Lecture 4: Scattering Theory

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Abstract

This lecture is an introduction to Scattering Theory in Quantum Mechanics. After introducing the asymptotic conditions and explaining their interpretation in terms of observable quantities, we introduce the Lippmann-Schwinger equation and the Born approximation. We then discuss Feynman diagrams and some differences between the non-relativistic and relativistic propagation of signals and particles.

1 Non-relativistic scattering theory

1.1 The asymptotic conditions.

We start by considering a particle of mass m moving in $\mathbb{R}^3$ in the time-dependent potential $V(\vec{x}, t)$ (whose support is not a priori assumed to be localized in the spatial directions). The evolution of the wave function $\psi(\vec{x}, t)$ is determined by the time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(\vec{x}, t) = H\psi(\vec{x}, t), \tag{1}$$

where the Hamiltonian is defined by $H = -\frac{1}{2m}\Delta_x + V$. We will assume for a while that $m = 1$.

We want to analyse the solutions of (1) with a certain behaviour in the far past and the far future. In the far past, we require that the solutions approach, as $t \to -\infty$, a solution of the Schrödinger equation corresponding to the *free* Hamiltonian $H_0 = -\frac{1}{2}\Delta$. Solutions of the free Schrödinger equation have the general form

$$\psi(\vec{x}, t) = \int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k}) e^{i(\vec{k}\cdot\vec{x} - \frac{k^2}{2}t)}, \tag{2}$$

where $f(\vec{k})$ represents the distribution of momenta at time $t = 0$. More specifically, we want to consider those solutions of (2) corresponding approximately to an incoming particle with velocity $\vec{v}$, which means that $f(\vec{k})$

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is localized near $\vec{k}_0 = \vec{v}$ (since m=1); a possible choice for f is

$$f(\vec{k}) = \exp(-\frac{1}{\alpha}(k-k_0)^2) \tag{3}$$

with small α. For large t, the integral in (2) is highly oscillatory so the main contribution comes from stationary phase; varying the exponent with respect to k gives $\vec{k} = \vec{x}/t$; if α is small then $\vec{k}$ has to be close to k_0, and the condition $\vec{x} = \vec{k}_0 t$ does indeed describe a free moving particle with velocity $\vec{k}_0$.

In the far future, we can no longer expect the wave function ψ to be localised near a definite momentum because of the scattering effect of the potential, so we will instead look for solutions of (1) which behave asymptotically like a sum of a localised solution of (2) and an outgoing spherical wave.

In order to find solutions of (1) we will first solve an eigenvalue problem for the Hamiltonian. We assume that there are no bound states, i.e. that H has no discrete spectrum. For each $\vec{k}$ we will search for a solution $\psi_{\vec{k}}(\vec{x})$ of the equation $H\psi_{\vec{k}}(\vec{x}) = \frac{k^2}{2}\psi_{\vec{k}}(\vec{x})$ with the following asymptotic behaviour at large distances:

$$\psi_{\vec{k}}(\vec{x}) \stackrel{x\to\infty}{\longrightarrow} e^{i\vec{k}\cdot\vec{x}} + \frac{1}{|x|}e^{i|k|\,|x|}F_{\vec{k}}(\Omega) + O\left(\frac{1}{|x|^2}\right). \tag{4}$$

The plus sign in the exponent of the second term is important, it will be needed in the construction of an *outgoing* wave solution of (1). The complex-valued function $F_{\vec{k}}$ is defined on the sphere of radius 1 and the notation Ω is a shorthand for a vector $\hat{x}$ on the sphere. Alternatively we can regard $F_{\vec{k}}$ as a function $F(\vec{k}', \vec{k})$ defined for $|\vec{k}'| = |\vec{k}|$.

The functions $\psi_{\vec{k}}$ can be used to construct exact solutions of the time-dependent Schrödinger equation, namely

$$\psi(\vec{x}, t) = \int \frac{d^3\vec{k}}{(2\pi)^3} f(\vec{k})\psi_{\vec{k}} e^{-i\frac{k^2}{2}t}. \tag{5}$$

Let us use (4) and (5) to see how does ψ look at infinity if f is assumed to be of the form (3). For $|t| \to \infty$ and $|x| \to \infty$ two terms contribute to the stationary phase; one of them is $\exp i(\vec{k}\cdot\vec{x} - k^2t/2)$ and has already been analysed– the stationary phase condition is $\vec{x} = \vec{k}_0 t$. The other one has, for large $|\vec{x}|$, the phase $|\vec{k}|\cdot|\vec{x}| - k^2t/2 + \arg F$; varying with respect to $|k|$ we find that the stationarity condition is

$$x = kt + \frac{\partial}{\partial k} \arg F_{\vec{k}} \tag{6}$$

Notice that if we ignored the term involving F we would get $x = kt$, which cannot be satified for negative $t-$ in agreement with the fact that we only want to have an *outgoing* spherical wave.

