \tag{16.2}$$

16.2 Short detour to classical mechanics

Now, the above diagram suggests that we take the ratio of $d\sigma = d\phi b\, db$ and $d\Omega = d\phi\, d(\cos\theta) = d\phi \sin\theta |d\theta|$ (note that we take the convention that $d\sigma > 0$ and $d(\cos\theta) > 0$).

$$\frac{d\sigma}{d\Omega} = \frac{2\pi b\, db}{2\pi \sin\theta |d\theta|} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| \tag{16.3}$$

As we make this statement, we are implicitly assuming classical mechanics! Why? In quantum mechanics, one cannot in general assign a definite path like we have drawn in the above diagram! A well-defined path for a motion is a classical concept, which must be replaced by the wave function in quantum mechanics. We shall explore the quantum mechanical case soon.

However, it is of some interest to consider the classical case a little while.

In particular, let us note this point. It may appear at this point that the total cross section is infinite for *any* problem! This is because $\int d\sigma = 2\pi \int_0^\infty b\, db = \pi\infty^2 = \infty$, where the 2π factor is the result of the integration over ϕ. While this is true mathematically, this does make the definition of σ quite useless! What have we missed here?

In reality, we distinguish between **scattered particles** and **un-scattered original particles**. Scattered particles are those particles that are affected by the interaction, while un-scattered particles those that are not. To illustrate this point, the **"hard sphere" potential** is interesting to consider. We can consider the hard sphere as represented by

$$V(r) = \begin{cases} 0 & r > R \\ \infty & r < R \end{cases} \tag{16.4}$$

For classical mechanics alone, we do not really need an infinite potential energy, but just a large value. However, the above definition serves us well both for quantum mechanical problems and for classical problems, so we will stick with it. Classically, the motion of the particle is that of a perfect bouncing off as pictured in Figure T11.2. Thus, we get

$$b = R\cos\left(\frac{\theta}{2}\right) \qquad b \le R \qquad \text{(scattered)} \tag{16.5}$$

$$b = b \qquad b > R \qquad \text{(un-scattered)} \tag{16.6}$$

Note that these un-scattered particles *will* be captured by the detector, but our interest is not in them. So, for the consideration of the cross section, it is ignored. Then, it follows that

$$\frac{d\sigma}{d\Omega} = \frac{R^2}{4} \qquad \text{using Eq. 16.3} \tag{16.7}$$

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi\frac{R^2}{4} = \pi R^2 \tag{16.8}$$

The last result seems to make a lot of sense. In classical mechanics, scattering occurs for a hard sphere potential, only if the impinging particle (if assumed to be a point particle, as here) has an impact parameter b, which is less than the circle of radius R of the sphere. **The effective area in which the scattering occurs is πR^2, the projected area of the sphere.**

Now, what would happen if the potential is changed to something like $V(\vec{r}) = V_0/(e^{(r-R)/W}+1)$? The sigmoidal factor $1/(e^{(r-R)/W}+1)$ makes the potential energy drop from V_0 for small $r \ll R$ to large $r \gg R$ at the "knee" (transition zone) positioned at $r = R$, with the width of the transition zone, $\sim W > 0$. In the limit of small W, and large V_0, the new potential will be practically identical with the above hard sphere potential. However, the question is for a very small but finite W—what would happen to the total cross section σ?

Perhaps your intuition says that $\sigma \sim \pi R^2$, and you would be correct! Except that the answer from classical mechanics is completely different. No matter how small the potential energy is, it will scatter the incoming particle if the force field is non-zero. So, the total cross section is actually infinite according to classical mechanics[6]. This completely incorrect answer can be remedied only by quantum mechanics, according to which a particle has only a probability to follow a certain path, while an infinite number of paths are possible.

What does this consideration actually mean for us? First of all, the above consideration should not bother you too much when you consider the scattering between

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[6] This argument here must be accepted with a grain of salt, however, in the sense that we are taking non-zero but very very small numbers too seriously. Nevertheless, the point of classical mechanics being unable to deal with the problem of scattering in a clean and nice way in general is a point well made here.

real classical particles, like two billiard balls colliding or two people walking past each other with a brief touch. For these cases, the interaction is indeed like a hard sphere, for all practical purposes. Second, it goes without saying that one should never think that everything is OK when applying classical mechanics to any problem involving fundamental particles like atoms, electrons, protons, etc. These small particles obey only quantum mechanics. If classical mechanics somehow gets the answer right for certain problems involving them (as for the famous Rutherford scattering problem!—Example T11.6 and problem T11.1), it may be a case for joy, but it should not be taken as a reason to relax guard against classical mechanics.

