

## CHAPTER 8

# 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:

$$H_0 = p^2/2m. \quad (8.1)$$

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

$$\psi_k = e^{ikx} \quad (8.2a)$$

$$p\psi_k = \hbar k\psi_k \quad (8.2b)$$

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

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  $\psi_k$  and  $\psi_{-k}$  is also an eigenfunction, e.g.

$$A\psi_k + B\psi_{-k} = Ae^{ikx} + Be^{-ikx} \quad (8.3a)$$

or

$$\Phi_k = \sin(kx + \delta). \quad (8.3b)$$

where  $A$ ,  $B$  and  $\delta$  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

$$\psi_{k0} = \cos kx \quad (8.4a)$$

$$\psi_{k1} = \sin kx \quad (8.4b)$$

$$P\psi_{k0} = \psi_{k0} \quad (8.5a)$$

$$P\psi_{k1} = -\psi_{k1}. \quad (8.5b)$$

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

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

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

The eigenvalue spectrum for  $E \geq 0$  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  $x > X$ :

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

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

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

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,

$$V(x) = V(-x) \quad (8.8a)$$

$$[P, V] = 0. \quad (8.8b)$$

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

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

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

These states differ from the corresponding free-particle parity eigenstates (8.4) by the 'phase shifts',  $\delta_0$  and  $\delta_1$ . 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

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

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

Thus:

$$S = \frac{1}{2}(e^{2i\delta_0} + e^{2i\delta_1}) = \frac{1}{2}[(e^{2i\delta_0} - 1) + (e^{2i\delta_1} - 1)] + 1 \\ = 1 + \sum_{l=0,1} ie^{i\delta_l} \sin \delta_l \quad (8.11a)$$

$$R = \frac{1}{2}(e^{2i\delta_0} - e^{2i\delta_1}) = \frac{1}{2}[(e^{2i\delta_0} - 1) - (e^{2i\delta_1} - 1)] \\ = \sum_{l=0,1} i(-1)^l e^{i\delta_l} \sin \delta_l. \quad (8.11b)$$

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  $180^\circ$  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

$$r = |x| \quad (8.12a)$$

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

In the one-dimensional case  $\theta$  has only two values, 0 and  $\pi$ , 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)

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

where

$$g(0) = S - 1 \quad (8.13b)$$

$$g(\pi) = R. \quad (8.13c)$$

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  $g(\theta)$  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.

$$|R|^2 + |S|^2 = 1. \quad (8.14)$$

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).

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

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

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

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

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

This relates  $f(\theta)$  to a dimensionless amplitude  $g(\theta)$  which is the natural generalization of the function  $g(6)$  appearing in the one-dimensional case. We therefore define for the one-dimensional scattering amplitude

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

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

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

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  $4\pi$  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 abso-

lute phase of the wave function has been fixed by choosing the coefficient of the incident wave to be real.

The scattering amplitude  $f(0)$  is very simply expressed in terms of the phase shifts by using eqs. (8.11), (8.13) and (8.16):

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

The generalization of eq. (8.18) to three dimensions is intuitively obvious. The scattering amplitude  $f(0)$  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.

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

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  $\theta$  by  $\pi - \theta$

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

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

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

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  $\theta$  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 0. Let  $\psi_1(\theta)$  and  $\varphi_2(\beta)$  be any two orthonormal functions of 0 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):

$$\psi_a^{(+)} = \phi_a(0)\psi_0^{(+)} + \phi_a(\pi)\psi_\pi^{(+)} = \sum_{\theta'=0,\pi} \phi_a(\theta')\psi_{\theta'}^{(+)} \quad (8.20a)$$

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

where

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

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

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

$$\sum_{a\beta\gamma} U_\gamma^* S_{\gamma\beta}^* U_\alpha S_{a\beta} = \sum_a U_a^* U_a. \quad (8.21a)$$

Since this must hold for all values of the coefficients  $U_a$ ,

$$\sum_{\beta=1,2} S_{a\beta} S_{\gamma\beta}^* = \delta_{a\gamma}. \quad (8.21b)$$

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

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

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  $\theta$  and  $\pi - \theta$  and taking the complex conjugate

$$[\psi_a^{(+)}(\pi - \theta)]^* = \phi_a^*(\theta) e^{ikr} + \sum_{\beta=1,2} S_{a\beta}^* \phi_\beta^*(\pi - \theta) e^{-ikr}. \quad (8.22b)$$

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  $\alpha$  to state  $\beta$  to be the same as that from  $\beta$  to  $\alpha$ .

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

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

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

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

$$\psi_i = e^{i\theta}[e^{-ikr} + (-1)^i e^{2i\delta_i}e^{ikr}]. \quad (8.23c)$$

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

$$\psi_i = -[e^{i\theta(\pi-\theta)}e^{-ikr} + e^{2i\delta_i}e^{i\theta}e^{ikr}]. \quad (8.23d)$$

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

$$\phi_i(\theta) = e^{i\theta} \quad (8.24a)$$

and the S-matrix is

$$S_{ii'} = e^{2i\delta_i} \delta_{ii'}. \quad (8.24b)$$

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  $\alpha$  and  $\beta$  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 momentum. We assume that the potential is invariant under reflections and also conserves isospin.

Consider systems of electric charge  $Q=+1$ ; i.e. the  $K^+n$  and  $K^0p$  systems for which charge exchange is possible. We do not consider the  $K^+p$  and  $K^0n$  systems, as only elastic scattering is allowed by charge conservation, and the treatment is exactly the same as the previous example, eq. (8.6). For positive energies the  $Q=+1$  states have a continuous spectrum and a fourfold degeneracy. The two-fold degeneracy of the uncharged example eq. (8.6) is doubled because there are  $K^+n$  and  $K^0p$  states for each eigenfunction of the Hamiltonian (8.6). In the regions  $x > X$  and  $x < -X$  the eigenfunctions of the KN Hamiltonian are the same as for free particles and any basis can be chosen to describe the four degenerate states. However we do not know the relation between the wave functions between the positive and negative domains. To describe a scattering problem with a  $K^+$  beam on a proton target, we need a wave function with the following properties:

In the region  $x < -X$ , it has an incident  $K^+n$  wave with momentum  $+k$  and reflected  $K^+n$  and  $K^0p$  waves with momentum  $-k$ . In the region  $x > X$  it has transmitted  $K^+n$  and  $K^0p$  waves with momentum  $+k$  but no waves with momentum  $-k$ . Thus it has an incident  $K^+$  wave coming from  $x = -\infty$  on a proton target and outgoing waves in both directions which can be either  $K^+n$  or  $K^0p$ .

Our formalism is easily generalized to describe these multichannel wave functions. We introduce an additional index  $q$  to label the charge channel,  $q=+$  for the  $K^+n$  state and  $q=0$  for  $K^0p$ . Then eq. (8.13a) can be written

$$\psi_q^{(+)} = U_q e^{ikx} + \sum_s g_{qs}(\theta) U_s e^{ikr}; \quad r > X \quad (8.25a)$$

where  $U_q$  describes the charge of the state, and  $g_{qs}(\theta)$  is a  $2 \times 2$  matrix in the charge space. Similarly eq. (8.20b) becomes

$$\psi_{q\alpha}^{(+)} = U_q \phi_\alpha(\pi - \theta) e^{-ikr} + \sum_{\beta=1,2} S_{q\alpha, q\beta} U_\beta \phi_\beta(\theta) e^{ikr}; \quad r > X. \quad (8.25b)$$

The S-matrix now has additional labels for the charge channel, and is given by the corresponding generalization of eq. (8.20c)

$$S_{q\alpha, q\beta} = \sum_{\theta, \theta'} \phi_\beta^*(\theta) [g_{q\beta}(\theta' - \theta) + \delta_{\theta\theta'} \delta_{q\beta}] \phi_\alpha(\theta'). \quad (8.25c)$$

Since isospin is conserved in the interaction, it is convenient to define isospin eigenfunctions.

$$U^{(1)} = \frac{1}{\sqrt{2}}(U_+ + U_0) \quad (8.26a)$$

$$U^{(0)} = \frac{1}{\sqrt{2}}(U_+ - U_0). \quad (8.26b)$$

We can then define simultaneous eigenfunctions of isospin and parity by generalizing eq. (8.23d)

$$\psi_i^{(T)} = -U^{(T)}[e^{iI(x-\theta)} e^{-ikr} + e^{2i\delta_i T} e^{iI\theta} e^{ikr}]. \quad (8.27a)$$

The four isospin and parity eigenfunctions are decoupled and each is characterized by its individual phase shift. The S-matrix is then

$$S_{Tl, T'l'} = e^{2i\delta_l T} \delta_{Tl} \delta_{ll'}. \quad (8.27b)$$

The scattering amplitudes  $g_{qr}(\theta)$  can then be expressed in terms of these phase shifts. For the case of incident  $K^+$ ,  $q=+$  and

$$g_{++}(\theta) = \frac{1}{2} \sum_{l,T} i e^{il\theta} e^{i\delta_l T} \sin \delta_l^T \quad (8.28a)$$

$$g_{+0}(\theta) = \frac{1}{2} \sum_{l,T} i e^{il\theta} (-1)^{T-1} e^{i\delta_l T} \sin \delta_l^T. \quad (8.28b)$$

The phase shift method thus allows the dependence on isospin and scattering angle to be unscrambled by the use of the isospin and parity eigenstates. In the general case any symmetry in the scattering problem allows a separation of the scattering amplitude into terms which are decoupled from one another because they correspond to different eigenvalues of a conserved quantity. One thus has partial waves for each set of eigenvalues and can express the corresponding partial-wave amplitudes in terms of the relevant phase shifts.

In a general collision problem there may be many possible channels for the reaction instead of only two,  $K^+n$  and  $K^0p$ , as in this simple example. For example in the scattering of protons on  $^{12}C$  there can be reactions in which there are outgoing neutrons, deuterons or alpha particles each leaving a different residual nucleus which can be either in its ground state or in some excited state. We can generalize the notation of eq. (8.25) for the wave function to apply to the case of an arbitrary number of channels. Let  $q$  describe all the ‘internal’ degrees of freedom of the incident and scattered particles. In a case like proton scattering on  $^{12}C$  the function  $U_q$  could describe not only the labels of the two particles but also the structure of the particular state of the residual nucleus. The function  $g_{qs}\theta$  is then an  $n \times n$  matrix where  $n$  is the number of channels, and the S-matrix is correspondingly enlarged. If there is no symmetry which allows us to separate the problem into uncoupled channels, then the phase shift method does not give a complete solution and the multichannel equation must be solved by other means. This would be the case in the proton- $^{12}C$  example.

## 8.6 The delta potential

Let us now consider the solution of the scattering problem for a short-range potential which exists only in a region very small compared to the wavelength of the scattered particle

$$kX \ll 1. \quad (8.29)$$

The Schrödinger equation

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right] \psi = E\psi = \frac{\hbar^2 k^2}{2m} \psi \quad (8.30a)$$

is commonly rewritten

$$\left( \frac{d^2}{dx^2} + k^2 \right) \psi = \frac{2mV}{\hbar^2} \psi = U\psi \quad (8.30b)$$

where

$$U(x) \equiv \frac{2m}{\hbar^2} V(x). \quad (8.30c)$$

Eq. (8.30b) can be integrated between the points  $-X$  and  $+X$  where the potential vanishes.

$$\frac{d\psi(+X)}{dx} - \frac{d\psi(-X)}{dx} + k^2 \int_{-X}^X \psi dx = \int_{-X}^X U\psi dx. \quad (8.31)$$

For a short-range potential satisfying eq. (8.29) the wave function does not change very much in the region of the potential, and eq. (8.31) gives the change in the derivative of the wave function from one side of the potential to the other. The right-hand side is just the product of the wave function and the integral of the potential. To simplify the calculations we assume a 'zero range' potential.

$$U(x) = -U_0 \delta(x). \quad (8.32)$$

We now let  $\rightarrow$  in eq. (8.31). Then for the even-parity solution (8.9a):

$$\frac{d\psi_0(0+)}{dx} - \frac{d\psi_0(0-)}{dx} = -2k \sin \delta_0 = -U_0 \psi_0(0) = U_0 \cos \delta_0. \quad (8.33)$$

The phase shift for the even-parity wave is thus

$$\tan \delta_0 = \frac{U_0}{2k} \quad (8.34a)$$

and the S-matrix element is

$$e^{2i\delta_0} = \frac{1 + i \tan \delta_0}{1 - i \tan \delta_0} = \frac{1 + i(U_0/2k)}{1 - i(U_0/2k)} = \frac{2k + iU_0}{2k - iU_0}. \quad (8.34b)$$

The odd-parity solution (8.34b) vanishes at the origin. Its phase shift thus vanishes for the zero-range potential.

$$\delta_1 = 0 \quad (8.35a)$$

$$e^{2i\delta_1} = 1. \quad (8.35b)$$

Substituting (8.34) and (8.35) into eq. (8.18) we obtain the scattering amplitude:

$$f(\theta) = \frac{1}{2ik} [e^{2i\delta_0} - 1] = \frac{U_0}{k[2k - iU_0]} \quad (8.36a)$$

$$g(\theta) = i[U_0/(2k - iU_0)]. \quad (8.36b)$$

We now have the complete solution to the scattering problem. The intensities of the forward and backward scattered waves are given by equation (8.36).

