QM-18 Lecture Notes Scattering in Quantum Mechanics* 18.1 Continuous Energy Solutions

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1 Asymptotic behaviour of scattering wave function

In this unit description of scattering and scheme of computation of cross section in quantum mechanics is introduced. This is achieved by imposing a suitable boundary condition on the solution of the time independent Schrödinger equation and converting Schrödinger equation into an integral equation using the Green function for the free particle Schrödinger equation. A perturbative solution of the integral equation leads to the Born approximation for the scattering amplitude.

Let us consider a scattering experiment in which a beam of particles is scattered from a target at rest. The frame of reference in which the

* KAPOOR //qm-lec-18001.tex;

December 12, 2016

target is at rest will be called the laboratory frame. After the scattering the particles, at large distances, will be moving, away from the target, like free particles. We assume the potential between an incident particle, position \vec{r}_1 , and the target, at position \vec{r}_2 , to be central potential V(r) which depends only on the relative position, $\vec{r} = \vec{r}_1 \vec{r}_2$, of the particle and the target. We recall that the two particle problem can then be reduced to the problem of one particle of reduced mass moving in a potential V(r). The cross section calculated for a particle moving in potential V(r) equals the scattering cross sections in the centre of mass frame and must be transformed to the lab frame to establish contact with experiments.

Knowledge of the classical trajectory of a particle, $\vec{r}(t)$ is sufficient to compute the cross section in classical mechanics. The classical physics being deterministic, the particles going into solid angle corresponding to a cone, covering small range $\theta, \theta + d\theta$ of the scattering angle, are precisely those which come from a corresponding range of impact parameter b. Hence we only need to know the relation between the impact parameter

and the scattering angle to compute the differential cross section $\sigma(\theta)$. The result is known to be

$$\sigma(\theta) = \frac{b}{\sin \theta} \left| \frac{db}{d\theta} \right| \tag{1}$$

In quantum mechanical framework the particles do not have a well defined trajectory and it is not meaningful to associate a well defined range of impact parameters with a given range of scattering angle. All information about a system has to be obtained from the wave function and must be extracted from the available statistical interpretation of the wave function.

The scattering process, like any other motion, is a problem of time evolution. In a scattering experiment, the incident particle is far off from the target and approaches towards the target reaching a point of closest approach. After that it moves away from the target and goes to infinity. A wave packet description the motion of a particle, in accordance with the time dependent Schrödinger equation, is the framework for a rigorous and a complete description of the scattering problem. It turns out that the scattering process can also the viewed as a stationary state problem and solution of the time independent Schrödinger equation turns out to be adequate as a first introduction for our present purpose.

Let us consider a thought experiment in which a beam of particles is incident and getting scattered for all times from $-\infty$ to ∞ . If take a snap shot of the beam in the experiment, it would look the same at all times. It should therefore not come as a surprise that one treat the scattering in terms of using stationary states. This is not something completely new, we are already used to treating motion of electrons in an atom as a stationary process in quantum mechanics. We will, therefore, formulate the scattering problem in terms of stationary state solutions, i.e.,

the solutions of the time independent Schrodinger equation. Boundary conditions for the wave function Assuming a spherically symmetric potential V(r) which goes to zero for large distances, E < 0 corresponds to possible bound states and the continuous energy solution for E > 0 is needed for a discussion of to the scattering. The Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + V(r)\psi = E\psi \tag{2}$$

has an infinite number of solutions E>0. To understand this we look at the free particle solutions. For a given energy the free particle solutions can be written as

$$\psi(\vec{r}) = N \exp(ik\hat{n} \cdot \vec{r}) \tag{3}$$

where $k = \sqrt{2E/2\hbar^2}$ and \hat{n} is a unit vector giving the direction of propagation. For a fixed energy E there are infinitely many plane wave solutions corresponding to the direction of propagation specified by the unit vector \hat{n} . Alternately, the solutions can also be written in terms of spherical waves of definite angular momentum ℓ and definite L_z value m

$$\psi(\vec{r}) = C j_{\ell}(kr) Y_{\ell m}(\theta, \phi) \tag{4}$$

The most general solution will be a superposition of the above special solutions. The free particle behaviour will hold for the scattering solutions for a potential which goes to zero for large distances, giving infinite number of solutions. Thus specifying the energy alone is not sufficient to pick a unique solution, it is necessary to specify a boundary condition suited to the scattering problem. In the stationary description, the solution to Schrodinger equation should describe the incident beam and an outgoing scattered wave. For short range potentials this will be a spherical wave with varying amplitude in different directions.

