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On the impulse approximation

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Abstract. The neglect-of-binding aspect of the impulse approximation—the 'impulse hypothesis'—is discussed by considering the scattering of a Gaussian wave packet by a particle bound to a fixed origin, when multiple scattering and shadow effects do not occur. It is shown that the impulse approximation for the transition amplitude is equivalent to the neglect of binding during the collision in this case. Conditions involving the collision time and binding potential are found for the neglect of binding during the collision to be valid, and are shown to closely resemble the corresponding classical conditions. The nature of collision time is discussed. The generalisation of the impulse approximation to a collision of a particle with a bound two-particle system is briefly indicated. Finally the suitability of the impulse approximation for atomic and molecular scattering problems is considered.

1. Introduction

The impulse approximation has been known for many years. In its present form it was introduced by Chew (1950), and subsequently found application to many scattering problems, both in nuclear and atomic physics.

The impulse approximation consists of three assumptions. In the case of a single particle incident upon a complex target system consisting of two or more particles bound together they are:

I. The range of interaction is small compared with the inter-particle distances, so that the incident particle interacts with only one particle of the target system during the collision.

II. The target system can be regarded as transparent, so that the amplitude of the incident particle is not appreciably diminished in crossing the target system. This is to say that the near particles of the target system do not cast shadows on the far ones.

III. The scattering occurs over such a short time that the effect of the binding forces during the collision may be neglected.

We thus think of the scattering as taking place from only one particle of the target system. The only part played by the initial state of the target system is to give a momentum distribution to the particles of the target system.

Assumption III is sometimes known as the 'impulse hypothesis' (Coleman, 1969), and we shall adopt this name here. In this paper we shall only be concerned with the impulse hypothesis.

The impulse hypothesis was first discussed by means of an iteration procedure soon after the original paper of Chew (Chew and Wick 1952, Ashkin and Wick 1952, Chew and Goldberger 1952). Epstein (1960) considered the case when the perturbation of the system is time-dependent, and showed that this is exact if the perturbation is an impulse. Although he did not use a perturbation treatment he assumed a

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potential which suddenly switches on at time $t = 0$ and suddenly switches off at time $t = T$. Myhrer (1975) discussed the validity of the impulse hypothesis in meson–nucleus scattering, again by examination of the first terms of a perturbation series. Coleman (1969) and Briggs (1977) also discussed the impulse hypothesis from a perturbation point of view.

As pointed out above, in this paper we shall examine the impulse hypothesis. In order to simplify matters we shall consider the scattering of a particle 1 by a particle 2 bound to a fixed origin O, where 1 does not interact with O. In this case assumptions I and II disappear, and the impulse approximation becomes identical with the impulse hypothesis. The use of perturbation theory or artificial switching on and off the potential will be avoided by consideration of the scattering of a Gaussian wave packet representing the initial motion of the incident particle. It then becomes possible to talk about the duration of the collision, and to give a clear meaning to such a phrase as 'during the collision' which occurs in the impulse hypothesis. We shall derive the impulse approximation in the case of the scattering of an incident particle by a bound particle described above, when assumptions I and II do not apply. The generalisation of the results to the collision of a particle with a complex target containing two bound particles is then easily made.

2. The impulse hypothesis

We shall denote the position vector of the incident particle 1 relative to the origin by $\boldsymbol{r}_1$, and the position vector of the target particle 2 relative to O by $\boldsymbol{r}_2$. The interaction between 1 and 2 will be assumed to be described by a potential $V = V(\boldsymbol{r}_1, \boldsymbol{r}_2)$, and the binding of 2 to the origin will be assumed to be described by a binding potential $W = W(\boldsymbol{r}_2)$.