Since  $f(\theta)$  is independent of  $\theta$  the forward and backward scattered amplitudes are equal. This is expected since only the even-parity wave is scattered by this potential and the odd-parity wave is not. Since both even and odd-parity waves have equal amplitudes forward and backward but opposite relative phase, there can be a difference between the forward and backward scattering amplitudes only when both waves are present. This can also be seen directly by examining eq. (8.23). The same result holds in three dimensions. Any difference between forward and backward scattering requires interference between even and odd-parity waves.

The expression (8.36b) substituted into the solution (8.13a) defines a solution to the Schrödinger differential equation (8.30a) for all values of  $k$ . It is instructive to examine the solutions for complex values of  $k$  as well as real values. If  $k$  is complex, the imaginary part of  $k$  contributes a real part to the exponents in eq. (8.36a). Either the incoming or outgoing wave has a positive real exponent corresponding to an amplitude which increases without limit at large distances. Such solutions do not represent physical states; they are excluded by the boundary conditions used with the Schrödinger equation. However, the scattering amplitude (8.36) and the S-matrix elements (8.34b) have a pole at the value  $k = iU_0$ . Thus as  $k$  approaches this value the amplitude of the scattered wave in (8.13a) increases without limit. If we normalize this solution to keep the amplitude of the

scattered wave constant, the first term approaches zero and vanishes at the pole. Thus at the value  $k = iU_0$ , eq. (8.13a) gives a solution in which there is only the outgoing wave and no incoming wave. For positive  $U_0$ ,  $k$  is pure imaginary and positive, the exponent is real and negative and the amplitude decreases to zero at large distances thus satisfying the boundary condition. Thus the imaginary value  $k = iU_0$  defines a physically admissible solution of the Schrödinger equation. Since the amplitude decreases to zero at large distances this solution corresponds to a bound state.

$$\psi_B(x) = e^{-\frac{1}{2}kx}. \quad (8.37a)$$

This bound-state wave function satisfies the Schrödinger equation:

$$H\psi_B(x) = E\psi_B(x) = -\frac{\hbar^2}{8m} \frac{U_0^2}{x^2} \psi_B(x). \quad (8.37b)$$

The wave function (8.37) has a very peculiar feature: its entire amplitude is outside the range of the potential. A measurement of the position of the particle therefore always finds it in a place where there is no force on it; yet the particle remains bound. Although this peculiarity is exaggerated by the unphysical delta function potential, a similar situation can exist with potentials of finite range and is related to wave-particle duality in quantum mechanics. If the range of the potential is small compared to the wavelength of the particle, the wave cannot be confined to the region of the potential. However, solutions may exist which have the form of standing waves with a tail that extends out beyond the potential. Thus there can be a very large probability of finding the particle in a region where there is no force on it. The binding is a result of the wave nature of the particle which spreads it over a finite region including the potential.

## 8.7 Analytical properties of scattering amplitudes

Interesting physical information is obtained by examining the properties of the scattering amplitude or the S-matrix considered as an analytic function in the complex plane. A pole in this function can reveal the existence of a bound state and give its energy.

The argument is general and applies to any scattering problem and not only to the delta potential. A pole implies the existence of a solution of a Schrödinger equation having the form of the second term in eq. (8.13a) with the incident wave missing. If such a solution exists for the time-independent Schrödinger equation, a solution of the time-dependent Schrödinger equation can be obtained by multiplying this solution by the factor  $e^{iEt/\hbar}$ .

$$\psi(t) = g(\theta)e^{ikr}e^{-iEt/\hbar}, \quad R > X, \quad (8.38a)$$

where the energy  $E$  is a complex number given by:

$$E = \hbar^2 k^2 / 2m. \quad (8.38b)$$

When the pole occurs at a purely imaginary value of  $k$ , as in eq. (8.36), the energy is real and negative and the solution (8.38a) corresponds to a bound state. If the pole occurs at a complex value of  $k$  with a positive imaginary part, a solution of the time-dependent Schrödinger equation of the form (8.38a) can also be written in which the wave function decreases exponentially to zero at large distances. If

$$k = k_1 + ik_2, \quad (8.39a)$$

then

$$E = \frac{\hbar^2}{2m} [k_1^2 - k_2^2 + 2ik_1 k_2], \quad (8.39b)$$

and

$$\psi(t) = g(\theta)e^{ikr}e^{-i[k_1^2 - k_2^2]t/m}e^{-k_2 r}e^{\hbar k_1 k_2 t/m}. \quad (8.39c)$$

The function (8.39c) satisfies all the proper boundary conditions for a Schrödinger wave function at any fixed value of the time  $t=t_0$ . It is well behaved and decreases to zero exponentially at large distances. This function can therefore represent a state of the physical system at the time  $t=t_0$ . However, since the Schrödinger equation is first order in time derivatives, a solution is completely specified for all time by giving its value at one time  $t=t_0$ . Since the function  $\psi(t)$  defined by eq. (8.39c) is a solution of the Schrödinger equation, it is the unique solution corresponding to the particular initial conditions chosen. However, if  $k_1 > 0$  the function (8.39c) increases exponentially with time and indicates that the scattering amplitude in some particular channel increases without limit. This contradicts conservation of probability and implies that no solutions with  $k_1 > 0$  can exist. Thus the S-matrix considered as an analytic function of the energy  $E$  is not allowed to have any poles in the upper complex half-plane; i.e. with a positive imaginary part. A pole in the lower half-plane,  $k_1 < 0$  is perfectly admissible since this corresponds to an exponentially decreasing probability in a given channel. This implies that the probability must increase in some other channel to give overall conservation of probability. However, an unlimited exponential increase of probability with time in any one channel cannot be compensated by decreases in other channels and is therefore not allowed.

Any scattering amplitude or S-matrix obtained from solving a Schrödinger equation exactly automatically has these analytic properties since conservation of probability is automatically incorporated in the Schrödinger equation. However, these analytic properties can be used in cases where we do not know the Schrödinger equation or have not solved it. The fact that a function is known to be analytic in a certain region of the complex plane allows us to use Cauchy's theorem in order to evaluate integrals of this function. The values of direct physical interest are only on the real axis. Thus one can consider contour integrals along the real axis from  $-\infty$  to  $+\infty$  which are closed by a circle in the upper half-plane. Relations are thus obtained between integrals of the scattering amplitude or of functions of the scattering amplitude on the real axis and the assumed asymptotic behavior at infinite energy which determines the contribution of the integral on the large circle. Such relations are called dispersion relations and are of particular importance in particle physics.

## 8.8 The double delta potential

The simple delta function potential lacks one important feature which characterizes physical potentials, namely, a characteristic range. Most physical potentials act in a finite region and there are physical scattering processes when the wavelength of the incident particles is short

compared to the size of the region in which the potential acts. There is also the possibility of resonances when a number of half wavelengths just fit in the region of the potential and can set up standing waves. These features are absent in the zero range delta potential.

A simple modification of the delta potential which introduces a finite range, is a potential of two delta functions separated by a finite distance. To keep the reflection symmetry we place the two delta functions at the points  $a$  and  $-a$

$$U(x) = \frac{2m}{\hbar^2} V(x) = -\frac{1}{2}U_0[\delta(x - \frac{1}{2}a) + \delta(x + \frac{1}{2}a)]. \quad (8.40)$$

We have defined the strength of each delta potential to be  $\frac{1}{2}U_0$ , to keep the same overall strength as for the single delta potential. The potential (8.40) thus reduces to the single delta potential (8.32) if  $a=0$ ,

To solve the Schrödinger equation we first integrate it between the points  $\pm a - \epsilon$  and  $\pm a + \epsilon$ , where  $\epsilon$  is very small,

$$\frac{d\psi}{dx}(\pm a + \epsilon) - \frac{d\psi}{dx}(\pm a - \epsilon) + k^2 \int_{\pm a - \epsilon}^{\pm a + \epsilon} \psi dx = \int_{\pm a - \epsilon}^{\pm a + \epsilon} U\psi dx = -\frac{1}{2}U_0\psi(\pm a). \quad (8.41a)$$

After dividing by  $\psi(\pm a)$  and neglecting the integral on the left-hand side which is of order  $\epsilon$ ,

$$\frac{1}{\psi} \frac{d\psi}{dx}(\pm a + \epsilon) - \frac{1}{\psi} \frac{d\psi}{dx}(\pm a - \epsilon) = -\frac{1}{2}U_0. \quad (8.41b)$$

Since  $\psi$  is continuous at  $\pm a$ , we can use the same value at  $\pm a \pm \epsilon$ . The expression (8.41b) is particularly useful because the logarithmic derivative is independent of the normalization.

We now use eq. (8.41b) to relate the solutions on the two sides of the delta function. The exact solutions of the Schrödinger equation for the interval  $-\frac{1}{2}a \leq x \leq \frac{1}{2}a$  with even and odd parity are just the corresponding solutions for a free particle.

$$\psi_0(x) = \cos kx; \quad \frac{1}{\psi_0} \frac{d\psi_0}{dx} = -k \tan kx; \quad -\frac{1}{2}a \leq x \leq \frac{1}{2}a \quad (8.42a)$$

$$\psi_1(x) = \sin kx; \quad \frac{1}{\psi_1} \frac{d\psi_1}{dx} = +k \cot kx; \quad -\frac{1}{2}a \leq x \leq \frac{1}{2}a. \quad (8.42b)$$

Outside the region of the potential, the parity eigenfunctions are expressed as usual in terms of phase shifts.

$$\psi_0(x) = \cos(kx \pm \delta_0); \quad \frac{1}{\psi_0} \frac{d\psi_0}{dx} = -k \tan(kx \pm \delta_0); \quad \pm x > \frac{1}{2}a \quad (8.43a)$$

$$\psi_1(x) = \sin(kx \pm \delta_1); \quad \frac{1}{\psi_1} \frac{d\psi_1}{dx} = +k \cot(kx \pm \delta_1); \quad \pm x > \frac{1}{2}a. \quad (8.43b)$$

The values of the phase shifts are determined by matching the two solutions (8.42) and (8.43) at the point  $x=\pm a$  using the condition (8.41b)

$$-k \tan(\frac{1}{2}ka + \delta_0) + k \tan(\frac{1}{2}ka) = -\frac{1}{2}U_0 \quad (8.44a)$$

$$k \cot(\frac{1}{2}ka + \delta_1) - k \cot(\frac{1}{2}ka) = -\frac{1}{2}U_0. \quad (8.44b)$$

Solving eqs. (8.44) for  $\delta_0$  and  $\delta_1$  gives

$$\cot \delta_0 = \tan \frac{1}{2}ka + \frac{2k}{U_0} \sec^2 \frac{1}{2}ka = \frac{4k/U_0 + \sin ka}{1 + \cos ka} \quad (8.45a)$$

$$\cot \delta_1 = -\cot \frac{1}{2}ka + \frac{2k}{U_0} \csc^2 \frac{1}{2}ka = \frac{4k/U_0 - \sin ka}{1 - \cos ka}. \quad (8.45b)$$

Eq. (8.45) show the following interesting features:

1. When  $ka=2n\pi$ , eqs. (8.45) reduce to the values (8.34) and (8.35) for a single delta potential. This includes the case  $a=0$ , when the potentials are equivalent and also all cases where there are an integral number of wavelengths between the two potentials.

2.  $\delta_0=0$  when  $ka=(2n+1)\pi$ ,  $\delta_1=0$  when  $ka=2n\pi$ , since the denominators of eqs. (8.45a) and (8.45b) vanish at these points. This can also be seen by looking at eq. (8.41a). Whenever  $\psi(\pm a)=0$ , the right-hand side of eq. (8.41a) vanishes, there is no discontinuity in the derivative at the point  $\pm a$ , and the solutions must be identical to those for a free particle in the absence of a potential; i.e. there is no phase shift. This occurs for the even-parity solution whenever an odd number of half wavelengths fit exactly in the interval between  $\pm a$  and for the odd-parity solution for an even number of half wavelengths. The even and odd-parity phase shifts thus show an oscillatory behavior as a function of  $k$  with periodic zeros.

3. For very small values of  $k$  eqs. (8.45) reduce to the form

$$\tan \delta_0 = \frac{U_0}{2k[1 + \frac{1}{2}aU_0]} \quad k \rightarrow 0 \quad (8.46a)$$

$$\tan \delta_1 = \frac{kU_0a^2}{8[1 - \frac{1}{2}aU_0]} \quad k \rightarrow 0. \quad (8.46b)$$

The odd-parity phase shift goes to zero and the even-parity phase shift has a form similar to that for a single delta function potential (8.34a). 4. For very large values of  $k$  eqs. (8.45) become

$$\tan \delta_0 = \frac{U_0}{4k} (1 + \cos ka) \quad k \rightarrow \infty \quad (8.47a)$$

$$\tan \delta_1 = \frac{U_0}{4k} (1 - \cos ka) \quad k \rightarrow \infty. \quad (8.47b)$$

The tangents of both phase shifts oscillate between zero and the value  $U_0/2k$  for a single delta function potential.

The most interesting region of values for  $k$  is the intermediate region where the numerators of eqs. (8.45a) and (8.54b) can vanish. The scattering amplitude is given by the expression

$$f(\theta) = \frac{1}{k} \sum_{l=0,1} e^{il\theta} e^{i\delta_l} \sin \delta_l = \frac{1}{k} \sum_{l=0,1} \frac{e^{il\theta}}{\cot \delta_l - i}. \quad (8.48)$$

The scattering amplitude thus has a maximum or resonance whenever  $\cot \delta_0 = 0$  or  $\cot \delta_1 = 0$ .

