ONE-DIMENSIONAL SCATTERING IN QUANTUM MECHANICS

8.1 The one-dimensional scattering problem

In a scattering experiment a beam of particles is scattered by a target, and the scattered particles are detected. The interaction between the beam and target takes place in a small volume of space. The region where the beam is prepared and the region where the scattered beam is detected are both outside the region of interaction between the beam and the target. Thus both in the initial and the final states the particles in the beam behave as free particles. Scattering processes are transitions from one free-particle state to another as a result of an interaction which takes place within a small volume. These features are all illustrated in the following one-dimensional example.

Consider a single particle of mass m and momentum p moving freely in one dimension. The Hamiltonian is:

$$H_0 = p^2/2m. \tag{8.1}$$

The momentum p commutes with H_0. Thus H_0 and p can be simultaneously diagonalized. The eigenfunctions are plane waves:

$$\psi_k = \mathrm{e}^{\mathrm{i}kx} \tag{8.2a}$$

$$p\psi_k = \hbar k\psi_k \tag{8.2b}$$

$$H_0\psi_k = \frac{(\hbar k)^2}{2m}\psi_k. \tag{8.2c}$$

The energy spectrum is continuous and doubly degenerate since the eigenvalue (8.2c) depends only on the magnitude of k and not on the sign. Any linear combination of the degenerate eigenfunctions ψ_k and ψ_{-k} is also an eigenfunction, e.g.

$$A\psi_k + B\psi_{-k} = A\mathrm{e}^{\mathrm{i}kx} + B\mathrm{e}^{-\mathrm{i}kx} \tag{8.3a}$$

or

$$\Phi_k = \sin(kx + \delta). \tag{8.3b}$$

where A, B and δ are constants.

The momentum eigenfunctions (8.2) describe travelling waves. The function (8.3a) is a linear combination of two travelling waves in opposite directions. The function (8.3b) describes a standing wave.

The Hamiltonian (8.1) is invariant under a reflection about the origin. The parity P thus commutes with the Hamiltonian and a complete set of simultaneous eigenfunctions of H and P can be found. The even and odd parity eigenfunctions are respectively

$$\psi_{k0} = \cos kx \tag{8.4a}$$

$$\psi_{k1} = \sin kx \tag{8.4b}$$

$$P\psi_{k0} = \psi_{k0} \tag{8.5a}$$

$$P\psi_{k1} = -\psi_{k1}. \tag{8.5b}$$

Let us now add to the Hamiltonian (8.1) a potential V, which is confined to a finite region bounded by the value $|x| = X$.

$$H = \frac{p^2}{2m} + V(x) \tag{8.6a}$$

$$V(x) = 0 \quad \text{for} \quad |x| > X. \tag{8.6b}$$

The eigenvalue spectrum for $E \geqq 0$ is not changed by the added potential. It is still continuous and doubly degenerate. The form of these eigenfunctions is also not changed in the region outside of the potential. One can find eigenfunctions which behave like any of the free-particle eigenfunctions (8.2a), (8.3) or (8.4b) for $x > X$, and similarly for $x < -X$. However we do not know the connection between the wave functions in the positive and negative domains. A wave function which has the form (8.2a) for $x > X$, must be some linear combination (8.3a) in the region $x < -X$, but we do not know a priori which linear combination. This depends upon the potential V.

Let $\psi^{(+)}(x)$ be an eigenfunction of H which has the form (8.2a) of a single plane wave for $x > X$:

$$\psi^{(+)}(x) = S e^{ikx} \quad \text{for} \quad x > X \tag{8.7a}$$

where S is a numerical coefficient. Then for $x < -X$, this eigenfunction has the form (8.3a),

$$\psi^{(+)}(x) = e^{ikx} + R e^{-ikx} \quad \text{for} \quad x < -X, \tag{8.7b}$$

where R is a numerical coefficient, and we have chosen the normalization so that the coefficient of the first term is one. This eigenfunction (8.7) has a very simple physical interpretation. For $x<-X$, there are waves travelling in both directions, whereas for $x>X$, there is only an 'outgoing' wave moving to the right. The first term on the right-hand side of (8.7b) can be interpreted as an incident wave, the second term as a reflected wave and the wave function (8.7a) as a transmitted wave. Then R and S are the reflection and transmission coefficients for the potential V. They can be determined by the explicit solution of the Schrödinger equation, including the region of the potential.