We demand that the wave function for a definite energy must satisfy the following boundary condition in the limit $r \to \infty$:

$$\lim \psi(\vec{r}) \to e^{ikz} + f(\theta) \frac{e^{ikr}}{r} \tag{5}$$

The above choice of the boundary condition requires an explanation. The first term has been written for the choice of z axis along the incident beam of definite energy E. In general, for incident beam having momentum k_i , one must replace the first term by $\exp(-i\vec{k}_i \cdot \vec{r})$. The second term represents an outgoing spherical wave, note that the time dependence of the wave function will $e^{-iEt/\hbar}$. The factor $f(\theta)/r$ represents the amplitude of the wave at large distances in the direction θ . Since the intensity of the scattered beam decreases as $1/r^2$ for large distance, the amplitude must decrease as 1/r for large r. As of now, it is not clear that such a solution does exist, in a later subsection we will show that a solution satisfying the boundary condition Eq.(5) does exist.

2 Cross section in quantum Theory

Now we come to computation of cross section for scattering from a potential spherical symmetric, finite range potential V(r). We wish to relate the differential cross section to the scattering amplitude $f(\theta)$. Let us consider a scattering experiment involving a total of N incident particles sent in time T. The number of particles detected per second by a detector in a direction θ will be proportional to the flux of the incident beam and the solid angle subtended by the detector and the constant of proportionality is just the differential cross section. For a detector placed at a distance r from the target and having an opening area ΔS , the solid angle will be $\Delta \Omega = \Delta S/r^2$ Thus we would get

No of particle detected per sec = $\sigma(\theta) \times \Delta\Omega \times$ Flux of the incident beam.

knowing the wave function, the number of particles detected per second can be computed using the probability current density \vec{j} . The opening of the detector is kept perpendicular to the radius vector and usually covers only a small solid angle, the probability of a particle entering the detector per sec is given by the surface integral

$$\iint_{S} j_r dS \approx j_r \Delta S \tag{6}$$

over the surface of the detector, where j_r is the radial component of the probability current. The total number of particles detected per sec will be N times the expression. Thus Eq.(2) becomes

$$N \times j_r \Delta S = \sigma(\theta) \times \Delta \Omega \times \text{Flux of the incident beam} = \sigma(\theta) \Delta \Omega \times N j_z.$$
 (7)

where j_z is the z component of the probability current. Using

$$\vec{j} = -\frac{\hbar}{2i\mu} (\psi^* \nabla \psi - \psi \nabla \psi^*) \tag{8}$$

the z component of the probability current for the incident beam e^{ikz} is easily found to be k/. Also the radial component of the of the probability current for the scattered wave is obtained by substituting $f(\theta)e^{ikr}/r$ for $\psi(r)$ in Eq.(8) and taking the radial component. Using

the most important term in the radial component of the current for the scattered wave becomes

$$j_r = \frac{|f(\theta)|^2}{r^2} + O(1/r^2). \tag{9}$$

Using Eq.(8)-Eq.(9) in Eq.(7) gives

$$(N(|f()|^2/r^2)\Delta S = \sigma(\theta)\Delta\Omega N \tag{10}$$

With $\Delta S = r^2 \Delta \Omega$, we get the desired relation

$$\sigma(\theta) = |f(\theta)|^2. \tag{11}$$

We have ignored the terms in the current coming from the interference of the incident and scattered waves. These are of the order of $1/r^2$, and are proportional to exp(ikr(1cos)). Due to the presence of large r in the exponential, this term oscillates rapidly with and contributes vanishingly small value to the cross section when summed over a small range of θ values.

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Created: Jul 2016 Ver 16.x

Printed December 12, 2016

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