From eqs. (8.45)

$$\cot \delta_0 = 0 \quad \text{when} \quad \sin ka = -4k/U_0 \quad (8.49a)$$

$$\cot \delta_1 = 0 \quad \text{when} \quad \sin ka = 4k/U_0. \quad (8.49b)$$

If  $U_0 a$  is large, eqs. (8.49) have many solutions and there are many such resonances. In the vicinity of a resonance where  $\delta_1 = 0$ , we can expand  $\cot \delta$ , as a power series in the energy and keep only the linear term

$$\cot \delta_l = \frac{2}{\Gamma} (E - E_0) \quad (8.50a)$$

where  $E_0$  is the value of the energy where  $\cot \delta_1 = 0$  and

$$\frac{2}{\Gamma} = \frac{d}{dE} (\cot \delta_l) \quad \text{at} \quad E = E_0. \quad (8.50b)$$

In the vicinity of  $E_0$  eq. (8.48) for the scattering amplitude can be written

$$f_1(\theta) = \frac{1}{k} \frac{\frac{1}{2} e^{i\theta} \Gamma}{(E - E_0) + \frac{1}{2} i\Gamma} \quad (8.51)$$

where  $f_1(\theta)$  is the contribution to the scattering amplitude of the particular partial wave having the resonance. The expression (8.51) has the typical form of a resonance curve where  $\Gamma$  is the width of the resonance at half maximum. The scattering amplitude (8.48) has poles when  $\cot(\delta_1) = i$ . From eqs. (8.45)

$$\begin{aligned} \cot \delta_0 - i &= \frac{(4k/U_0 + \sin ka) - i(1 + \cos ka)}{(1 + \cos ka)} \\ &= -i \frac{[1 + e^{ika} + 4ik/U_0]}{(1 + \cos ka)} \end{aligned} \quad (8.52a)$$

$$\begin{aligned} \cot \delta_1 - i &= \frac{(4k/U_0 - \sin ka) - i(1 - \cos ka)}{(1 - \cos ka)} \\ &= -i \frac{[1 - e^{ika} + 4ik/U_0]}{(1 - \cos ka)}. \end{aligned} \quad (8.52b)$$

A pole in the scattering amplitude thus occurs at a pure imaginary value of  $k$ ,  $ik = -\lambda$  if

$$(1 + e^{-\lambda a}) - 4\lambda/U_0 = 0 \quad \text{for} \quad \delta_0 \quad (8.53a)$$

$$(1 - e^{-\lambda a}) - 4\lambda/U_0 = 0 \quad \text{for} \quad \delta_1. \quad (8.53b)$$

Eq. (8.53a) shows that there is always one such bound state of even parity. This can be seen

graphically by drawing the functions  $1 + e^{-\lambda a}$  and  $4\lambda/U_0$  and noting that they must intersect at one point. Eq. (8.53b) shows that for large values of  $U_0$  there is one odd-parity bound state whereas for small values of  $U_0$  there will be no bound state. This is seen graphically by drawing the curves  $1 - e^{\lambda a}$  and  $4\lambda/U_0$ . The critical value of  $U_0$  is the one for which both curves have the same slope at  $\lambda = 0$ ,

$$U_0 = 4/a. \quad (8.54)$$

A bound state is found for values of  $U_0$  greater than this value (8.54). This can also be verified by solving the Schrödinger equation directly for the bound states.

## 8.9 A delta potential with an excited state

Another instructive example obtainable by simple modification of the delta potential is the scattering by a system with an excited state which can be excited during the scattering. This corresponds to the physical problems of scattering of a particle by an atom, nucleus or molecule with the possibility of inelastic scattering with the excitation of the scatterer. We assume that the scatterer is very heavy and fixed at the origin and has only two states, the ground state and an excited state. The only scatterer degree of freedom which need be considered is the internal one which specifies whether it is in the ground state or the excited state. The wave function describing this system then is a function of the coordinate  $x$  of the particle being scattered and the internal degrees of freedom of the scatterer. The most general such wave function can be written as a linear combination of two terms, one having the scatterer in the ground state and the other having the scatterer in the excited state.

$$|\psi\rangle = a_g^\dagger |0\rangle \psi_g(x) + a_e^\dagger |0\rangle \psi_e(x) \quad (8.55)$$

where  $a^\dagger$  and  $a^\dagger$  create the scatterer in the ground and excited states respectively.

The Hamiltonian for this system includes the kinetic energy of the particle and the energy of the excited and ground states of the scatterer. For the interaction we choose a delta function potential with two terms, an elastic scattering term which does not change the state of the scatterer and an inelastic scattering term which induces transitions between the ground and the excited states.

$$\begin{aligned} H &= \frac{p^2}{2m} - \frac{\hbar^2}{2m} \delta(x)[U_0(a_g^\dagger a_g + a_e^\dagger a_e) + U_1(a_g^\dagger a_e + a_e^\dagger a_g)] \\ &\quad + E_e a_e^\dagger a_e + E_g a_g^\dagger a_g. \end{aligned} \quad (8.56)$$

The Schrödinger equation for the system is easily solved by the standard techniques used with delta function potentials. For all values of  $x$  except at the origin the solution is just a solution for a free particle with no interaction. The derivative of the solution is discontinuous at the

origin. The discontinuity is given in terms of the strength of the potential by integrating the Schrödinger equation between  $x = -\varepsilon$  and  $x = +\varepsilon$ . In the limit  $\varepsilon \rightarrow 0$  the only terms which contribute are the discontinuity in the derivative and the integral over the delta function potential. For the Hamiltonian (8.56) we obtain

$$-\frac{\hbar^2}{2m} \frac{d\psi}{dx} \Bigg|_{-\varepsilon}^{+\varepsilon} - \frac{\hbar^2}{2m} [U_0 \{a_s^\dagger a_s + a_e^\dagger a_e\} + U_1 \{a_s^\dagger a_e + a_e^\dagger a_s\}] \psi(0) = 0. \quad (8.57)$$

Substituting the wave function (8.55) into eq. (8.57) we obtain

$$\begin{aligned} a_s^\dagger |0\rangle \frac{d\psi_s}{dx} \Bigg|_{-\varepsilon}^{+\varepsilon} + a_e^\dagger |0\rangle \frac{d\psi_e}{dx} \Bigg|_{-\varepsilon}^{+\varepsilon} + [U_0 \psi_s(0) + U_1 \psi_e(0)] a_s^\dagger |0\rangle \\ + [U_0 \psi_e(0) + U_1 \psi_s(0)] a_e^\dagger |0\rangle = 0. \end{aligned} \quad (8.58)$$

Since the ground and excited states of the scatterer are orthogonal, the terms involving these two states must vanish separately, thus

$$\frac{d\psi_s}{dx} \Bigg|_{-\varepsilon}^{+\varepsilon} + U_0 \psi_s(0) + U_1 \psi_e(0) = 0 \quad (8.59a)$$

$$\frac{d\psi_e}{dx} \Bigg|_{-\varepsilon}^{+\varepsilon} + U_0 \psi_e(0) + U_1 \psi_s(0) = 0. \quad (8.59b)$$

These equations (8.59) are sufficient to determine the exact solutions, once we have specified the desired boundary conditions. Consider a scattering problem in which the scatterer is initially in its ground state. Since the interaction conserves parity and the odd-parity solution is always unaffected by a delta function potential at the origin, we consider the even-parity solution. This has the usual form with a phase shift for the function  $\psi_g(x)$ . For  $\psi(x)$  however, we wish a solution which has only outgoing waves and no incoming waves. Thus we set

$$\psi_g(x) = \alpha \cos(k|x| + \delta_0) \quad (8.60a)$$

$$\psi_e(x) = \beta e^{ik_e|x|} \quad (8.60b)$$

where  $\alpha$  and  $\beta$  are coefficients to be determined and

$$k^2 = \frac{2m(E - E_g)}{\hbar} \quad (8.60c)$$

$$k_e^2 = \frac{2m(E - E_e)}{\hbar} = k^2 - \frac{2m}{\hbar} [E_e - E_g]. \quad (8.60d)$$

Substituting eqs. (8.60) into eqs. (8.59) we obtain

$$-2k\alpha \sin \delta_0 + U_0 \alpha \cos \delta_0 + U_1 \beta = 0 \quad (8.61a)$$

$$2ik_e \beta + U_0 \beta + U_1 \alpha \cos \delta_0 = 0. \quad (8.61b)$$

Solving these equations for  $\beta/\alpha$  we obtain

$$\frac{\beta}{\alpha} = -\frac{U_1 \cos \delta_0}{U_0 + 2ik_e} = \frac{2k \sin \delta_0 - U_0 \cos \delta_0}{U_1}. \quad (8.62a)$$

Solving eq. (8.62a) for the phase shift  $\delta_0$  we obtain

$$\begin{aligned} \tan \delta_0 &= \frac{U_0}{2k} - \frac{U_1^2}{2k(U_0 + 2ik_e)} \\ &= \frac{U_0}{2k} \left[ 1 - \frac{U_1^2}{U_0^2 + 4k_e^2} \right] + \frac{ik_e U_1^2}{k[U_0^2 + 4k_e^2]}. \end{aligned} \quad (8.62b)$$

Eq. (8.62b) shows that the phase shift can be complex. The meaning of a complex phase shift is easily seen from the expressions (8.11) for the amplitudes of the reflected wave  $R$  and the transmitted wave  $S$  as functions of the phase shift. For complex phase shifts the total intensity of the reflected and transmitted waves is given by

$$|R|^2 + |S|^2 = \frac{1}{2} [e^{2i(\delta_0 - \delta_0^*)} + e^{2i(\delta_1 - \delta_1^*)}] = \frac{1}{2} [e^{-4 \operatorname{Im} \delta_0} + e^{-4 \operatorname{Im} \delta_1}] \leq 1. \quad (8.63)$$

Thus, if the phase shifts have an imaginary part the total intensity of the outgoing waves is less than the intensity of the incoming waves. This is perfectly reasonable for the case where there can be inelastic scattering. The elastic scattered wave does not necessarily have the full intensity of the incoming wave.

The expression (8.62b) has exactly the right properties to describe the inelastic scattering. If the energy of the incident beam is too low to excite the excited state, then  $k_e$  as given by eq. (8.60d) is imaginary, the phase shift as given by eq. (8.62b) is purely real, and there is no loss of intensity in the scattered beam. Once the energy is high enough to excite the scatterer,  $k_1$  is real. It is defined in eq. (8.60b) to be positive in order to describe outgoing waves. Thus the imaginary part of the phase shift given by eqs. (8.62b) is positive so that the elastic scattered intensity as given by eq. (8.63) is less than one.

Let us now examine the poles in the scattering amplitude. These occur when

$$\tan \delta_0 = \frac{U_0}{2k} - \frac{U_1^2}{2k(U_0 + 2ik_e)} = -i. \quad (8.64)$$

This can be reduced to the form

$$(U_0 + 2ik)(U_0 + 2ik_e) = U_1^2. \quad (8.65)$$

In the limit  $U_1 = 0$  where there is no inelastic scattering, there are two solutions to eq. (8.65) both giving pure imaginary values of  $k$  and  $k_e$ . Let us write

$$ik = -\lambda \quad (8.66a)$$

$$ik_e = -\lambda_e. \quad (8.66b)$$

The values of  $\lambda$  and  $X_e$  for the case  $U_x = 0$  are just the poles expected for a delta function potential. They correspond to the bound states of the particle, together with either the ground state or the excited state of the scatterer.

For the case where  $U_i$  is finite but small, it is convenient to rewrite eq. (8.65) in the form

$$\lambda = \frac{U_0}{2} - \frac{U_1^2}{2(U_0 - 2\lambda_e)} \quad (8.67a)$$

$$\lambda_e = \frac{U_0}{2} - \frac{U_1^2}{2(U_0 - 2\lambda)} = \frac{U_0}{2} - \frac{U_1^2 U_0}{2[U_0^2 - 4\lambda^2]} - \frac{U_1^2 \lambda}{[U_0^2 - 4\lambda^2]} \quad (8.67b)$$

where  $\lambda$  and  $k_1$  are related by

$$\lambda^2 = \lambda_e^2 - \frac{2m}{\hbar^2} (E_e - E_s). \quad (8.67c)$$

We now note the following interesting feature. If the binding energy  $+U_0$  is larger than the excitation energy  $E_e - E_g$  of the scatterer, then the two bound states are stable. However, if the binding energy is less than the excitation energy of the excited state, the bound state of the particle with the excited state of the scatterer can decay to the ground state of the scatterer and a free particle. This is clearly seen from eqs. (8.76b) and (8.67c). If  $A_e$  is chosen to correspond to the bound state of the particle with the scatterer in the excited state, then eq. (8.67c) shows that  $\lambda$  is real if the binding energy is greater than the excitation energy but will be imaginary if the binding energy is less than the excitation energy. If  $\lambda$  is real, then  $A_e$  is given by eq. (8.67b) also to be real, and corresponds to a bound state. If however,  $\lambda$  is imaginary, then  $A_e$  given by eq. (8.67b) has an imaginary part and corresponds to a decaying state or a resonance. For this case we should substitute eq. (8.66) back in (8.67b) to obtain

$$\lambda_e = \frac{U_0}{2} - \frac{U_1^2 U_0}{2[U_0^2 + 4k^2]} + i \frac{U_1^2 k}{U_0^2 + 4k^2}. \quad (8.68a)$$

The resonance energy is then given by

$$\begin{aligned} E_r &= \frac{\hbar^2}{2m} \lambda_e^2 \\ &= \frac{\hbar^2}{2m} \left[ \left( \frac{U_0}{2} - \frac{U_1^2 U_0}{2[U_0^2 + 4k^2]} \right)^2 - \frac{U_1^4 k^2}{(U_0^2 + 4k^2)^2} \right] + \frac{1}{2} i \Gamma \end{aligned} \quad (8.68b)$$

where

$$\Gamma = \frac{\hbar^2 k U_0 U_1^2}{2m[U_0^2 + 4k^2]} \left[ 1 - \frac{U_1^2}{U_0^2 + 4k^2} \right]. \quad (8.68c)$$

The decay of the resonant state can also be treated by time-dependent perturbation theory.