The states of the system in the absence of the interaction V are described by ket vectors

$$|\boldsymbol{k}, n\rangle = |\boldsymbol{k}\rangle|n\rangle \tag{2.1}$$

where $|\boldsymbol{k}\rangle$ represents a δ-function normalised plane-wave state of 1 moving freely with momentum $\hbar\boldsymbol{k}$ while $|n\rangle$ represents a state of the particle 2 in the potential W. In order that the states $|\boldsymbol{k}, n\rangle$ form a complete set it may be necessary for some of the states $|n\rangle$ to lie in the continuum. The wavefunction of the state (2.1) will be

$$\langle \boldsymbol{r}_1, \boldsymbol{r}_2|\boldsymbol{k}, n\rangle = \langle \boldsymbol{r}_1|\boldsymbol{k}\rangle\langle \boldsymbol{r}_2|n\rangle = (2\pi)^{-3/2} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r}_1)\langle \boldsymbol{r}_2|n\rangle, \tag{2.2}$$

$\langle \boldsymbol{r}_2|n\rangle$ being the wavefunction of particle 2 in the state $|n\rangle$.

If K_1 and K_2 are the kinetic energy operators associated with particles 1 and 2 respectively, and m_1 and m_2 are their masses, the energy of particle 1 in the absence of V is

$$E_k = \hbar^2 k^2 / 2m_1 \tag{2.3}$$

and so $|\boldsymbol{k}\rangle$ satisfies the eigenvalue equation

$$K_1|\boldsymbol{k}\rangle = E_k|\boldsymbol{k}\rangle. \tag{2.4}$$

Similarly if E_n is the energy associated with the state $|n\rangle$ the latter satisfies the eigenvalue equation

$$(K_2 + W)|n\rangle = E_n|n\rangle. \tag{2.5}$$

It follows from (2.1), (2.4) and (2.5) that the state $|\boldsymbol{k}, n\rangle$ satisfies the eigenvalue equation

$$H_0|\boldsymbol{k}, n\rangle = E_{kn}|\boldsymbol{k}, n\rangle \tag{2.6}$$

where

$$H_0 = K_1 + K_2 + W \tag{2.7}$$

is the Hamiltonian of the unperturbed system while

$$E_{kn} = E_k + E_n \tag{2.8}$$

is its total energy.

We now suppose that the initial state of the system consists of the incident particle 1 with momentum $\hbar\boldsymbol{k}_i$ while the bound particle 2 is in a state $|i\rangle$, so that the initial state of the system is represented by the ket $|\boldsymbol{k}_i, i\rangle$. Similarly we suppose the final state to be represented by the ket $|\boldsymbol{k}_f, f\rangle$ so that $\hbar\boldsymbol{k}_f$ is the momentum of the incident particle 1 after the collision while the target particle 2 is left in a state $|f\rangle$.

The exact transition amplitude $T(\boldsymbol{k}_i, i \to \boldsymbol{k}_f, f)$ is given by the standard expression

$$T(\boldsymbol{k}_i, i \to \boldsymbol{k}_f, f) = \langle \boldsymbol{k}_f, f|V|\boldsymbol{k}_i, i, +\rangle \tag{2.9}$$

where $|\boldsymbol{k}_i, i, +\rangle$ represents the scattering state obtained from $|\boldsymbol{k}_i, i\rangle$ by the perturbation V which obeys outgoing wave boundary conditions. The state $|\boldsymbol{k}_i, i, +\rangle$ satisfies the well known Schwinger–Lippmann equation

$$|\boldsymbol{k}_i, i, +\rangle = |\boldsymbol{k}_i, i\rangle + (E - H_0 + i\epsilon)^{-1} V|\boldsymbol{k}_i, i, +\rangle \tag{2.10}$$

where E is the energy of the system and ϵ is a positive number. By energy conservation E is the energy of both the initial state $|\boldsymbol{k}_i, i\rangle$ and of the final state $|\boldsymbol{k}_f, f\rangle$. The positive number ϵ is allowed to tend to zero at the end of any calculation. In particular, if H is the perturbed Hamiltonian

$$H = H_0 + V \tag{2.11}$$

the state $|\boldsymbol{k}_i, i, +\rangle$ satisfies the eigenvalue equation

$$H|\boldsymbol{k}_i, i, +\rangle = E|\boldsymbol{k}_i, i, +\rangle \tag{2.12}$$

as $\epsilon \to 0+$.