The extra term in the right-hand side is a finite time advance or delay describing the fact that the moment when the scattered particles arrive at a detector is affected by the interaction with the target. The stationarity condition shows that the advance/delay is the radial derivative of the phase of F, called the *phase shift*.

1.2 Relation with experiments.

It is now time to relate the above constructions to quantities which are actually measurable in scattering experiments. The function $F(\Omega)$ is called the *scattering amplitude*. The reason for this is that the measure $|F(\Omega)|^2 d^2\Omega$ on the sphere $S_1 = \{|x| = 1\}$ can be interpreted as the number of scattered particles per unit solid angle if there is one incident particle per unit area ($d^2\Omega$ denotes the usual measure on the 2-sphere). Notice that only the absolute value of F is relevant here. The integral

$$\sigma = \int_{S_1} |F(\Omega)|^2 d^2\Omega \tag{7}$$

is called the *total cross-section* and represents the total number of scattered particles (per unit incoming particle in unit area). As such, σ can also be viewed as the *effective cross-sectional area* of the target: if the target is thought to remove a fraction of the incoming particles of momentum $\vec{k}_0$, then σ is the total number of removed particles if there is one particle per unit area. The relationship between σ and F is usually written as

$$\frac{d\sigma}{d\Omega} = |F(\Omega)|^2. \tag{8}$$

1.3 The Lippmann-Schwinger equation.

We have so far used the eigenfunctions of the Hamiltonian to solve the time-dependent Schrödinger equation. The question now is how to solve the eigenvalue problem for H. One possibility is to start from the free Hamiltonian $H_0 = -\frac{1}{2}\Delta$ whose eigenfunctions are $\exp(i\vec{k} \cdot \vec{x})$ (corresponding to the eigenvalues $k^2/2$). We will search for eigenfunctions $\psi_{\vec{k}}$ of H of the form $\psi_{\vec{k}} = \exp(i\vec{k}\cdot\vec{x}) + \alpha_{\vec{k}}$. Since $H = H_0 + V$ we have

$$0 = \left(H - \frac{k^2}{2}\right)\psi_{\vec{k}} = V\psi_{\vec{k}} + \left(H_0 - \frac{k^2}{2}\right)\alpha_{\vec{k}} \tag{9}$$

which implies

$$\alpha_{\vec{k}} = -\frac{1}{H_0 - \frac{k^2}{2}} V\psi_{\vec{k}}, \tag{10}$$

where the operator $1/(H_0 - k^2/2)$ is supposed to be a right-inverse to $H_0 - k^2/2$.

Although the operator $H_0 - k^2/2$ is not invertible, we still can construct a right-inverse of it In momentum space, for instance, the operator $H_0 - k^2/2$ is roughly speaking a multiplication operator

$$\left(H_0 - \frac{k^2}{2}\right) e^{i\vec{q}\cdot\vec{x}} = \frac{1}{2}(q^2 - k^2)e^{i\vec{q}\cdot\vec{x}} \tag{11}$$

so we should have

$$\frac{1}{H_0 - \frac{k^2}{2}} = \frac{1}{\frac{1}{2}(q^2 - k^2)}. \tag{12}$$

Because of the pole, there are several ways of making sense of the above; one possibility, in the usual notation, is:

$$\frac{1}{H_0 - \frac{k^2}{2}} = \frac{1}{\frac{1}{2}(q^2 - k^2) - i\epsilon}. \tag{13}$$

The conversion to position space is realised through the following

Exercise. Show that the integral kernel (in position space) of the operator defined by (13) is

$$G(\vec{x}, \vec{y}) = \frac{1}{2\pi}\frac{e^{i|k|\cdot|x-y|}}{|x-y|}. \tag{14}$$

By using the exercise, (10) leads to the *Lippmann-Schwinger equation*

$$\psi_{\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} - \frac{1}{2\pi}\int d^3\vec{y}\,\frac{e^{i|k|\cdot|x-y|}}{|x-y|}V(\vec{y})\psi_{\vec{k}}(\vec{y}). \tag{15}$$