We describe the system with unperturbed wave functions for which  $U_1 = 0$ , but  $U_0$  is included in the unperturbed Hamiltonian to give the bound states. In the absence of the perturbation  $U_1$  both bound states are stable. In first-order time-dependent perturbation theory the decay rate of the excited bound state is given by the golden rule formula and the width is therefore

$$\Gamma = \hbar W_{i \rightarrow f} = 2\pi |\langle f | V | i \rangle|^2 \varrho(E_f). \quad (8.69)$$

The interaction matrix element is

$$\langle f | V | i \rangle = \frac{\hbar^2}{2m} U_1 \lambda_e^{\frac{1}{2}} \cos \delta_0 \quad (8.70a)$$

where the last two factors come from the normalization of the bound-state wave function and the value of the continuum wave function at the origin. The density of final states in one dimension is given by

$$\varrho(E_f) = \frac{1}{\hbar} \frac{dp}{dE} = \frac{m}{2\pi\hbar^2 k}. \quad (8.70b)$$

Substituting eqs. (8.70) into (8.69), and inserting the unperturbed values for  $\lambda$ , and  $\cos \delta_0$  gives exactly the first term of eq. (8.68c). This is to be expected since the second term is of higher order in the perturbation  $V_x$  and the perturbation theory result is good only to first order.

## 8.10 Kaon decay and scattering problems

Another instructive example is pion-pion scattering in one dimension resulting from the interaction between kaons and pions responsible for the kaon decay. The interaction can change an initial two-pion state into a one-kaon state and then into another two-pion state. Consider the Hamiltonian used in the treatment of kaon decay in ch. 7,

$$H = H_K + H_\pi + V \quad (8.71a)$$

where

$$H_K = \int E_{Kq} a_{Kq}^\dagger a_{Kq} dq \quad (8.71b)$$

$$H_\pi = \int E_{\pi q} a_{\pi q}^\dagger a_{\pi q} dq \quad (8.71c)$$

and we consider the momentum variable  $q$  in a one-dimensional space. For the interaction  $V$  we use the local interaction (7.13a)

$$V = g \int dx a_n^\dagger(x) a_n^\dagger(x) a_K(x) + h.c. \quad (8.72)$$

Our treatment of pion-pion scattering is not relevant to the scattering of physical pions, whose additional strong interactions completely overwhelm the weak interaction (7.13a). Furthermore, we shall be making non-relativistic approximations which are not valid for pions in this energy region. The treatment would apply to the case where the scattering of two

nonrelativistic particles is dominated by a metastable state which decays into these two particles, i.e. a resonance.

We wish to describe pion-pion scattering in the center-of-mass system; i.e. in a state of total momentum zero. The only kaon state which is coupled to this system is the zero-momentum kaon state because of momentum conservation. To handle the local interaction most conveniently the pion creation operators are expressed in configuration space as a function of two coordinates  $y$  and  $z$ . We therefore look for a solution of the Schrödinger equation having the form

$$|\psi\rangle = |\int \alpha(y-z) a_s^\dagger(y) a_s^\dagger(z) dy dz + \beta a_{K_0}^\dagger|0\rangle \quad (8.73)$$

where the coefficients  $\alpha(y-z)$  and  $\beta$  are to be determined by substituting in the Schrödinger equation. For a zero-momentum state  $\alpha$  depends only on the relative coordinate  $(y-z)$  of two pions.

We now express the Hamiltonian (8.71) in terms of the variables appearing in the wave function (8.73), namely, the pion coordinates and the kaon momentum. The interaction  $V$  is expressed as function of coordinates. We therefore Fourier-transform the kaon operator to momentum space. We also write the pion operators at points  $y$  and  $z$ , as in the wave function in (8.73) and introduce a factor  $\delta(y-z)$

$$V = (2\pi)^{-\frac{1}{2}} g \int dy \int dz \int dq a_s^\dagger(y) a_s^\dagger(z) a_{K_0} e^{\pm iq(y+z)} \delta(y-z) + \text{h.c.} \quad (8.74)$$

The kaon Hamiltonian (8.71b) is already in the desired form, but the pion Hamiltonian (8.71c) must be expressed in terms of configuration space variables. To simplify this calculation we assume the non-relativistic relation

$$E_{sq} = mc^2 + \frac{\hbar^2 q^2}{2m}. \quad (8.75)$$

This approximation allows the use of the non-relativistic Schrödinger equation in configuration space. The treatment is easily generalized to the case where the pions are described by the Klein-Gordon equation. The pion Hamiltonian (8.71c) can now be written in configuration space

$$H_s = \frac{1}{2\pi} \int dx \int dx' \int dq \left[ mc^2 + \frac{\hbar^2 q^2}{2m} \right] e^{-iqx} a_s^\dagger(x) e^{iqx'} a_s(x'). \quad (8.76a)$$

This can be rewritten

$$H_s = \frac{1}{2\pi} \int dx a_s^\dagger(x) \int dx' \int dq \left[ mc^2 - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] e^{iq(x'-x)} a_s(x'). \quad (8.76b)$$

Performing the integrations over  $q$  and  $x'$ , we obtain

$$H_s = \int dx a_s^\dagger(x) \int dx' \left[ mc^2 - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] \delta(x' - x) a_s(x') \quad (8.77a)$$

$$H_s = \int dx a_s^\dagger(x) \left[ mc^2 - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] a_s(x). \quad (8.77b)$$

We now substitute the wave function (8.73) into the Schrödinger equation. We first calculate  $H_x |\psi\rangle$  using eqs. (8.77b) and (8.73).

$$\begin{aligned} H_s |\psi\rangle &= \int dx a_s^\dagger(x) \left[ mc^2 - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] \\ &\times a_s(x) \int dy \int dz \alpha(y-z) a_s^\dagger(y) a_s^\dagger(z) |0\rangle. \end{aligned} \quad (8.78a)$$

Moving the annihilation operator to the right and using boson commutation relations we obtain

$$\begin{aligned} H_s |\psi\rangle &= \int dx a_s^\dagger(x) \left[ mc^2 - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] \\ &\times \int dy \int dz \alpha(y-z) [\delta(x-y) a_s^\dagger(z) + \delta(x-z) a_s^\dagger(y)] |0\rangle. \end{aligned} \quad (8.78b)$$

The dummy integration variables  $y$  and  $z$  can be interchanged in the last term on the right-hand side of eq. (8.78b) and the two terms combined

$$\begin{aligned} H_s |\psi\rangle &= \int dx a_s^\dagger(x) \left[ mc^2 - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] \\ &\times \int dy \int dz [\alpha(y-z) + \alpha(z-y)] \delta(x-y) a_s^\dagger(z) |0\rangle. \end{aligned} \quad (8.78c)$$

Eq. (8.78c) illustrates the symmetry requirements of the pion Bose statistics. If  $\alpha(y-z)$  is an odd function the two-pion component in the wave function (8.73) vanishes. Only the even part of  $\alpha(y-z)$  has any physical significance. We therefore assume that  $\alpha(y-z)$  is an even function. The integration of eq. (8.78c) over the variable  $y$  is trivial because of the  $\delta(x-y)$ .

$$H_s |\psi\rangle = \int dx a_s^\dagger(x) \left[ 2mc^2 - \frac{\hbar^2}{m} \frac{d^2}{dx^2} \right] \int dz \alpha(x-z) a_s^\dagger(z) |0\rangle. \quad (8.79)$$

To evaluate  $\nu |\psi\rangle$  we note that

$$\begin{aligned} V a_{K_0}^\dagger |0\rangle &= (2\pi)^{-\frac{1}{2}} g \int dy \int dz \int dq a_s^\dagger(y) a_s^\dagger(z) e^{\pm iq(y+z)} \delta(q) \delta(y-z) |0\rangle \\ &= (2\pi)^{-\frac{1}{2}} g \int dy \int dz a_s^\dagger(y) a_s^\dagger(z) \delta(y-z) |0\rangle \end{aligned} \quad (8.80a)$$

$$\begin{aligned} V \int dy \int dz \alpha(y-z) a_s^\dagger(y) a_s^\dagger(z) |0\rangle &= \\ &= 2(2\pi)^{-\frac{1}{2}} g^* \int dy \int dz \int dy' \int dz' \int dq \delta(y-y') \delta(z-z') \alpha(y-z) \delta(y'-z') \\ &\times e^{-\pm iq(y+z)} a_{K_0}^\dagger |0\rangle \\ &= 2(2\pi)^{-\frac{1}{2}} g^* \int dz \int dq \alpha(0) e^{-iqz} a_{K_0}^\dagger |0\rangle = 2(2\pi)^{\frac{1}{2}} \alpha(0) g^* a_{K_0}^\dagger |0\rangle. \end{aligned} \quad (8.80b)$$

Thus

$$V|\psi\rangle = (2\pi)^{-\frac{1}{2}}\beta g \int dy \int dz a_{\pi}^{\dagger}(y)a_{\pi}^{\dagger}(z)\delta(y-z)|0\rangle + 2\alpha(0)g^*(2\pi)^{\frac{1}{2}}a_{K_0}^{\dagger}|0\rangle. \quad (8.81)$$

We also have

$$H_K|\psi\rangle = \beta m_K c^2 a_{K_0}^{\dagger}|0\rangle. \quad (8.82)$$

Using eqs. (8.79), (8.81) and (8.82), we can now write the Schrödinger equation for the solution (8.73).

$$(H - E)|\psi\rangle = 0 = \int dy \int dz [a_{\pi}^{\dagger}(y)a_{\pi}^{\dagger}(z)]|0\rangle \times \left[ 2mc^2 - \frac{\hbar^2}{m} \frac{d^2}{dy^2} - E \right] \alpha(y-z) + (2\pi)^{-\frac{1}{2}}\beta g \delta(y-z) + a_{K_0}^{\dagger}|0\rangle \{(m_K c^2 - E)\beta + 2\alpha(0)g^*(2\pi)^{\frac{1}{2}}\}. \quad (8.83)$$

Equating separately the coefficients of the kaon and pion states we obtain the equations for the coefficients  $\beta$  and  $\alpha(y-z)$

$$(m_K c^2 - E)\beta + 2\alpha(0)g^*(2\pi)^{\frac{1}{2}} = 0 \quad (8.84a)$$

$$\left[ 2mc^2 - \frac{\hbar^2}{m} \frac{d^2}{dy^2} - E \right] \alpha(y-z) + (2\pi)^{-\frac{1}{2}}\beta g \delta(y-z) = 0. \quad (8.84b)$$

Eliminating  $\beta$  between these two equations we obtain

$$\left[ 2mc^2 - \frac{\hbar^2}{m} \frac{d^2}{dx^2} - E \right] \alpha(x) = \frac{2|g|^2}{(m_K c^2 - E)} \delta(x)\alpha(0) \quad (8.85a)$$

where

$$x = y - z \quad (8.85b)$$

is the relative coordinate.

Eq. (8.85a) is just a Schrödinger equation for a particle of mass  $m$  (the reduced mass) in a delta function potential.

$$\left[ \frac{d^2}{dx^2} + k^2 \right] \alpha = -U_0 \delta(x) \quad (8.86a)$$

where

$$E_r = \frac{\hbar^2}{2m} \lambda_e^2 = \frac{\hbar^2}{2m} \left[ \left( \frac{U_0}{2} - \frac{U_1^2 U_0}{2[U_0^2 + 4k^2]} \right)^2 - \frac{U_1^4 k^2}{(U_0^2 + 4k^2)^2} \right] + \frac{1}{2}i\Gamma \quad (8.86b)$$

and

$$U_0 = \frac{2m|g|^2}{\hbar^2[m_K c^2 - E]}. \quad (8.86c)$$

We have thus derived a one-body Schrödinger equation starting from the second-quantized Hamiltonian (8.71a). This is just the reverse of second quantization which begins with a one-body Schrödinger equation and develops a formalism capable of dealing with many particles and creation and annihilation. One might say that we have ‘un-second-quantized’ the Hamiltonian (8.71a) to get the one-body eq. (8.86). From the solution of eq. (8.86) in section 8.6, we can write

$$\alpha(x) = \cos(k|x| + \delta_0) \quad (8.87a)$$

where the phase shift  $\delta_0$  is given by eq. (8.34a)

$$\tan \delta_0 = \frac{U_0}{2k} = \frac{m|g|^2}{\hbar^2 k[m_K c^2 - E]}. \quad (8.87b)$$

The scattering amplitude is given by eq. (8.36a)

$$f(\theta) = \frac{1}{k[2k/U_0 - i]} = \frac{m|g|^2}{k[\hbar^2 k[m_K c^2 - E] - im|g|^2]}. \quad (8.88a)$$

This can be written as a Lorentzian resonance curve

$$f(\theta) = \frac{1}{k} \frac{\frac{1}{2}\Gamma}{(m_K c^2 - E) - \frac{1}{2}i\Gamma} \quad (8.88b)$$

where the width  $\Gamma$  is

$$\Gamma = \frac{2m|g|^2}{\hbar^2 k}. \quad (8.88c)$$

This is just the value for the width obtained from the golden rule formula for the transition probability per unit time:

$$\frac{\Gamma}{\hbar} = \frac{2\pi}{\hbar} |g|^2 \varrho(E) \quad (8.89a)$$

where the density of states in one dimension in a box of unit volume is

$$\varrho(E) = \frac{1}{h} \frac{dp}{dE} = \frac{2m}{hp} = \frac{2m}{2\pi\hbar^2 k}. \quad (8.89b)$$

Thus the pion-pion scattering amplitude is given by a resonance curve whose width is just that calculated for the decaying state by time-dependent perturbation theory. Note, however, that the result (8.88c) is *exact*, as we have made no approximation in the solution of the Schrödinger equation for the given Hamiltonian.