Let us consider the system in the absence of the binding W. The Hamiltonian h of the system is now given by

$$h = K_1 + K_2 + V \tag{2.13}$$

and the unperturbed Hamiltonian h_0 is given by

$$h_0 = K_1 + K_2. \tag{2.14}$$

The eigenstates of h_0 are represented by kets of the form

$$|\boldsymbol{k}, \boldsymbol{\kappa}\rangle = |\boldsymbol{k}\rangle|\boldsymbol{\kappa}\rangle \tag{2.15}$$

which describe a state of motion in which both particles are free, particle 1 with momentum $\hbar\boldsymbol{k}$ and particle 2 with momentum $\hbar\boldsymbol{\kappa}$. If E_k is defined by (2.3) while

$$E_\kappa = \hbar^2\kappa^2/2m_2 \tag{2.16}$$

is the energy of the freely moving particle 2, the energy of the state $|\boldsymbol{k}, \boldsymbol{\kappa}\rangle$ is

$$E_{k\kappa} = E_k + E_\kappa \tag{2.17}$$

and, from (2.14)

$$h_0|\boldsymbol{k}, \boldsymbol{\kappa}\rangle = E_{k\kappa}|\boldsymbol{k}, \boldsymbol{\kappa}\rangle. \tag{2.18}$$

Associated with the free state $|\boldsymbol{k}, \boldsymbol{\kappa}\rangle$ there is a scattering state $|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle$ which satisfies the Schwinger–Lippmann equation

$$|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle = |\boldsymbol{k}, \boldsymbol{\kappa}\rangle + (E_{k\kappa} - h_0 + i\epsilon)^{-1} V|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle. \tag{2.19}$$

As before the state $|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle$ obeys outgoing wave boundary conditions and, when $\epsilon \to 0+$, the eigenvalue equation

$$h|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle = E_{k\kappa}|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle. \tag{2.20}$$

Thus $|\boldsymbol{k}_i, i, +\rangle$ represents scattering of particle 1 with unperturbed momentum $\hbar\boldsymbol{k}_i$ by particle 2 when initially bound to the origin O in a state $|i\rangle$, the scattering taking place through the interaction V between 1 and 2, while $|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle$ represents the scattering of particle 1 with unperturbed momentum $\hbar\boldsymbol{k}$ by a free particle 2 with unperturbed momentum $\hbar\boldsymbol{\kappa}$, the scattering again taking place through the interaction V.

Chew (1950) introduced the hypothesis that assumption III is equivalent to replacing the exact state $|\boldsymbol{k}_i, i, +\rangle$ in (2.9) by means of the approximation

$$|\boldsymbol{k}_i, i, +\rangle \simeq \int |\boldsymbol{k}_i, \boldsymbol{\kappa}, +\rangle\langle\boldsymbol{\kappa}, i\rangle \, \mathrm{d}\boldsymbol{\kappa} \tag{2.21}$$

where $\langle\boldsymbol{\kappa}|i\rangle$ is the amplitude for particle 2 to have momentum $\hbar\boldsymbol{\kappa}$ when in the state $|i\rangle$. In other words, he assumed that the impulse hypothesis is equivalent to the assertion that the transition amplitude may be approximated by the expression

$$T(\boldsymbol{k}_i, i \to \boldsymbol{k}_f, f) \simeq \int \langle\boldsymbol{k}_f, f|V|\boldsymbol{k}_i, \boldsymbol{\kappa}, +\rangle\langle\boldsymbol{\kappa}|i\rangle \, \mathrm{d}\boldsymbol{\kappa}. \tag{2.22}$$

If we expand the final state $|f\rangle$ of particle 2 in terms of a complete set of plane wave states $|\boldsymbol{\kappa}'\rangle$ we obtain

$$T(\boldsymbol{k}_i, i \to \boldsymbol{k}_f, f) \simeq \int\int \langle f|\boldsymbol{\kappa}'\rangle\langle\boldsymbol{k}_f, \boldsymbol{\kappa}'|V|\boldsymbol{k}_i, \boldsymbol{\kappa}, +\rangle\langle\boldsymbol{\kappa}|i\rangle \, \mathrm{d}\boldsymbol{\kappa} \, \mathrm{d}\boldsymbol{\kappa}'. \tag{2.23}$$