If the potential V has compact support then any solution of (15) has the boundary conditions required by the asymptotic condition built in. This can be seen by using the fact that for large $|x|$ and $\vec{y}$ in a compact set we have $|x-y| = |x| - \hat{x}\cdot\vec{y} + O(1/|x|)$, where $\hat{x} = \vec{x}/|x|$. Indeed, if we use this approximation then (15) becomes

$$\psi_{\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} - \frac{1}{2\pi}\frac{e^{i|k|\cdot|x|}}{|x|}\int d^3\vec{y}e^{-i|k|\,\hat{x}\cdot\vec{y}}V(\vec{y})\psi_{\vec{k}}(\vec{y}) + O\left(\frac{1}{x^2}\right), \tag{16}$$

which shows the existence of a scattered wave of the promised type.

Remark. The procedure used in (13) for going around the pole is chosen precisely in order to guarantee the existence of the outgoing spherical wave.

Notice that (16) gives an expression for the scattering amplitude: for any point $\Omega = \hat{x}$ on the sphere of radius 1 we have

$$F(\Omega) = -\frac{1}{2\pi}\int d^3\vec{y}e^{-i|k|\,\hat{x}\cdot\vec{y}}V(\vec{y})\psi_{\vec{k}}(\vec{y}). \tag{17}$$

Remark. We can reinterpret the function F as a function of k' and k such that $|k'| = |k|$, in agreement with the idea that after scattering the particle moves in the $\hat{x}$ direction with the same speed as before.

Although the Lippmann-Schwinger equation cannot be solved exactly, it can be used to compute $\psi_{\vec{k}}$ in perturbation theory as an expansion in the powers of the potential (assumed to be sufficiently weak). This can be done by an iterative procedure: we first calculate $\psi_{\vec{k}}$ to order V by using the free eigenfunction $\exp(i\vec{k}\cdot\vec{y})$ in the right-hand side of (15) instead of $\psi_{\vec{k}}(\vec{y})$; once we know $\psi_{\vec{k}}$ to order V we plug it back into (15) to get the answer to order V^2 and so on.

1.4 The Born approximation.

We have seen above an expression of the scattering amplitude in terms of the eigenfunctions $\psi_{\vec{k}}$. The *first Born approximation* is the computation of the scattering amplitude with $\psi_{\vec{k}}$ replaced in (17) by the free plane wave $\exp(i\vec{k}\cdot\vec{y})$. We have seen that the scattered wave travels with the same speed as the incoming one so we can write, for $|\vec{k}'| = |\vec{k}|$,

$$F(\vec{k}', \vec{k}) = -\frac{1}{2\pi}\int d^3\vec{y}e^{-i\vec{k}'\cdot\vec{y}}V(\vec{y})\psi_{\vec{k}}(\vec{y}). \tag{18}$$

In the first Born approximation this becomes

$$F(\vec{k}', \vec{k})_{Born} = -\frac{1}{2\pi}\int d^3\vec{y}e^{-i(\vec{k}-\vec{k}')\cdot\vec{y}}V(\vec{y}). \tag{19}$$

If we introduce the *momentum transfer* $\vec{q} = \vec{k}' - \vec{k}$ we see that $F(\vec{k}', \vec{k})_{Born}$ is the Fourier transform of the potential in the $\vec{q}$ variable.

Remark. This fact is important since it shows that the less smooth V is, the less rapidly does $F(\vec{k}', \vec{k})$ decay as a function of $\vec{k}' - \vec{k}$ (for fixed $\vec{k}$). This led Rutherford to postulate the existence of the atomic nucleus (based on his scattering experiments). Later on, when similar experiments were performed with protons instead of atoms, the same reasoning suggested the composite structure of the proton (existence of quarks).

There are also higher Born approximations for the transition amplitudes: it is enough to use the successive approximations to $\psi_{\vec{k}}$ in the expression (17) of $F(\vec{k}', \vec{k})$. It turns out that in general the Born approximations lead to very precise computations.

Remark. Instead of considering a particle incident on a target we can regard our previous discussion as a description of the interaction of two particles. The center of mass decouples and the same results go through for the relative motion of the particles.