8.2 Reflection and rotation symmetry and phase shifts

Suppose that the potential is invariant under reflections,

$$V(x) = V(-x) \tag{8.8a}$$

$$[P, V] = 0. \tag{8.8b}$$

Then the Hamiltonian (8.6) and the parity operator P can be simultaneously diagonalized to give even and odd standing-wave solutions. These can be written in the convenient form

$$\psi_0 = \cos(kx + \delta_0) \quad (x > X); \qquad \psi_0 = \cos(kx - \delta_0) \quad (x < -X) \tag{8.9a}$$

$$\psi_1 = \sin(kx + \delta_1) \quad (x > X); \qquad \psi_1 = \sin(kx - \delta_1) \quad (x < -X). \tag{8.9b}$$

These states differ from the corresponding free-particle parity eigenstates (8.4) by the 'phase shifts', δ_0 and δ_1. The values of these phase shifts depend upon the potential V and are obtained by the explicit solution of the Schrödinger equation.

The particular linear combination of the parity eigenstates (8.9) which has the form (8.7) is easily constructed

$$\psi^{(+)} = e^{+i\delta_0}\psi_0 + ie^{+i\delta_1}\psi_1 = \tfrac{1}{2}(e^{2i\delta_0} + e^{2i\delta_1})e^{ikx} \qquad (x > X) \tag{8.10a}$$

$$= e^{ikx} + \tfrac{1}{2}(e^{2i\delta_0} - e^{2i\delta_1})e^{-ikx} \qquad (x < -X) \tag{8.10b}$$

Thus:

$$S = \tfrac{1}{2}(e^{2i\delta_0} + e^{2i\delta_1}) = \tfrac{1}{2}[(e^{2i\delta_0} - 1) + (e^{2i\delta_1} - 1)] + 1$$

$$= 1 + \sum_{l=0,1} ie^{i\delta_l} \sin\delta_l \tag{8.11a}$$

$$R = \tfrac{1}{2}(e^{2i\delta_0} - e^{2i\delta_1}) = \tfrac{1}{2}[(e^{2i\delta_0} - 1) - (e^{2i\delta_1} - 1)]$$

$$= \sum_{l=0,1} i(-1)^l e^{i\delta_l} \sin\delta_l. \tag{8.11b}$$

The transmission and reflection coefficients are determined completely by the values of the phase shifts of the even and odd solutions.

Let us now express these results in a language which is more easily generalized to the physical three-dimensional case. The one-dimensional reflection symmetry of the potential, eq. (8.8a) can also be called invariance under a 180° rotation about an axis perpendicular to the x-axis. The natural generalization to three dimensions is full rotational invariance under an arbitrary rotation. Since the most convenient coordinates for discussing rotational invariance in three dimensions are spherical polar coordinates, our one-dimensional results will be more easily generalized to three dimensions if we express them in terms of 'one-dimensional polar variables'. We therefore define

$$r = |x| \tag{8.12a}$$

$$\theta = 0 \quad \text{if} \quad x > 0; \qquad \theta = \pi \quad \text{if} \quad x < 0. \tag{8.12b}$$

In the one-dimensional case θ has only two values, 0 and π, for the forward and backward directions respectively. However the dependence of the wave functions and the scattering process on this two-valued angular variable already gives considerable insight into the angular dependence for the three-dimensional case.

In three-dimensional scattering problems, a combination of cartesian and polar coordinates is often used, to write a wave function as a linear combination of an incident plane wave and an outgoing spherical wave. The wave function (8.7) can be rewritten as a single equation in this form, using our one-dimensional polar variables (8.12)

$$\psi^{(+)}(x) = e^{ikx} + g(\theta)e^{ikr}; \qquad (r > X) \tag{8.13a}$$

where

$$g(0) = S - 1 \tag{8.13b}$$

$$g(\pi) = R. \tag{8.13c}$$

The first term e^{ikx} in eq. (8.13a) is present not only for $x < -X$ but also for $x > X$. It describes, therefore, not only the incoming incident wave but also an outgoing wave which would be the complete solution of the Schrödinger equation in the absence of the potential. The two terms in the wave function (8.13a) thus describe an unperturbed incident wave which is the complete solution in the absence of the potential and a scattered wave which is entirely due to the potential. The function $g(\theta)$ describes the 'angular dependence' of the scattered amplitude.