## 8.11 Perturbation theory and the T-matrix

In one-dimensional scattering problems partial-wave analysis (8.18) expresses the exact so-

lution in terms of two phase shifts. In three dimensions there are an infinite number of phase shifts and the method is practical only if a general closed form is found for all phase shifts or if it is possible to neglect the contributions from all partial waves above some value of  $l$ .

Another approach uses perturbation theory to solve the Schrödinger equation by a series of successive approximations. However, a straightforward application of the perturbation methods commonly used to treat bound-state problems leads to difficulties. Consider for example, the matrix elements of the potential  $V$  in a scattering problem between the exact solution (8.13) of the scattering problem and an unperturbed plane-wave state. Such matrix elements arise in perturbation theory and it is important to be able to evaluate them properly. From the Schrödinger equation,

$$\langle e^{\pm ikx} | V | \psi^{(+)}(x) \rangle = \langle e^{\pm ikx} | H - H_0 | \psi^{(+)}(x) \rangle \quad (8.90a)$$

Since  $\psi^{(+)}(x)$  is an eigenfunction of  $H$  with the eigenvalue  $E = (hk)^2/2m$

$$H|\psi^{(+)}(x)\rangle = E|\psi^{(+)}(x)\rangle = \frac{\hbar^2 k^2}{2m} |\psi^{(+)}(x)\rangle. \quad (8.90b)$$

Since  $e^{\pm ikx}$  is an eigenfunction of the Hermitean operator  $H_0$  with the same eigenvalue  $E$

$$\langle e^{\pm ikx} | H_0 = E \langle e^{\pm ikx} | = \frac{\hbar^2 k^2}{2m} \langle e^{\pm ikx} |. \quad (8.90c)$$

Thus:

$$\langle e^{\pm ikx} | V | \psi^{(+)}(x) \rangle = \langle e^{\pm ikx} | \psi^{(+)}(x) \rangle (E - E) = 0. \quad (8.91)$$

This result is clearly incorrect. What is wrong? Try and figure this out before reading further!

Another example of this trouble appears in the following equation obtained by algebraic manipulation of the Schrödinger equation.

$$\Psi = \frac{1}{E - H_0} V \Psi. \quad (8.92)$$

This expression might be used for perturbation theory. With a zero-order wave function on the right-hand side, the first approximation is calculated from eq. (8.92) and higher approximations are obtained by iteration. However, there are eigenfunctions of  $H_0$  with the eigenvalue  $E$  and the operator  $1/(E - H_0)$  blows up for these states.

These difficulties arise from the use of wave functions which are plane waves extending over all space. These wave functions are not square integrable and their normalization integrals are infinite. One way to avoid these difficulties is by normalizing wave functions in a box of finite volume. This procedure gives a discrete energy level spectrum with the allowed values of  $k$  determined by the boundary conditions on the eigenfunctions (8.9) at the boundary of the box. Since these allowed values of  $k$  depend upon the phase shift, the eigenvalues  $E$  of the exact

Hamiltonian  $H$  are different from those of the unperturbed Hamiltonian  $H_Q$ . The expression (8.90) can be evaluated without inconsistencies and there are no vanishing denominators in eq. (8.92). However, the boundary conditions choose different values of  $k$  for the even and odd-parity states and remove the two-fold degeneracy of the eigenfunctions. The parity eigenfunctions provide a unique basis and there are no eigenfunctions describing a single incident wave and scattered waves. This is expected since the boundary conditions transform outgoing scattered waves into incoming waves which are re-scattered. Functions normalized in a box are thus not convenient for scattering calculations.

The use of a time-dependent description with wave packets confined to a finite region of space leads to a consistent formalism and corresponds more closely to physical scattering experiments performed in the laboratory. However, it is simpler to use the time-independent plane-wave states and the stationary eigenfunctions (8.13), with the normalization properly formulated.

We can avoid the above difficulties by replacing the usual orthonormality conditions for a discrete spectrum by the relation

$$\int_{-\infty}^{\infty} e^{-ik'x} e^{ik''x} dx = 2\pi\delta(k' - k''). \quad (8.93)$$

The Dirac delta function is a peculiar object which is zero everywhere except at the point  $k' = k''$  where it is infinite. However this singular function is useful in calculations. It never appears in a result for a physically measurable quantity but only in integrands at intermediate stages. The singularity always disappears in an integration necessary to obtain the physical results. For example in using results calculated with plane waves to obtain physical results described by wave packets, the construction of a wave packet from plane-wave states involves just such an integral over the variables appearing in the argument of the delta function.

There are two kinds of contributions to matrix elements calculated with these plane-wave states: (1) Singular expressions like (8.93) where the infinite volume of space contributes to the integral and the result contains a delta function, (2) Non-singular integrals which are finite and vary smoothly with  $k$ .

These have contributions only from a finite volume, like the left-hand side of eq. (8.90a) or contributions from large distances which decrease sufficiently rapidly to make the integral converge. Both the singular and non-singular contributions give reasonable answers when integrated over the variable  $k$ .

We now resolve the paradox of eq. (8.91) and evaluate properly the integral defined by the right-hand side of eq. (8.90a). Using eq. (8.90b) but not eq. (8.90c), and substituting eq. (8.1)

we obtain

$$\begin{aligned}\langle e^{\pm ikx} | V | \psi^{(+)}(x) \rangle &= \int_{-x}^{+x} e^{\mp ikx} (H - H_0) \psi^{(+)}(x) dx \\ &= \frac{\hbar^2}{2m} \int_{-x}^{+x} e^{\mp ikx} \left( k^2 + \frac{d^2}{dx^2} \right) \psi^{(+)}(x) dx.\end{aligned}\quad (8.94a)$$

We must now be careful about allowing differential operators to operate to the left, as in eq.

(8.90c) for these non-normalizable states. The standard method for making the differential operator in the expression (8.94a) operate to the left is integration by parts. Two integrations shift the differential operator to operate on the plane wave  $e^{\pm ikx}$  and gives a contribution which exactly cancels the  $k^2$ -term to give zero in agreement with the naive result (8.91).

However in each partial integration there is also the integrated part. This vanishes if the wave functions go to zero sufficiently rapidly at large distances, but plane-wave functions manifestly do not vanish at large distances. Therefore the integrated part is finite and in this case gives the entire result

$$\langle e^{\pm ikx} | V | \psi^{(+)}(x) \rangle = \frac{\hbar^2}{2m} e^{\mp ikx} \left( \frac{d\psi^{(+)}}{dx} \pm ik\psi^{(+)}(x) \right) \Big|_{-x}^x. \quad (8.94b)$$

Substituting eq. (8.13a) for  $\varphi^{(+)}(x)$  shows that the unperturbed plane wave gives an equal contribution at both limits and does not contribute to the expression (8.94b). The only contribution comes from the particular scattered wave which is in the same direction as the plane wave on the left-hand side of the matrix element. Using the form (8.19c) for the wave function, we obtain

$$\langle e^{ikx \cos \alpha} | V | \psi_{\beta}^{(+)}(x) \rangle = \frac{i\hbar^2}{m} g(\alpha - \beta) \quad (8.95)$$

where  $\alpha=0$  or  $\pi$  and  $\beta=0$  or  $\pi$ .

The matrix elements of  $V$  between all possible scattering states (8.19) and all possible plane-wave states are now defined. However this is not the usual expression for the matrix element of an operator since it is defined between states expressed in different bases.

The result (8.95) can be expressed in the single basis of the unperturbed plane-wave states by defining a new operator. The  $\Gamma$ -matrix is defined for this purpose by the relation

$$V\psi_{\alpha}^{(+)} = T\phi_{\alpha} \quad (8.96a)$$

where  $\phi_{\alpha}$  is the unperturbed plane-wave state corresponding to the exact solution  $\delta_{\alpha}^{(+)}$

$$\phi_{\alpha} = e^{ikx \cos \alpha}. \quad (8.96b)$$

The matrix elements of  $\Gamma$  are directly obtained from eq. (8.95)

$$\langle \phi_{\beta} | T | \phi_{\alpha} \rangle = \frac{ik\hbar^2}{m} g(\alpha - \beta). \quad (8.97)$$

The  $\Gamma$ -matrix gives a complete description of the scattering since all the information about the scattering process is contained in the elements of the  $\Gamma$ -matrix. The  $S$  and  $\Gamma$ -matrices can be related by comparing eqs. (8.97) and (8.20):

$$S_{\alpha\beta} = \delta_{\alpha\beta} + \frac{m}{ik\hbar^2} T_{\alpha\beta}. \quad (8.98)$$

The  $\Gamma$ -matrix, as defined by eq. (8.98) has elements formally defined also between states having different energies, while the  $S$ -matrix as defined by eq. (8.20) connects only states of the same energy. Eqs. (8.97) and (8.98) apply only to matrix elements between states of the same energy. The  $\Gamma$ -matrix vanishes if there is no potential; i.e. no scattering, whereas the  $S$ -matrix becomes the unit matrix in that case. In the three-dimensional case the numerical factor (8.98) in the relation between  $S$  and  $\Gamma$ -matrices is different owing to the different dimensions of the various quantities.

An other expression for the  $S$ -matrix is obtained by evaluating matrix elements between the states (8.20b) with scattered outgoing waves and (8.22a) with scattered incoming waves. These have a singular part which comes from the region outside the potential.

$$\begin{aligned}\langle \psi_{\gamma}^{(-)} | \psi_{\alpha}^{(+)} \rangle &= \sum_{\theta=0,\pi} \int_0^{\infty} dr \left[ \sum_{\beta=1,2} \phi_{\beta}^{*}(\pi - \theta) S_{\beta} \phi_{\beta}(\theta) e^{ikr} + \phi_{\gamma}^{*}(\theta) e^{-ikr} \right] \\ &\times [\phi_{\alpha}(\pi - \theta) e^{-ikr} + \sum_{\beta=1,2} S_{\alpha\beta} \phi_{\beta}(\theta) e^{ikr}] = S_{\alpha\gamma} \times 2 \int_0^{\infty} dr.\end{aligned}\quad (8.99)$$

The divergent integral can be expressed as a delta function by using states and with slightly different values of  $k$  and applying eq. (8.93).

Thus the  $S$ -matrix element for the transition  $a-y$  is given by the matrix element between the solution with outgoing scattered waves and the one with incoming scattered waves with unperturbed states  $\alpha$  and  $\gamma$  respectively.

## 8.12 Green's functions and the Born series

We now return to the formulation of perturbation theory for the scattering problem and the impossibility of using eq. (8.92) as it stands. Perturbation theory gives an approximation to the exact solution of the Schrödinger equation starting from a plane wave as the unperturbed solution. However, we do not want *any* exact solution of the Schrödinger equation. We want a solution having the form (8.20b) with outgoing waves added to the unperturbed wave. We do not want solutions like (8.22a) containing *incoming* waves added to the unperturbed wave. In the absence of the potential when  $g(\theta)=0$  and  $S_{\alpha\beta}=\delta_{\alpha\beta}$  eqs. (8.20b) and (8.22a) become

identical. The same is true for any linear combination of (8.20b) and (8.22a). Thus a given unperturbed solution of the free-particle Schrödinger equation can correspond to several different solutions of the Schrödinger equation when the interaction is present, not only the desired one in which the interaction produces additional outgoing waves but also others in which it produces incoming waves. A one-to-one correspondence does not exist.

Perturbation theory is thus ambiguous if it simply attempts to find a solution of the perturbed Schrödinger equation which corresponds to a particular solution of the unperturbed Schrödinger equation. This ambiguity is reflected in the presence of the denominator in eq. (8.92) which can vanish and therefore does not define a perturbation expansion. To obtain a useful perturbation formulation we must re-define our problem as finding a solution of the perturbed Schrödinger equation which not only corresponds to a particular unperturbed state but is also restricted to having only additional outgoing waves. This problem does not arise for the case where the wave functions are normalized in a box. There a one-to-one correspondence does exist between perturbed and unperturbed, solutions and eq. (8.92) has no vanishing denominators.