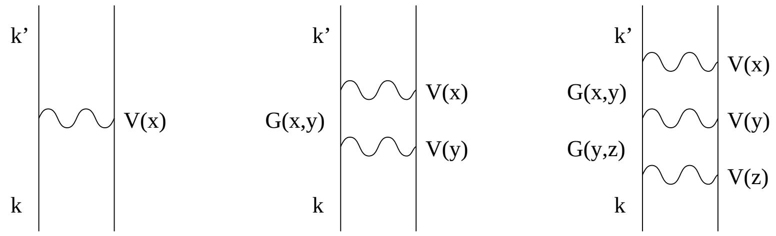
Remark. We can also generalize the preceding arguments for the case of n interacting particles. Let us note that this time we won't be able to simultaneously normalize the masses to 1 and that we need one spherical wave centered at each interaction point. The exact solutions of the Schrödinger equation $\psi_{\vec{k}_1,\ldots,\vec{k}_n}$ will be sums of free and spherical waves away from the diagonals (i.e. whenever $\vec{k}_i \neq \vec{k}_j$ for $i \neq j$).

1.5 Feynman diagrams.

Starting from (17) and the Lippmann-Schwinger equation we can compute the transition amplitude as an infinite sum

$$\begin{aligned} F(\vec{k}', \vec{k}) &= -\frac{1}{2\pi} \int d^3\vec{x} e^{-i(\vec{k}'-\vec{k})\cdot\vec{x}} V(\vec{x}) \\ &+ \frac{1}{4\pi^2} \int d^3\vec{x} d^3\vec{y} e^{-i\vec{k}'\cdot\vec{x}} V(\vec{x}) G(\vec{x}, \vec{y}) V(\vec{y}) e^{i\vec{k}\cdot\vec{y}} \\ &- \frac{1}{8\pi^3} \int d^3\vec{x} d^3\vec{y} d^3\vec{z} e^{-i\vec{k}'\cdot\vec{x}} V(\vec{x}) G(\vec{x}, \vec{y}) V(\vec{y}) G(\vec{y}, \vec{z}) V(\vec{z}) e^{i\vec{k}\cdot\vec{z}} \\ &+ \cdots \end{aligned}$$

Given our experience with Feynman diagrams, it is easy to see that the terms of the sum can be represented graphically (for instance, the graphs corresponding to the first three terms in the sum are shown below).



Each curly line represents an interaction due to the potential V. In-between interactions, the particles move freely (hence the free propagator $G(x,y)$). The incoming and outgoing particles have definite momentum ($\vec{k}, \vec{k}'$, respectively). The diagrams can be thought to encode either the relative motion of two particles or the evolution of one particle scattered by a fixed target. Notice that only very simple (ladder) diagrams appear, corresponding to that fact that there are no creation/annihilation phenomena in this non-relativistic description.

2 Relativistic versus non-relativistic scattering theory

We will now analyse some differences between the non-relativistic picture we have been considering so far and the relativistic treatment of scattering theory.

2.1 Propagation of particles

Going back to the time-dependent Schrödinger equation (1), we can try to solve it directly by imitating the method used in 1.3 to derive the Lippmann-Schwinger equation. We can use the plane wave solutions $\exp i(\vec{k}\cdot\vec{x} - \frac{k^2}{2}t)$ of the *free* Schrödinger equation to transform the Schrödinger equation for H into an integral equation: any solution of the perturbed Schrödinger equation satisfies the following analogue of Lippmann-Schwinger:

$$\psi = e^{i(\vec{k}\cdot\vec{x} - \frac{k^2}{2}t)} - \frac{1}{i\frac{\partial}{\partial t} - \frac{1}{2}\Delta} V\psi. \tag{20}$$

As in Subsection 1.3., the easiest way of making sense of the inverse of $i\frac{\partial}{\partial t} - \frac{1}{2}\Delta$ is in momentum space. Since

$$\left(i\frac{\partial}{\partial t} - \frac{1}{2}\Delta\right) e^{i(\vec{q}\cdot\vec{x} - Et)} = \left(E - \frac{q^2}{2}\right) e^{i(\vec{q}\cdot\vec{x} - Et)}, \tag{21}$$

an inverse (in momentum space) can be found by prescribing the way to go around the pole $E = q^2/2$. For instance, we could use

$$\frac{1}{i\frac{\partial}{\partial t} - \frac{1}{2}\Delta} e^{i(\vec{q}\cdot\vec{x} - Et)} = \frac{1}{E - \frac{q^2}{2} + i\epsilon} e^{i(\vec{q}\cdot\vec{x} - Et)}. \tag{22}$$

The integral kernel of the chosen inverse, in position space, is given by the inverse Fourier transform

$$G(\vec{x}, t; \vec{x}', t') = \int \frac{d^3\vec{q}}{(2\pi)^4} e^{i\vec{q}\cdot\vec{x}} \int_{-\infty}^{\infty} dE \frac{e^{-iE(t-t')}}{E - \frac{q^2}{2} + i\epsilon}. \tag{23}$$