The separation of the wave function into unperturbed and scattered waves differs from the separation in eqs. (8.7) into incoming and outgoing waves,

where the outgoing waves include the continuation of the incident wave after it has passed the potential. This difference between the two descriptions appears as an additional term in the expression (8.13b) relating the forward scattering amplitude $g(0)$ to the transmission coefficient S. There is no such additional term in the relation (8.13c) between the backward scattering amplitude $g(\pi)$ and the reflection coefficient R.

These two alternative descriptions are both useful in the treatment of scattering phenomena. The division into incoming and outgoing waves is convenient for the discussion of conservation of probability, which requires that the current carried by the incoming waves be equal to the current carried by the outgoing waves. The division into an unperturbed wave and a scattered wave is useful for the treatment in perturbation theory where one begins with the unperturbed wave as the zero-order solution and calculates the scattered wave by a method of successive approximations.

8.3 Conservation of probability and the optical theorem

From conservation of probability the currents carried by the two outgoing waves must be equal to the current from the incoming wave. Since all waves in this elastic scattering process have the same wave number and velocity, the currents are all proportional to the densities, with the same proportionality factor. Thus the sum of the densities of the two outgoing waves must be equal to the density of the incoming wave.

$$|R|^2 + |S|^2 = 1. \tag{8.14}$$

Note that the solution (8.11) satisfies this condition.

The total scattered intensity is the sum of the intensities of the forward and backward scattered waves (in the three-dimensional case it would be the integral of the scattered intensity over all angles).

$$|g(0)|^2 + |g(\pi)|^2 = |R|^2 + |S - 1|^2 = 2\mathrm{Re}(1-S) = -2\mathrm{Re}\ g(0), \tag{8.15}$$

where we have used eq. (8.14).

The function $g(\theta)$ is dimensionless and its square defines a scattering probability. In three dimensions, the scattering amplitude is naturally defined to give it the dimensions of length and its square defines the scattering cross section. The extra factor with dimensions of length arises naturally in three-dimensions because the free-particle solution corresponding to an outgoing wave is e^{ikr}/r rather than e^{ikr}. The three-dimensional analog of eq. (8.13a) is

$$\psi^{(+)}(x) = e^{ikx} + f(\theta)e^{ikr}/r \tag{8.16a}$$

where $f(\theta)$ is the scattering amplitude having the dimensions of length. Let us write

$$f(\theta)\frac{e^{ikr}}{r} = g(\theta)\frac{e^{ikr}}{ikr}. \tag{8.16b}$$

This relates $f(\theta)$ to a dimensionless amplitude $g(\theta)$ which is the natural generalization of the function $g(\theta)$ appearing in the one-dimensional case. We therefore define for the one-dimensional scattering amplitude

$$f(\theta) \equiv \frac{1}{ik} g(\theta). \tag{8.16c}$$

Substituting eq. (8.16c) into eq. (8.15), we obtain:

$$\sum_{l=0,\pi} |f(\theta)|^2 = -2k^2 \operatorname{Re}[ikf(0)] = 2k^{-1} \operatorname{Im}[f(0)]. \tag{8.17}$$

This relation showing that the total scattered intensity is proportional to the imaginary part of the forward scattering amplitude is called the 'optical theorem'. In the three-dimensional case the numerical factor is 4π instead of 2. This non-linear relation has a left-hand side quadratic in the scattering amplitudes and a linear right-hand side. The non-linearity arises because the scale of the wave functions has already been set by normalizing the coefficient of the incident wave to unity in the right-hand side of eq. (8.14). The occurrence of the imaginary part of an amplitude on the right-hand side of eq. (8.17) does not indicate a physical significance to the absolute phase in a wave function. This is a relative phase because the absolute phase of the wave function has been fixed by choosing the coefficient of the incident wave to be real.