The desired perturbation formulation can be developed with the aid of the solution for the delta function potential already considered. Substituting the potential (8.32) and the solution (8.36) into the Schrödinger equation (8.30) we obtain

$$\frac{\hbar^2}{2m} \left[ \frac{d^2}{dx^2} + k^2 + U_0 \delta(x) \right] \left[ e^{ikx} + \frac{iU_0}{2k - iU_0} e^{ikr} \right] = 0. \quad (8.100a)$$

This can be rewritten

$$\frac{\hbar^2}{2m} \left[ \frac{d^2}{dx^2} + k^2 \right] e^{ikr} = \frac{i\hbar^2 k}{m} \delta(x). \quad (8.100b)$$

This expression can be used for a delta function potential at any point  $x'$ , not necessarily at the origin, by substituting  $x-x'$  for  $x$  in equation (8.100b)

$$\frac{\hbar^2}{2m} \left[ \frac{d^2}{dx^2} + k^2 \right] e^{ik|x-x'|} = \frac{i\hbar^2 k}{m} \delta(x-x'). \quad (8.100c)$$

It is now convenient to define the Green's functions

$$G^\pm(x, x') = \frac{m}{i\hbar^2 k} e^{\pm ik|x-x'|}. \quad (8.101a)$$

From eq. (8.100c) the functions  $G^\pm(x, x')$  are seen to satisfy the equation

$$\frac{\hbar^2}{2m} \left[ \frac{d^2}{dx^2} + k^2 \right] G^\pm(x, x') = \delta(x - x'). \quad (8.101b)$$

With an intuitive picture of a potential  $V(x)$  built up of a continuum of delta function poten-

tials at each point  $x'$  with strength  $V(x')$  we can write the Schrödinger equation in the form:

$$\frac{\hbar^2}{2m} \left[ \frac{d^2}{dx^2} + k^2 \right] \psi(x) = V(x)\psi(x) = \int_{-\infty}^{+\infty} V(x') \delta(x - x') \psi(x') dx'. \quad (8.102a)$$

We can now write formal solutions of the Schrödinger equation by using the Green's functions (8.101b) which are solutions for the delta function potential. The function

$$\psi_\alpha^{(\pm)}(x) = \phi_\alpha + \int_{-\infty}^{+\infty} G^\pm(x, x') V(x') \psi_\alpha^{(\pm)}(x') dx' \quad (8.102b)$$

satisfies the Schrödinger equation (8.30b) if  $\phi_\alpha$  is any solution of the free-particle Schrödinger equation. This is sometimes described by considering eq. (8.30b) as an inhomogeneous equation. Adding any solution of the homogeneous equation to a given solution of the inhomogeneous equation gives another solution.

However, eq. (8.30b) is not really inhomogenous as the 'inhomogeneous term' contains a factor  $\psi$ . Thus eq. (8.102b) is not really a *solution* of the equation, as  $\psi$  appears on the right-hand side as well as on the left. For a delta function potential, eq. (8.102b) gives the solution, because  $\psi$  at one

point is a single number, determined later by normalization. For any other potential,  $\phi(x)$  appears as an unknown function whose value can only be found by solving the whole equation. Thus in deriving eq. (8.102b) we have converted the Schrödinger equation to an integral equation which still must be solved to get  $\psi(x)$ .

This integral equation (8.102b) differs from the Schrödinger equation in a very useful way. All solutions of the integral equation are also solutions of the Schrödinger equation. However, not all solutions of the Schrödinger equation are solutions of the integral equation. We have chosen eq. (8.102b) to give only those solutions which have the desired properties at large values of  $x$ . They consist of an unperturbed wave having the given form  $\phi_\alpha$  plus outgoing scattered waves and no incoming waves if  $G^+(x, x')$  is used and the reverse if  $G^-(x, x')$  is used. This has been achieved by choosing the first term on the right-hand side of eq. (8.102b) to be the desired unperturbed wave and by choosing the Green's function in the integral to be that solution of eq. (8.101b) which has only outgoing or only incoming waves. Other solutions of the Schrödinger equation could be obtained by replacing the first term in eq. (8.102b) by any solution of the free-particle Schrödinger equation and by replacing the Green's function  $G^\pm(x, x')$  by any solution of eq. (8.101b).

Eq. (8.102b) is a possible starting point for a perturbation treatment. We have removed the ambiguity implied by eq. (8.92) which cannot choose between the solutions (8.20b) and

(8.22a). Consider the expansion of the wave function (8.102) in a perturbation theory. We consider  $\psi^{(+)}(x)$ , choose the zero order term  $\varphi_\alpha$  to be unperturbed wave  $e^{ikx}$ , and define  $\varphi_\eta$  to be the  $\eta$ th-order term in the perturbation series

$$\psi^{(+)}(x) = e^{ikx} + \psi_1 + \psi_2 + \dots + \psi_n + \dots \quad (8.103)$$

The entire perturbation series can be obtained from eq. (8.102b) by iteration. The substitution of the zero-order term into the integral on the right-hand side of eq. (8.102b) gives on the left-hand side the sum of the zero-order term and a first-order term which is proportional to the potential. The substitution of this function into the integral on the right-hand side gives back the unperturbed solution plus the same first-order solution and a second-order term which is proportional to the square of the potential. Each iteration gives the next higher term in the perturbation expansion. The approximate solution in each order has the desired asymptotic properties, the unperturbed plane wave plus outgoing scattered waves. This iteration is called the Born series for the scattering amplitude. The first term which is the result of first-order perturbation theory is called the Born approximation. This result is

exactly the same as would be obtained by using the golden rule and first-order time-dependent perturbation theory.

The above one-dimensional discussion is presented as a simplification of the physical three-dimensional problems in order to give an intuitive picture with a minimum of complicated mathematics. In this connection it is worth mentioning some differences between the one and three-dimensional cases which follow from purely dimensional considerations. The analogs of the Green's function equations (8.100c) and (8.101) involve a delta function in three-dimensional space and outgoing or incoming waves in three dimensions which have the form  $e^{\pm ikr} j_r$ . The delta function in a one-dimensional space has dimensions  $1/r$  while the free-particle plane wave is dimensionless. In three dimensions, the delta function has dimensions  $1/r^3$  and the free-particle solution has dimension  $1/r$ . The factor  $k$  on the right-hand side of eq. (8.100c) is required by dimensional considerations for the one-dimensional case but not for the three-dimensional case. Thus the momentum dependence in the definition of the one-dimensional Green's function (8.101) disappears in the three-dimensional case.

We now return to the formal perturbation expression (8.92) and consider a simple modification which allows us to remove its difficulties and ambiguities and to obtain a formal expression equivalent to the integral equation (8.102).

We write the product  $V\psi$  in the form indicated by eq. (8.102a) and express the delta function as a Fourier transform

$$\begin{aligned} V(x)\psi(x) &= \int_{-\infty}^{\infty} dx' \delta(x - x')V(x')\psi(x') \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk' \int_{-\infty}^{\infty} dx' e^{ik'(x-x')}V(x')\psi(x'). \end{aligned} \quad (8.104)$$

We can write

$$\frac{1}{E - H_0} e^{ik'x} = \frac{2m}{\hbar^2(\kappa^2 - k'^2)} e^{ik'x} \quad (8.105a)$$

where

$$\kappa^2 = \frac{2m}{\hbar^2} E. \quad (8.105b)$$

Substituting eqs. (8.104) and (8.105) into the right-hand side of eq. (8.92) we obtain

$$\begin{aligned} \frac{1}{E - H_0} V(x)\psi(x) &= \frac{m}{\pi\hbar^2} \int_{-\infty}^{+\infty} dx' \int_{-\infty}^{+\infty} dk' \frac{e^{ik'(x-x')}}{(\kappa - k')(k + k')} V(x')\psi(x'). \end{aligned} \quad (8.106a)$$

The difficulty due to the singular denominator  $E - H_0$  is still present and appears in the denominators of the integrand on the right-hand side. However, if we add to  $E$  a small imaginary part, which we later allow to go to zero, we can evaluate the integral. The integrand remains finite along the path of integration as soon as the poles are moved off the real axis. Since the integrand is analytic in the complex  $k'$ -plane except for poles at  $k' = \pm \kappa$ , the integral over  $k'$  is conveniently evaluated by contour integration, closing the contour with the addition of a semicircle at infinity. The contribution of the semicircle to the integral vanishes if the semicircle is in the upper half plane for positive values of  $x - x'$  and in the lower half plane for negative values of  $x - x'$ . The contour integrals are then evaluated by taking the residues at the two poles  $k' = \kappa$  and  $k' = -\kappa$ . One of these is in the upper half plane and contributes to the integral for positive  $x - x'$ . The other is in the lower half plane and contributes to the integral for negative  $x - x'$ . Which of the two poles  $\pm \kappa$  is in the upper and which is in the lower half plane depends on the sign of the imaginary part of  $\kappa$  and not on its magnitude. We thus obtain two possible values for the integral

$$\frac{1}{E - H_0} V(x)\psi(x) = \frac{m}{i\hbar^2} \int_{-\infty}^{\infty} dx' \frac{e^{ix|x-x'|}}{\kappa} V(x')\psi(x') \quad \text{if } \text{Im } \kappa > 0 \quad (8.106b)$$

$$\frac{1}{E - H_0} V(x)\psi(x) = \frac{m}{i\hbar^2} \int_{-\infty}^{\infty} dx' \frac{e^{-ix|x-x'|}}{\kappa} V(x')\psi(x') \quad \text{if } \text{Im } \kappa < 0. \quad (8.106c)$$

The integrands on the right-hand sides of eq. (8.106b) and (8.106c) contain just the Green's functions  $G^\pm(x, x')$  defined by eq. (8.101a). Thus eq. (8.106) can be rewritten:

$$\lim_{\epsilon \rightarrow 0} \frac{1}{E - H_0 \pm i\epsilon} V(x)\psi(x) = \int_{-\infty}^{\infty} dx' G^\pm(x, x') V(x')\psi(x'). \quad (8.107)$$

Substituting this result into eq. (8.102b), we obtain

$$\psi_a^{(\pm)}(x) = \phi_a(x) + \lim_{\epsilon \rightarrow 0} \frac{1}{E - H_0 \pm i\epsilon} \psi_a^{(\pm)}(x). \quad (8.108)$$

This is the formal operator representation of the integral equation (8.102b).

We have 'fixed up' eq. (8.92) by adding a small imaginary part to  $E$ , which is allowed to approach zero, and adding a 'solution of the homogeneous equation'  $(E - H_0)\psi = 0$ . The sign of the imaginary part determines whether the solution with incoming or outgoing scattered waves is chosen.

Eq. (8.108) can be used to obtain an integral equation for the T-matrix. Multiplying the equation for  $\psi$  by  $V$  and using the definition (8.96a) of  $T$ , we obtain

$$V\psi_a^{(+)}(x) = T\phi_a(x) = V\phi_a(x) + V \frac{1}{E - H_0 + i\epsilon} T\phi_a(x) \quad (8.109)$$

where we have used the notation common in scattering theory, of implying the limit  $\epsilon \rightarrow 0$  without writing it explicitly.

The integral equation for the matrix elements of  $T$  is obtained by taking the scalar product of eq. (8.109) with any unperturbed state  $\varphi_\beta$ . We thus obtain the operator equation

$$T = V + V \frac{1}{E - H_0 + i\epsilon} T. \quad (8.110)$$

The  $\Gamma$ -matrix is defined by eq. (8.96a) to have matrix elements between states which do not have the same energy as well as states which have the same energy. Only the matrix elements between states which have the same energy are given by eq. (8.97) and related to physically

observable scattering amplitudes. However, the operator relation (8.110) must involve also matrix elements of  $T$  between states of different energies, since  $V$  has such matrix elements. We have seen that the evaluation of the integrand, eq. (8.106) involves other values of  $k'$ .

Eq. (8.110) also provides a basis for a perturbation calculation of the  $\Gamma$ -matrix. The unperturbed value of  $\Gamma$  is  $T=0$ . Substitution of this value on the right-hand side of eq. (8.110) gives the first-order result  $T=V$ , which is just the Born approximation. Continued iteration gives the higher-order results.

The relation between eqs. (8.108) and (8.102b) is characteristic of two approaches to quantum mechanics. The analytical approach, which began with Schrödinger, uses differential and integral equations and other analytical mathematical tools. The algebraic approach, which began with Heisenberg, uses matrices and vectors and operators in Hilbert space, and other algebraic mathematical tools. The physical results obtained by the two methods are always equivalent. Once a result is obtained with one approach, it is easy to translate the work into the other language, and obtain the same result. However, the best method to use in a given case depends upon the problem and on the taste of the individual who is trying to solve it. It is good for a student to be familiar with both approaches. Then, when he encounters a difficulty in one approach, he can translate the problem into the other and perhaps see it more clearly. In the present example, the difficulty was encountered in the algebraic statement, eq. (8.92), clarified by going to the analytical approach to obtain eq. (8.102b) and then 'translated' back into algebra to obtain the equivalent expression (8.107).

### 8.13 A particle in a one-dimensional periodic potential

The phase shifts used in scattering problems can also be used to treat the problem of a particle moving in a one-dimensional periodic potential. Let us modify the scattering problem (8.6) by adding an infinite number of potentials, identical to the potential  $V(x)$ , but centered at periodic intervals with period  $a \geq 2X$ . This new periodic potential is

$$V_p(x) = \sum_{n=-\infty}^{n=\infty} V(x - na) \quad (8.111a)$$

and the Hamiltonian is

$$H = \frac{p^2}{2m} + V_p(x). \quad (8.111b)$$

Such a Hamiltonian is often used to describe the motion of electrons in a crystal, where the ions produce a periodically varying electric field.