The only pole of the E integral is at $E = \frac{q^2}{2} - i\epsilon$ and so, *if* $t - t' < 0$ we get $G = 0$(because we can then avoid the pole by closing the integration contour in the upper half-plane). This result has an important implication: *particles can only travel forward in time.*

This is no longer true in a relativistic context: we have seen that the typical propagator of a particle of a mass m is

$$\frac{1}{q_0^2 - \vec{q}^2 + m^2 + i\epsilon}$$

in momentum space; in position space, the inverse Fourier transform gives (for $x = (\vec{x}, t)$)

$$G(x, x') = \int \frac{d^3\vec{q}}{(2\pi)^4} e^{i\vec{q}\cdot\vec{x}} \int_{-\infty}^{\infty} dE \frac{e^{-iE(t-t')}}{q_0^2 - \vec{q}^2 + m^2 + i\epsilon}. \tag{24}$$

No matter whether we close the integration contour in the upper or lower half-plane, we cannot avoid both poles, therefore it is no longer true that G vanishes if the time coordinates of the points x and x' satisfy $t < t'$. As a consequence, particles can make zig-zags in time, a phenomenon which is interpreted as the creation or annihilation of particle/antiparticle pairs (the particles traveling forward in time and the antiparticles backwards).

2.2 Propagation of signals

Non-relativistically, interactions are instantaneous. However, this is no longer true in the relativistic case.

Let us consider the example of the electromagnetic field; the interaction is transmitted by photons traveling at the speed of light (since the interaction is not instantaneous, we model it by some particles moving at finite speed).

The photon propagator in momentum space equals $1/(q_0^2 - \vec{q}^{\,2} + i\epsilon)$, an expression whose non-relativistic limit (given by $q_0 \to 0$) is formally $-1/\vec{q}^{\,2}$. This has to be reinterpreted since non-relativistically there is no creation and annihilation of particles (so the only way we can think about the photon non-relativistically is to consider that it only exists at the time t_0 when the interaction occurs).

Notice that the (four-dimensional) inverse Fourier transform of $-1/\vec{q}^{\,2}$ equals

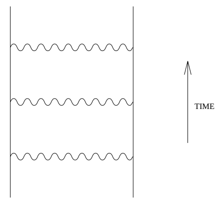
$$-\int \frac{d^4q}{(2\pi)^4}\frac{e^{iq\cdot y}}{\vec{q}^{\,2}} = -\delta(t)\frac{1}{|\vec{y}|}, \tag{25}$$

which is precisely a delta-function in time multiplied by the Coulomb potential. Therefore the non-relativistic limit corresponds to an *instantaneous* interaction (i.e. scattering in the Coulomb potential). Relativistically,

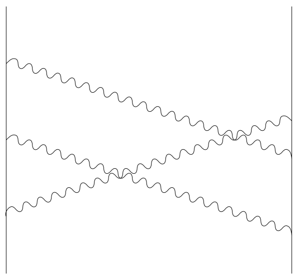
$$-\int \frac{d^4q}{(2\pi)^4}\frac{e^{iq\cdot y}}{q_0^2 - \vec{q}^{\,2} + i\epsilon} \tag{26}$$

is no longer supported at a fixed point in time, so the interaction is not instantaneous.

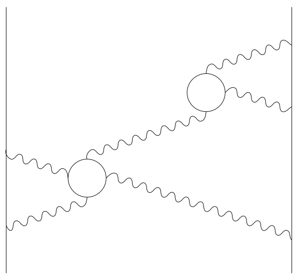
We can also illustrate the results on the propagation of particles and interactions in perturbation theory. It was shown that non-relativistically only ladder diagrams are encountered; intuitively, if time flows in the vertical direction, these diagrams represent particles moving forward with the horizontal curly lines being instantaneous interactions.



By contrast, in the relativistic case interactions travel at the speed of light and particle/antiparticle pairs can appear, so more complicated Feynman diagrams such as the ones below have to be considered.



This diagram illustrates the fact that photons traveling at the speed of light replace the non-relativistic instantaneous interaction. The curly line which represents the interaction in the non-relativistic case is relativistically a photon. In the second diagram we show the creation and annihilation of particle pairs. (Of course there are also diagrams in which both effects are present.) The diagram also illustrates another important fact: in a local theory, the presence of electron/positron pairs makes it impossible to count 'the total number of particles in the universe'. The totality of electrons can be accounted for by a single electron zig-zagging in time or even a sigle closed loop.



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