The scattering amplitude $f(\theta)$ is very simply expressed in terms of the phase shifts by using eqs. (8.11), (8.13) and (8.16):

$$f(\theta) = k^{-1} \sum_{l=0,1} e^{il\theta} e^{i\delta_l} \sin \delta_l. \tag{8.18}$$

The generalization of eq. (8.18) to three dimensions is intuitively obvious. The scattering amplitude $f(\theta)$ is a function of continuous angular variables describing the scattering in any direction rather than only forward and backward. The parity symmetry of the potential becomes a rotational symmetry, expressing the invariance of the potential with respect to all changes of direction in space, rather than only the change from forward to backward. The conserved quantity corresponding to rotational invariance is angular momentum. The two parity eigenstates (8.9) are thus replaced by an infinite discrete series of angular momentum eigenstates each having its own phase

shift. The expansion of a scattering wave function into angular momentum eigenstates is called a partial wave expansion. In three dimensions the scattering amplitude (8.18) is also expressed as the sum of the contributions of the partial waves with each contribution expressed as a function of the corresponding phase shift.

8.4 The *S*-matrix

The wave function (8.13) can be expressed as the sum of incoming and outgoing waves by writing the first term in polar coordinates as well as the second term.

$$\psi_0^{(+)} = \delta_{\theta\pi} e^{-ikr} + [g(\theta) + \delta_{\theta 0}] e^{ikr}; \qquad r > X \tag{8.19a}$$

where the subscript zero on the wave function indicates that its incident wave is in the forward direction. Since our potential is invariant under reflections we can construct another solution of the Schrödinger equation from eq. (8.19a) by performing a reflection on this wave function. In polar coordinates a reflection replaces θ by $\pi - \theta$

$$\psi_\pi^{(+)} = \delta_{\theta 0} e^{-ikr} + [g(\pi - \theta) + \delta_{\theta\pi}] e^{ikr}; \qquad r > X, \tag{8.19b}$$

where the subscript π indicates that the incident wave is in the backward direction. Eqs. (8.19a) and (8.19b) can be combined in the form

$$\psi_{\theta'}^{(+)} = \delta_{\theta(\pi-\theta')} e^{-ikr} + [g(\theta' - \theta) + \delta_{\theta\theta'}] e^{ikr}; \qquad r > X. \tag{8.19c}$$

Any linear combination of eqs. (8.19a) and (8.19b) is also a solution of the Schrödinger equation. Since any function of the two-valued variable θ can be expressed as a linear combination of $\delta_{\theta\pi}$ and $\delta_{\theta 0}$, we can construct solutions with an incoming wave e^{-ikr} multiplied by an arbitrary function of θ. Let $\phi_1(\theta)$ and $\phi_2(\theta)$ be any two orthonormal functions of θ in the two-dimensional vector space defined by the values $\theta = 0$ and $\theta = \pi$. Then we can construct the two corresponding solutions by combining the solutions (8.19a) and (8.19b):

$$\psi_\alpha^{(+)} = \phi_\alpha(0)\psi_0^{(+)} + \phi_\alpha(\pi)\psi_\pi^{(+)} = \sum_{\theta'=0,\pi} \phi_\alpha(\theta')\psi_{\theta'}^{(+)} \tag{8.20a}$$

$$\psi_\alpha^{(+)} = \phi_\alpha(\pi - \theta)e^{-ikr} + \sum_{\beta=1,2} S_{\alpha\beta}\phi_\beta(\theta)e^{ikr}; \qquad r > X, \quad \alpha = 1, 2 \tag{8.20b}$$

where

$$S_{\alpha\beta} = \sum_{\theta,\theta'} \phi_\beta^*(\theta)[g(\theta' - \theta) + \delta_{\theta\theta'}]\phi_\alpha(\theta'). \tag{8.20c}$$

The matrix $S_{\alpha\beta}$ is called the S-matrix and gives the amplitude of the outgoing wave of type β corresponding to an incoming wave of type α.

Conservation of probability requires that the total intensity of outgoing waves be equal to the intensity of incoming waves for any linear combination $\sum U_\alpha \psi_\alpha^{(+)}$ ($\alpha = 1, 2$) of the states (8.20b). Since the functions ϕ_α and ϕ_β are orthonormal, equating intensities of outgoing and incoming waves gives

$$\sum_{\alpha\beta\gamma} U_\gamma^* S_{\gamma\beta}^* U_\alpha S_{\alpha\beta} = \sum_\alpha U_\alpha^* U_\alpha. \tag{8.21a}$$

Since this must hold for all values of the coefficients U_α,

$$\sum_{\beta=1,2} S_{\alpha\beta} S_{\gamma\beta}^* = \delta_{\alpha\gamma}. \tag{8.21b}$$

Thus the S-matrix is unitary.