While we are on this topic, let us note that even for many classical mechanics problem, the force exchange occurs on a very short length scale, which can be too short to be described in classical mechanical terms. For many quantum scattering problems that we will consider, the interaction range is either atomic (~ Å; screened Coulomb interaction) or sub-atomic (~ fm; nuclear interaction). So, the assumption that the detector length scale $r \gg$ the interaction range is an excellent one in general for our purpose. We will make this assumption for the most part. A notable exception is when the interaction is long-ranged, like the Coulomb interaction (as in the Rutherford scattering problem). Such problem must be treated more carefully.

16.3 Back to quantum mechanics

How would we describe the scattering like the one that we have been considering so far, i.e. an elastic scattering by a potential, in quantum mechanics?

The appropriate wave function[7] to use is

$$\psi(r,\theta) = A\left(e^{ikz} + f(\theta)\,\frac{e^{ikr}}{r}\right) \qquad \text{large } r \qquad (16.9)$$

where we assumed that the z direction is the direction of the original beam (see diagram in page 2), and "large r" means that r is greater than the interaction range, as we discussed above. Here, we are assuming that the initial beam comes in with $\vec{k}_i$ and the final beam has $\vec{k}_f$, with

$$k \equiv |\vec{k}_i| = |\vec{k}_f| \qquad \text{elastic scattering} \qquad (16.10)$$

$$E = \frac{\hbar k^2}{2m} \qquad \text{energy} \qquad (16.11)$$

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[7] Note that we do not include the time dependence in the wave function, since we are considering an elastic scattering. So, the above wave function must be considered as a solution of the time-independent Schrödinger equation. For an inelastic scattering, the outgoing spherical wave will have a different k value than the incoming plane wave, and will also carry a different time evolution factor.

and $\vec{k}_i$ is along the z direction (and so the initial beam is represented by e^{ikz}) while $\vec{k}_f$ has an angular distribution according to $f(\theta)$. The complex function $f(\theta)$ is the so-called **scattering amplitude**. It determines the differential cross section completely:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \tag{16.12}$$

Let us see how we can derive this important result. Deriving it is equivalent to understanding why we wrote what we wrote in Eq. 16.9.

There is *some trick* being used in writing down Eq. 16.9, actually. Normally, we write the plane wave solution for a single particle as something like $\exp(ikz)/\sqrt{2\pi}$ (particle in an infinite space) or $\exp(ikz)/\sqrt{\mathcal{V}}$ (particle in a box of volume $\mathcal{V}$). Such a wave function can be written formally as Ae^{ikz}, with A left as a constant to be determined later. If we now consider the **probability current** $\vec{j}$ (Homework 5.4) for this wave function, we can easily compute that $\vec{j}$ is given by

$$\vec{j} = |A|^2 \frac{\hbar k}{m} \vec{e}_3 \qquad \text{probability current for } \psi = Ae^{ikz} \tag{16.13}$$

This has a direction interpretation: $|A|^2$ is the probability density and $\frac{\hbar k}{m}\vec{e}_3$ is the velocity with which it flows, so it fits the intuition that it must be something like $\rho\vec{v}$ (cf. Homework 5.4(b)).

The trick is the following. **Instead of interpreting $|A|^2$ as the probability density of the incoming particle, we can interpret it as the particle density of the incoming particle beam**[8]. With this re-interpretation of A, what we then have is

$$j = |A|^2 \frac{\hbar k}{m} = I_{in} \tag{16.14}$$

where I_{in} is what we defined when we introduced Eq. 16.1.

Now, how about I_{out}? Considering a small solid angle $d\Omega$, one can take the spherical wave $Af(\theta)e^{ikr}/r$ and interpret it as precisely the same way as we just did for a plane wave, since its wave front is "just a plane wave" with amplitude $Af(\theta)/r$, when examined in a small region defined by $d\Omega$. Then, I_{out} is obtained as

$$I_{out} = \overbrace{\left|\frac{Af(\theta)}{r}\right|^2 \frac{\hbar k}{m}}^{\#\text{ per unit time per unit area}} \times \underbrace{\overbrace{\frac{r^2 d\Omega}{d\Omega}}^{\text{area}}}_{\text{per unit solid angle}} \tag{16.15}$$

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[8] This interpretation makes sense only if we assume that particles in the beam are uncorrelated, which is a good assumption for many experiments.

Combining the last two equations, it follows easily that

$$\frac{d\sigma}{d\Omega} \equiv \frac{I_{out}}{I_{in}} = |f(\theta)|^2$$

proving our assertion in Eq. 16.12.

Note that the cross section is concerned with the scattered portion of the wave function only, consistent with our discussion in page 4.