The Hamiltonian  $H$  is invariant under the translation  $x \rightarrow x+a$ . Thus if  $\psi(x)$  is an eigenfunc-

tion of if,  $\psi(x+\alpha)$  is also an eigenfunction with the same eigenvalue.

$$H\psi(x) = E\psi(x), \quad (8.112a)$$

$$H\psi(x + a) = E\psi(x + a). \quad (8.112b)$$

If the energy value  $E$  is non-degenerate, the two solutions (8.112a) and (8.112b) describe the same state and can differ only by a factor. This factor must be of modulus unity since  $\psi(x+\alpha)$  and  $\varphi(x)$  have the same normalization. Thus

$$\psi(x + a) = e^{i\phi}\psi(x). \quad (8.113)$$

A function satisfying this condition can be written in the following form

$$\psi_k(x) = e^{ikx}u_k(x) \quad (8.114a)$$

where

$$\phi = ka \quad (8.114b)$$

and  $u_k(x)$  is a periodic function with period  $a$ ,

$$u_k(x + a) = u_k(x). \quad (8.114c)$$

In this form (8.114) the wave function is seen to be the product of a free-particle wave function and a periodic function which expresses the effect of the potential. These wave functions are called Bloch waves and are used in the description of conduction electrons in a lattice.

If the potential is an even function of  $x$ , i.e. invariant under a reflection about the origin,

$$V(x) = V(-x). \quad (8.115)$$

The Hamiltonian (8.1 lib) and the parity  $P$  can therefore be simultaneously diagonalized. From our experience with the scattering problem, we expect a two-fold degeneracy of eigenfunctions,\* and that one can choose parity eigenfunctions which describe standing waves, or the Bloch wave functions (8.114a) which describe traveling waves.

We can now investigate the properties of these Bloch waves by using an approach similar to the one used in scattering problems, namely by using phase shifts to describe the effect of the potential on the wave functions. If we know a Bloch wave solution in the interval  $-\frac{1}{2}a \leq x \leq \frac{1}{2}a$  and we know the phase factor  $\phi$  or the Bloch wave number  $k$ , then we can determine the solution everywhere by using the periodicity condition (8.113) or the equivalent relation (8.114). We therefore only have to solve the Schrödinger equation in the region  $|x| \leq a$ . But for  $|x| \leq a$  the periodic potential is identical to that of the scattering problem, eq. (8.6), and the solutions of the scattering problem can be used for the periodic potential.

If we substitute a solution of the scattering problem for the region  $|x| \leq a$  into the periodicity condition (8.113) we obtain a solution of the Schrödinger differential equation for the periodic potential, but it will generally be discontinuous at the points  $x = (n + \frac{1}{2})a$ . To construct

an acceptable solution, we must find a solution of the Schrödinger equation in the region  $|x| \leq a$  which also satisfies the periodicity condition (8.113) as boundary conditions on the function and on its derivative at the points  $x = \pm \frac{1}{2}a$ . Such a function will be continuous and have a continuous derivative when it is extended outside the region  $|x| \leq a$  by use of the periodicity condition (8.113).

The periodic boundary condition is conveniently formulated by writing the Bloch wave solution as a linear combination of parity eigenfunctions.

$$\psi(x) = \psi_0(x) + \psi_1(x) \quad (8.116a)$$

where  $\psi_0(x)$  and  $\psi_1(x)$  are eigenfunctions of  $H$  with even and odd parity respectively and are not normalized. Then

$$\psi(-x) = \psi_0(x) - \psi_1(x). \quad (8.116b)$$

The derivative of this solution is

$$\psi'(x) = \psi'_0(x) + \psi'_1(x), \quad (8.117a)$$

$$\psi'(-x) = -\psi'_0(x) + \psi'_1(x). \quad (8.117b)$$

We now impose the periodicity condition (8.113) on  $\psi(x)$  and  $\psi'(x)$  at the points  $x = \pm ia$

$$\frac{\psi(+\frac{1}{2}a)}{\psi(-\frac{1}{2}a)} = \frac{\psi_0 + \psi_1}{\psi_0 - \psi_1} = e^{ika} \quad (8.118a)$$

$$\frac{\psi'(+\frac{1}{2}a)}{\psi'(-\frac{1}{2}a)} = \frac{\psi'_0 + \psi'_1}{-\psi'_0 + \psi'_1} = e^{ika}, \quad (8.118b)$$

where we have used the shortened notation  $\psi_0$ ,  $\psi_1$  and  $\psi_1'$  to denote the values of these functions at  $x = ia$ . Combining these equations gives the relations

$$\frac{\psi_0 + \psi_1}{\psi_0 - \psi_1} - \frac{\psi'_0 + \psi'_1}{-\psi'_0 + \psi'_1} = 0 = \psi_1\psi'_1 - \psi_0\psi'_0 \quad (8.119a)$$

$$\cos ka = \frac{e^{ika} + e^{-ika}}{2} = \frac{1}{2} \left[ \frac{\psi_0 + \psi_1}{\psi_0 - \psi_1} + \frac{\psi'_0 - \psi'_1}{\psi'_1 + \psi'_0} \right] = \frac{\psi_0\psi'_1 + \psi_1\psi'_0}{\psi_0\psi'_1 - \psi_1\psi'_0}, \quad (8.119b)$$

where we have used eq. (8.119a) to simplify eq. (8.119b).

Eqs. (8.119) express the boundary conditions on the solution of the Schrödinger equation in the region in terms of the even and odd-

parity eigenfunctions. These can be taken from the scattering solution, since they are the same as those for the periodic potential in this interval. Thus from eq. (8.9), which is valid for  $|x| \leq a$  and therefore for

$$\psi_0 = A \cos(\frac{1}{2}ka + \delta_0) \quad (8.120a)$$

$$\psi_1 = B \sin(\frac{1}{2}ka + \delta_1) \quad (8.120b)$$

$$\psi'_0 = -\kappa A \sin(\frac{1}{2}ka + \delta_0) \quad (8.120c)$$

$$\psi'_1 = \kappa B \cos(\frac{1}{2}ka + \delta_1) \quad (8.120d)$$

where  $A$  and  $B$  are coefficients to be determined and

$$\kappa = (2mE/\hbar)^{\frac{1}{2}}. \quad (8.120e)$$

The wave number  $\kappa$  is to be distinguished from the Bloch wave number  $k$  defined by eq. (8.114). For a free particle  $K=k$ . In the presence of a periodic potential, the boundary conditions (8.119) determine the relation between  $\kappa$  and  $k$ ; i.e. between the energy and the momentum.

We can now substitute the values (8.120) into the boundary conditions (8.119). We first note that

$$2\psi_0\psi'_0 = -\kappa a A^2 \sin(\kappa a + 2\delta_0) \quad (8.121a)$$

$$2\psi_1\psi'_1 = \kappa B^2 \sin(\kappa a + 2\delta_1) \quad (8.121b)$$

$$2\psi_0\psi'_1 = \kappa AB \cos(\kappa a + \delta_0 + \delta_1) + \cos(\delta_0 - \delta_1) \quad (8.121c)$$

$$2\psi'_0\psi_1 = \kappa AB \cos(\kappa a + \delta_0 + \delta_1) - \cos(\delta_0 - \delta_1). \quad (8.121d)$$

Substituting eqs. (8.121) into eqs. (8.119) we obtain

$$B^2 \sin(\kappa a + 2\delta_1) + A^2 \sin(\kappa a + 2\delta_0) = 0. \quad (8.122a)$$

$$\cos ka = \frac{\cos(\kappa a + \delta_0 + \delta_1)}{\cos(\delta_0 - \delta_1)}. \quad (8.122b)$$

$$\cos(\kappa a + \delta_0 + \delta_1) = \cos \kappa a \cos(\delta_0 - \delta_1). \quad (8.122c)$$

This can be rewritten

The left-hand sides of both equations (8.122b) and (8.122c) are cosine functions restricted to be less than unity. The right-hand side of eq. (8.122c) is a product of two cosine functions with the same restrictions. Thus for any given Bloch wave number  $k$  there always exists a value of  $\kappa$  from eq. (8.122c) and a solution of the Schrödinger equation. All values are thus allowed for the Bloch wave number  $k$  which has a continuous spectrum analogous to the free electron momentum.

The right-hand side of eq. (8.122b) is the quotient of two cosine functions. It is greater than unity for some values of  $\kappa$  and eq. (8.122b) then has no solution for  $k$ . The energy spectrum thus has a band structure with discontinuities and forbidden regions whenever the right-hand side of eq. (8.122b) becomes greater than unity. If the value of  $\kappa$  or of the energy is plotted against the Bloch wave number  $k$  the curve has discontinuities in  $K$  or  $2s$  at a fixed value of  $k$ .

## 8.14 Some properties of the band spectrum

Eqs. (8.122) have been obtained from general symmetry arguments without assumptions about the detailed shape of the potential  $V(x)$ , because the boundary conditions (8.199)

depend on the solutions of the Schrödinger equation in the interior only through two parameters, the logarithmic derivatives of the even and odd-parity solutions at  $x=a$ . These parameters are directly related to the scattering phase shifts. Thus the conditions (8.122) which determine the band structure are expressed completely in terms of these phase shifts and do not depend upon other details of the solution of the Schrödinger equation or of the potential.

We now use these results to determine specific properties of the band spectrum. The function  $\cot(ka+\delta_0+\delta_1)$  oscillates between  $-1$  and  $+1$ . At the extrema of these oscillations when it is equal to  $\pm 1$ , eq. (8.122b) has no solution for  $k$  if  $\delta_0+\delta_1$ . The forbidden regions around these extrema are seen from eq. (8.122b) to be defined by the condition

$$-|\delta_0 - \delta_1| < (\kappa a + \delta_0 + \delta_1 - n\pi) < |\delta_0 - \delta_1| \quad (8.123a)$$

where  $n$  is an integer chosen to minimize the absolute value of  $\kappa a + \delta_0 + \delta_1 - n\pi$ .

At the boundaries of the forbidden regions (8.123a) eqs. (8.122) show that the solutions have the following properties

$$B = 0 \quad \text{and} \quad ka = n\pi = (\kappa a + \delta_1 + \delta_0) + (\delta_0 - \delta_1) \\ \text{when } \kappa a = n\pi - 2\delta_0 \quad (8.123b)$$

$$A = 0 \quad \text{and} \quad ka = n\pi = (\kappa a + \delta_1 + \delta_0) - (\delta_0 - \delta_1) \\ \text{when } \kappa a = n\pi - 2\delta_1. \quad (8.123c)$$

The forbidden regions thus occur whenever  $ka=nn$  and appear as jump in the value of  $\kappa a$  between the values  $n\pi-2\delta_0$  and  $n\pi-2\delta_1$ . At the limits of the forbidden bands the Bloch waves are also parity eigenstates having odd parity when  $\kappa a=n\pi-2\delta_0$  and even parity when  $\kappa a=n\pi-2\delta_1$ . When  $\kappa a+\delta_0+\delta_1=(n+\frac{1}{2})\pi$ , eq. (8.122c) vanishes. Thus

$$\kappa a = (n + \frac{1}{2})\pi = \kappa a + \delta_0 + \delta_1 \quad \text{when} \quad \kappa a = (n + \frac{1}{2})\pi - \delta_0 - \delta_1. \quad (8.123d)$$

In the neighborhood of this point, eq. (8.122c) gives the inequality

$$|\kappa a + \delta_0 + \delta_1 - (n + \frac{1}{2})\pi| \leq |\kappa a - (n + \frac{1}{2})\pi|. \quad (8.123e)$$

The energy spectrum of the Bloch waves thus consists of alternating allowed and forbidden bands. The forbidden bands occur at the Bloch wave numbers  $ka-n\pi$  where there are an integral number of half wavelengths in a lattice period. A plot of  $\kappa a + \delta_0 + \delta_1$  thus has the form shown in fig. 8.1. The points at  $ka=(n+i)n$  lie on the dotted fine  $\kappa a + \delta_0 + \delta_1 = ka$ , as indicated by eq. (8.123d), but the slope of the curve is less than unity as indicated by the inequality (8.123e). At  $ka-n\pi$ , the curve jumps from a point  $|\delta_0 - \delta_1|$  below the dotted line to a point  $|\delta_0 - \delta_1|$  above. The forbidden values of  $\kappa + \delta_0 + \delta_1$  lie between these two values.

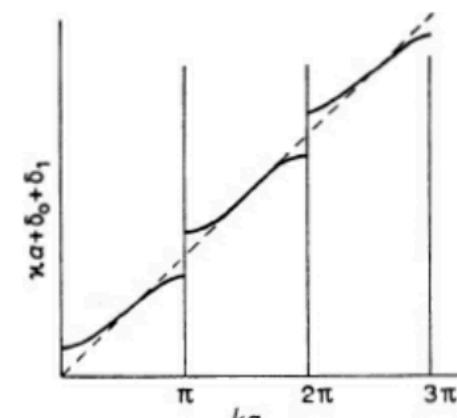


Fig. 8.1. Typical band spectrum for a periodic potential.

This band structure has been shown to be responsible for the classification of solids as conductors and insulators. Conduction occurs when it is easy to move electrons. In the absence of an applied electric field, there is no net current as the numbers of electrons moving in opposite directions are equal. An applied field can disturb this balance by putting more electrons in states moving in the direction of the field than in the reverse direction, provided that energy levels with a very small excitation energy are available for these electrons. In a system of free electrons there is a continuous spectrum and levels are always available at a very small excitation above the highest filled level. However, in a periodic potential with a band spectrum no very small excitations are possible if the electrons exactly fill a set of allowed energy bands. The lowest excitations then involve raising the energy of electrons across the forbidden region. This is not possible with a weak external field. Thus solids in which the number of electrons just fills the set of allowed bands are insulators; those in which the highest band is only partly filled are conductors.