If there is no potential, the outgoing wave is the same as the incoming wave and the S-matrix is seen from eq. (8.20b) to be equal to the unit matrix.

Using the unitarity relation (8.21b) we can construct another set of two corresponding solutions

$$\begin{aligned}\psi_\gamma^{(-)} &= \sum_{\alpha=1,2} \psi_\alpha^{(+)} S_{\alpha\gamma}^* \\ &= \sum_{\alpha=1,2} \phi_\alpha(\pi - \theta) S_{\alpha\gamma}^* e^{-ikr} + \phi_\gamma(\theta) e^{ikr}; \quad r > X, \quad \alpha = 1, 2. \end{aligned} \tag{8.22a}$$

These solutions have a single outgoing wave and a sum of incoming waves, rather than a single incoming wave and a sum of outgoing waves. Note that a function having these properties can also be generated from any solution (8.20b) by interchanging θ and $\pi - \theta$ and taking the complex conjugate

$$[\psi_\alpha^{(+)}(\pi - 0)]^* = \phi_\alpha^*(0) e^{ikr} + \sum_{\beta=1,2} S_{\alpha\beta}^* \phi_\beta^*(\pi - 0) e^{-ikr}. \tag{8.22b}$$

Substituting the functions (8.22b) into the Schrödinger equation shows that they are solutions if the potential is *real*, i.e. if the potential is invariant under time reversal. In that case the solutions (8.22a) and (8.22b) must describe the same physical states, differing only by phases. This gives conditions on the S-matrix imposed by time reversal invariance. For the case where the phases of the basic states $\phi_\alpha(\theta)$ are chosen to be real, e.g. the states (8.19), time reversal invariance requires the S-matrix to be *symmetric*. This agrees with an intuitive picture of time reversal which would require the transition probability from state α to state β to be the same as that from β to α.

The S-matrix can be diagonalized for a reflection-symmetric potential by choosing the parity eigenstates (8.9) as our basic states. In polar coordinates,

these are

$$\psi_0 = \cos(kr + \delta_0) = \tfrac{1}{2}e^{-i\delta_0}[e^{-ikr} + e^{2i\delta_0}e^{ikr}]; \qquad r > X \tag{8.23a}$$

$$\psi_1 = e^{i\theta}\sin(kr + \delta_1) = \tfrac{1}{2}ie^{-i\delta_1}e^{i\theta}[e^{-ikr} - e^{2i\delta_1}e^{ikr}]; \qquad r > X. \tag{8.23b}$$

These two can be combined with new normalization and phase factors in the form

$$\psi_l = e^{il\theta}[e^{-ikr} + (-1)^l e^{2i\delta_l}e^{ikr}]. \tag{8.23c}$$

This can also be written in a form resembling eq. (8.20b)

$$\psi_l = -[e^{il(\pi-\theta)}e^{-ikr} + e^{2i\delta_l}e^{i\theta}e^{ikr}]. \tag{8.23d}$$

By comparison with eqs. (8.20b) we see that

$$\phi_l(\theta) = e^{il\theta} \tag{8.24a}$$

and the S-matrix is

$$S_{ll'} = e^{2i\delta_l}\delta_{ll'}. \tag{8.24b}$$

A knowledge of the S-matrix gives a complete description of the scattering process. The S-matrix gives the scattered waves for all possible incident waves. In the general case where there are inelastic scattering processes as well as elastic, the S-matrix relates all possible states which are coupled together by the scattering process, the indices α and β take on values for all possible 'channels' rather than just the two values for the forward and backward channels. There are some schools of thought in particle physics which see the S-matrix as the most basic and fundamental quantity in particle physics, since the elements of the S-matrix are measured in scattering experiments rather than the Hamiltonian or other dynamical variables like fields.

8.5 KN charge exchange and multichannel scattering

As an example of multichannel scattering processes we can consider particles having additional internal degrees of freedom, such as electric charge. This introduces the possibility of inelastic processes, such as charge exchange scattering in addition to elastic scattering. Consider the scattering of a kaon by a potential due to a nucleon held fixed at the origin. The motion of the nucleon is neglected, but it can be either a proton or a neutron and exchange charge with the kaon which can be either a K^+ or K^0. If the initial state is a K^+ and a neutron, a charge exchange scattering can occur to a final state which is a K^0 and a proton. The n–p and K^0–K^+ mass differences are neglected so that charge exchange occurs with no change in energy or