The transition amplitude is therefore expressed in terms of the amplitude $\langle\boldsymbol{k}_f, \boldsymbol{\kappa}'|V|\boldsymbol{k}_i, \boldsymbol{\kappa}, +\rangle$ for free particle scattering. Since the double integral in (2.23) goes over all values of $\boldsymbol{\kappa}$ and $\boldsymbol{\kappa}'$, 'off-the-energy shell' matrix elements appear when the energies of the states $|k_i, \boldsymbol{\kappa}\rangle$ and $|\boldsymbol{k}_f, \boldsymbol{\kappa}'\rangle$ are unequal.

3. Derivation of the impulse by hypothesis

The states discussed in § 2 were all time-independent, but the impulse hypothesis as formulated in assumption III of § 1 clearly refers to a process which takes place in time. If we are to relate the approximation (2.22) to assumption III we must consider the time-dependent formulation of scattering theory.

Initially particle 2 is in a bound state $|i, t\rangle = |i\rangle \exp(-iE_i t/\hbar)$. Particle 1 cannot have a precise momentum $\hbar\boldsymbol{k}_i$, and so its state must be described by a wave packet. In

order to minimise the spread in momentum and space we choose a Gaussian wave packet. It is natural to take for the Gaussian wave packet one whose centre moves in a straight line through the origin and coincides with the origin at time $t = 0$ when we assume the packet to be minimal. Its mean momentum will be taken to be $\hbar \boldsymbol{k}_i$, and we shall assume that the spread of momentum is sufficiently small so that the relevant transition amplitudes do not vary significantly for values of $\boldsymbol{k}$ for which the momentum distribution is not small. This can always be done by taking the spatial spread of the packet to be sufficiently large.

If we put $\hbar \boldsymbol{k}_i = m_1 \boldsymbol{v}$ then $\boldsymbol{v}$ is the velocity of its centre. Assuming further the minimum half-width to be L, the Gaussian $|g(t)\rangle$ for the initial motion of particle 1 will have a position probability distribution

$$|\langle \boldsymbol{r}_1 | g(t) \rangle|^2 = \pi^{-3/2} L_t^{-3} \exp[-(\boldsymbol{r}_1 - \boldsymbol{v}t|^2 / L_t^2] \tag{3.1}$$

where

$$L_t^2 = L^2 + \frac{\hbar^2 t^2}{m_1^2 L^2}. \tag{3.2}$$

The wave packet therefore spreads out at a rate $\hbar / m_1 L$ as we go into the past or future. The representative in momentum space of the Gaussian at $t = 0$ will be

$$G(\boldsymbol{k}) = \langle \boldsymbol{k} | g(0) \rangle = \pi^{-3/4} L^{3/2} \exp[-\tfrac{1}{2} L^2 (\boldsymbol{k} - \boldsymbol{k}_i)^2]. \tag{3.3}$$

The initial unperturbed state of the system is now $|g(t)\rangle |i, t\rangle$, and we shall denote this simply by $|t\rangle$. The energy of the time-independent unperturbed state $|\boldsymbol{k}, i\rangle$ is E_{ki} (cf equation (2.6)), and so $|t\rangle$ is given by

$$|t\rangle = \int G(\boldsymbol{k}) |\boldsymbol{k}, i\rangle \exp(-iE_{ki}t/\hbar)\, \mathrm{d}\boldsymbol{k}. \tag{3.4}$$

In particular, at $t = 0$

$$|0\rangle = \int G(\boldsymbol{k}) |\boldsymbol{k}, i\rangle \, \mathrm{d}\boldsymbol{k}. \tag{3.5}$$

When the interaction V is present (3.4) represents the state of the system only asymptotically as $t \to -\infty$. At finite times $|\boldsymbol{k}, i\rangle$ in (3.4) must be replaced by the Schwinger–Lippmann state $|\boldsymbol{k}, i, +\rangle$. It follows that if $|t, +\rangle$ is the perturbed state of the system at time t then at $t = 0$ $|t, +\rangle$ is given by replacing $|\boldsymbol{k}, i\rangle$ by $|\boldsymbol{k}, i, +\rangle$ in (3.5); that is, by

$$|0, +\rangle = \int G(\boldsymbol{k}) |\boldsymbol{k}, i, +\rangle \, \mathrm{d}\boldsymbol{k}. \tag{3.6}$$