### 8.15 Lattice dynamics. Bloch electrons and phonons

In a real crystal the potential that an electron sees is not strictly periodic. The ions may be displaced slightly from their equilibrium positions in the lattice. We can take this into account by modifying the potential (8.111a) to allow for small displacements  $\xi_\eta$  of each ion from its equilibrium position

$$V(x, \xi_n) = \sum_n V(x - na - \xi_n) \approx V_p(x) - \sum_n \xi_n \frac{\partial V(x - na)}{\partial x}. \quad (8.124)$$

Since these displacements are small we can expand the potential in a Taylor's series and keep only first order terms.

The displacements  $\xi_\eta$  are not given parameters but dynamical variables whose motion should be described in our Hamiltonian. We thus generalize the Hamiltonian to include three parts describing the electron, the ions and the interaction between the electron and ions.

$$H = H_e + H_i + H_{int}. \quad (8.125a)$$

In the electron Hamiltonian we include the kinetic energy and the first term of the right-hand side of eq. (8.124).

$$H_e = \frac{p^2}{2m} + V_p(x). \quad (8.125b)$$

The ion Hamiltonian consists of the sum of the kinetic energies of all the ions and the potentials of the interatomic forces. Since the displacements  $\xi_\eta$  are small, we expand the interatomic potential in powers of  $\xi_\eta$  and keep only terms to second order. The constant term is removed by changing the zero of the energy. Linear terms are absent since the variables  $\xi_\eta$  are measured from

their equilibrium position. Thus,

$$H_i = \sum_n \frac{\pi_n^2}{2M} + \sum_{nn'} C_{nn'} \xi_n \xi_{n'}, \quad (8.125c)$$

where  $\pi_n$  is the momentum canonically conjugate to  $\xi_n$ ,  $M$  is the ion mass, and  $C_{nn'}$  is the appropriate coefficient in the expansion of the interionic potential. Since the potential depends only upon the distance between the interacting ions and not on the position of the individual ions in the lattice,  $C_{nn'}$  depends only on the difference  $n-n'$ .

The electron-ion interaction contains only one term in the approximation we are considering; namely the second term on the right-hand side of eq. (8.124)

$$H_{int} = - \sum_n \xi_n \frac{\partial V}{\partial x} (x - na). \quad (8.125d)$$

Although this term was initially introduced to describe the effect of the displacement of the ion on the potential seen by the electron, the same interaction also affects the motion of the ion. The electric force between an electron and the positive ions affects the motion of the ions as well as the motion of the electron.

Although the periodic symmetry in the electron motion has been broken, there is an overall periodic symmetry for the whole lattice. We now define the transformation on the dynamical variables induced by a translation by a lattice period  $a$

$$x \rightarrow x + a, \quad p \rightarrow p \quad (8.126a)$$

$$\xi_n \rightarrow \xi_{n-1}, \quad \pi_n \rightarrow \pi_{n-1}. \quad (8.126b)$$

The Hamiltonian (8.125) is seen to be invariant under this transformation since  $C_{nn'}$  depends only on  $n-n'$ .

In order to proceed further, we consider a finite number of ions and use periodic boundary conditions in order to keep the invariance under the transformation (8.126b). This is common

in solid state physics and field theory. We thus let  $\eta$  vary in steps of unity from  $-N$  to  $+JV$  and set

We have already seen how the periodic symmetry of the electron Hamiltonian  $H_e$  is used to find its eigenfunctions. The same symmetry is useful in treating the ion Hamiltonian  $H_x$ . Here we wish to transform the variables  $\xi_\eta$  to normal mode variables by diagonalizing the matrix  $C_{nn}$  with a linear transformation in the vector space of the dynamical variables  $\xi_\eta$ . The electron Hamiltonian was diagonalized by a transformation on vectors in Hubert

space, not in a space of dynamical variables. However, the symmetry is used the same way in both cases. Since the matrix to be diagonalized is invariant under a particular transformation, we look for eigenvectors of the matrix which are also simultaneous eigenvectors of this transformation.

As we have already seen in the example in Hubert space, the eigenvectors of translations are just the Fourier transforms of the coordinates undergoing the translation, i.e. plane waves. We can therefore define our normal-mode variables immediately

$$a_q = \frac{1}{2}(N\hbar\alpha_q)^{-\frac{1}{2}} \sum_{n=-N}^{+N-1} (\xi_n + i\alpha_q n) e^{-iqna} \quad (8.127a)$$

$$a_q^\dagger = \frac{1}{2}(N\hbar\alpha_q)^{-\frac{1}{2}} \sum_{n=-N}^{+N-1} (\xi_n - i\alpha_q n) e^{iqna} \quad (8.127b)$$

where  $x_q$  is a constant to be determined which depends on the index  $q$ . We have chosen those linear combinations of the coordinates  $\xi_\eta$  and momenta  $n_n$  which make the normal-mode variables satisfy the commutation relations of boson annihilation and creation operators. The values of  $q$  are chosen to satisfy the periodic boundary conditions.

$$q = \frac{n'\pi}{Na}; \quad -N \leq n' \leq N-1 \quad (8.127c)$$

$$a_{q+2\pi/a} \equiv a_q. \quad (8.127d)$$

We choose  $\alpha_q$  to be an even function of  $q$

$$\alpha_q = \alpha_{-q}, \quad (8.127e)$$

and note the orthogonality relation

$$\sum_{q=-\pi/a}^{q=(1-N^{-1})\pi/a} e^{-iq(n-n')a} = 2N\delta_{nn'}. \quad (8.127f)$$

The variables (8.127) are seen to be eigenfunctions of the transformation (8.126b) with the eigenvalues  $e^{\pm iq a}$ . Using the orthogonality relation (8.127f) we see that they also satisfy the boson commutation relation:

$$[a_q, a_{q'}^\dagger] = \delta_{qq'}. \quad (8.127g)$$

When the ion Hamiltonian (8.125c) is expressed in terms of the normal-mode variables it reduces to the form:

$$H_I = \sum_q \frac{1}{2}\hbar\omega_q(a_q^\dagger a_q + a_q a_q^\dagger) \quad (8.128a)$$

where

$$\omega_q = 2 \sum_r \alpha_q C_{0r} e^{iqra} = (M\alpha_q)^{-1} \quad (8.128b)$$

$$\alpha_q = [2M \sum_r C_{0r} e^{iqra}]^{-\frac{1}{2}} \quad (8.128c)$$

and

$$C_{0r} = C_{n,n+r}. \quad (8.128d)$$

This is just the Hamiltonian for a system of free bosons, with the relation between frequency and wave number given by eq. (8.128b).

We can now express the interaction (8.125d) in terms of the normal coordinates by writing the potential as a Fourier transform.

$$\frac{\partial V}{\partial x}(x-na) \equiv \sum_q (N\hbar\alpha_q)^{-\frac{1}{2}} v_q e^{iq(x-na)}. \quad (8.129a)$$

We then have

$$H_{int} = - \sum_q \sum_n (N\hbar\alpha_q)^{-\frac{1}{2}} v_q e^{iqx} \xi_n e^{-iqna} = - \sum_q v_q e^{iqx} (a_q + a_q^\dagger). \quad (8.129b)$$

The interaction (8.129b) thus describes a change in the electron momentum by an amount  $hq$ , accompanied by either the absorption of a boson of wave vector  $q$ , or the creation of a boson of wave vector  $-q$ .

We now see the physical significance of the periodic symmetry, expressed by the invariance of the Hamiltonian under the generalized discrete translation (8.126). The Bloch wave number  $k$  or momentum of the electron is no longer a constant of the motion, but is changed by the interaction (8.129b). However, an overall ‘momentum conservation’ when the phonon variables are considered can be shown as follows.

The operator  $t^{iqx}$  in eq. (8.129b) describes a momentum transfer of  $hq$  to the electron and has a simple interpretation if the electron is in a momentum eigenstate. However, the eigenfunctions of the electron Hamiltonian (8.125b) are the Bloch waves (8.114) and not ordinary plane waves. These are not momentum eigenstates since an electron moving through any potential which is not constant has its momentum changed as it moves through the potential. Although the wave vector  $k$  associated with the Bloch wave function formally resembles the wave vector of a plane wave, the difference between this momentum and ordinary momentum is illustrated by calculating the matrix element of the operator  $t^{iqx}$  between two Bloch

wave functions.

$$\langle k' | e^{iqx} | k \rangle = \int_{-\infty}^{\infty} u_k^*(x) e^{-ik'x} e^{iqx} e^{ikx} u_k(x) dx. \quad (8.130a)$$

If the functions  $u_k(x)$  were constant, as in the case of plane waves, the integral in eq. (8.130a) would give a single delta function corresponding to momentum conservation. Since the functions  $u_k(x)$  are not constant but are periodic with period  $a$ , they can be expanded in a Fourier series in this interval. Thus the integral (8.130a) gives a delta function contribution whenever the difference  $k' - k - q$  is equal to an allowed value for a Fourier component in the expansion of  $u_k(x)$ . Thus

$$\langle k' | e^{iqx} | k \rangle = \sum_n 2\pi\delta(k' - k - q - 2n\pi/a) \int_{-\frac{1}{2}a}^{\frac{1}{2}a} u_k^*(x) e^{-i2n\pi x/a} u_k(x) dx. \quad (8.130b)$$

We assume that the functions  $u_k(x)$  are normalized in the interval from  $-\frac{1}{2}a$  to  $\frac{1}{2}a$ . They are not required to be orthogonal for different values of  $k$ , because the orthogonality condition applies to the entire wave function including the factor  $e^{ifx}$ .

The Bloch wave number or crystal momentum is thus conserved modulo  $2\pi/a$ . This is reasonable, since the Hamiltonian is not invariant under the continuous group of translations, but only under the discrete translation by a lattice vector  $a$ , and the Bloch wave number is only defined modulo  $2\eta\pi/a$ . Translation symmetry is discussed further in ch. 14.

We can easily generalize the Hamiltonian  $H$  to apply to many electrons instead of a single electron, if we disregard the direct Coulomb interaction between the electrons. This is justified in the Hartree-Fock approximation (see ch. 9) where we only consider the average interaction of a given electron with all other electrons, and neglect the fluctuations. The average interaction is included by changing the parameters of the periodic potential. If  $c_j$  denotes the creation operator of the Bloch wave vector  $k$ , we can rewrite eqs. (8.125b) and (8.129).

$$H_e = \sum_k E_k c_k^\dagger c_k \quad (8.131a)$$

$$R = \frac{1}{2}(e^{2i\delta_0} - e^{2i\delta_1}) = \frac{1}{2}[(e^{2i\delta_0} - 1) - (e^{2i\delta_1} - 1)] \\ = \sum_{l=0,1} i(-1)^l e^{i\delta_l} \sin \delta_l. \quad (8.11b)$$

$$E_k = \frac{\hbar^2}{2m} [\kappa(k)]^2 \quad (8.131c)$$

$$v_{knq} = \langle k + q + 2n\pi/a | e^{iqx} | k \rangle v_q \quad (8.131d)$$

where

and  $K(k)$  is given by eq. (8.122c).

The Hamiltonian defined by eqs. (8.131) and (8.128) is formally the same as the phenomenological Hamiltonians constructed to treat boson emission, absorption and decay processes, such as eqs. (4.2) and (7.12). However, we

have here constructed the Hamiltonian explicitly from the electron-ion and ion-ion interactions. We have derived, rather than postulated the existence of lattice vibration (phonon) creation and annihilation operators (8.129) which satisfy boson commutation rules. We have also derived interaction terms describing the emission and absorption of phonons by an electron, and can express the parameters of this interaction directly in terms of the electron-ion interaction.

This one-dimensional electron-phonon Hamiltonian provides a model which can be used to treat many interesting physical processes. For example:

*Phonon-electron scattering* is a second-order process in perturbation theory between an initial state  $|c_k c_l|0\rangle$  and a final state  $|c_k' c_l'|0\rangle$  each containing one electron and one phonon, via intermediate states  $|c_k c_l|0\rangle$  or  $|c_k' c_l' c_l|0\rangle$  containing either none or two phonons.

*Electron-electron scattering via a phonon exchange* is a second-order process in perturbation theory between an initial state  $|c_k c_l|0\rangle$  and a final state  $|c_k' c_l'|0\rangle$  each containing two electrons via intermediate states  $|c_k c_l c_l'|0\rangle$  containing two electrons and a phonon. Thus there is an effective electron-electron interaction via the lattice analogous to the ordinary electromagnetic interaction which arises from the exchange of photons. This electron-electron interaction mediated by the lattice can give rise to the pairing correlations which result in superconductivity.

*The polaron* is an electron which creates a potential well around itself by polarizing the lattice, repelling negative ions and attracting positive ions. It then oscillates in this well while at the same time moving through the lattice and carrying the well along with it. This can be treated by various methods.

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\* If the eigenvalue  $E$  is degenerate, the eigenfunctions are not required to have the form (8.113) or (8.114). However, we can define an operator which performs the translation  $x \rightarrow x + a$ , and which commutes with the Hamiltonian (8.111b). This is discussed in detail in ch. 14. Thus, it is always possible to choose a basis of eigenfunctions of  $H$  which are also eigenfunctions of the translation operator and have the form (8.114).