We now note that (3.5) can be expressed in terms of the plane wave states $|\boldsymbol{\kappa}\rangle$ of free motion of particle 2 according to

$$|0\rangle = \int\int G(\boldsymbol{k}) \langle \boldsymbol{\kappa} | i \rangle |\boldsymbol{k}, \boldsymbol{\kappa}\rangle \, \mathrm{d}\boldsymbol{k} \, \mathrm{d}\boldsymbol{\kappa}. \tag{3.7}$$

The state of unbound motion (that is, free motion of both particles) which coincides with this at time $t = 0$ is

$$|t\rangle_{\mathrm{u}} = \int\int G(\boldsymbol{k}) \langle \boldsymbol{\kappa} | i \rangle |\boldsymbol{k}, \boldsymbol{\kappa}\rangle \exp(-\mathrm{i}\hbar^{-1} E_{k\kappa} t) \, \mathrm{d}\boldsymbol{k} \, \mathrm{d}\boldsymbol{\kappa} \tag{3.8}$$

(cf equation (2.18)). If such a state were perturbed only by the interaction V, $|t\rangle_u$ is its asymptotic form as $t \to -\infty$. At $t = 0$ such a perturbed state would be given by

$$|0, +\rangle_u = \int\int G(\boldsymbol{k})\langle \boldsymbol{\kappa}|i\rangle |\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle \, d\boldsymbol{k} \, d\boldsymbol{\kappa} \tag{3.9}$$

where $|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle$ is the Schwinger–Lippmann state described in § 2.

The evolution operator in the interaction picture is

$$U(t_1, t_2) = \exp(iH_0 t_1/\hbar) \exp[-iH(t_1 - t_2)/\hbar] \exp(-iH_0 t_2/\hbar). \tag{3.10}$$

On use of (2.11), (2.7) and (2.14) this may be written

$$U(t_1, t_2) = \exp[i(h_0 + W)t_1/\hbar] \exp[-i(h_0 + W + V)(t_1 - t_2)/\hbar] \exp[-i(h_0 + W)t_2/\hbar]. \tag{3.11}$$

It is well known that

$$|0, +\rangle = U(0, -\infty)|0\rangle \tag{3.12}$$

if $U(0, -\infty)$ is the strong limit as $t \to -\infty$ of $U(0, t)$, provided V and W are not too singular when $\boldsymbol{r}_1 = \boldsymbol{r}_2$ or $\boldsymbol{r}_2 = \boldsymbol{0}$, and fall off sufficiently fast as $|\boldsymbol{r}_1 - \boldsymbol{r}_2|$ or $\boldsymbol{r}_2 \to +\infty$, respectively. There is therefore a time $\tau > 0$ such that, effectively,

$$|0, +\rangle = U(0, -\tau)|0\rangle. \tag{3.13}$$

We now insert (3.13) into (3.6), premultiply by V and take the inner product with the final state $|\boldsymbol{k}_f, f\rangle$ to obtain

$$\langle \boldsymbol{k}_f, f|VU(0, -\tau)|0\rangle = \int G(\boldsymbol{k})\langle \boldsymbol{k}_f, f|V|\boldsymbol{k}, i, +\rangle \, d\boldsymbol{k}. \tag{3.14}$$

The quantity $\langle \boldsymbol{k}_f, f|V|\boldsymbol{k}, i, +\rangle$ is the exact transition amplitude $T(\boldsymbol{k}, i \to \boldsymbol{k}_f, f)$ for the process $|\boldsymbol{k}, i\rangle \to |\boldsymbol{k}_f, f\rangle$ and so (3.14) can be written

$$\langle \boldsymbol{k}_f, f|VU(0, -\tau)|0\rangle = \int G(\boldsymbol{k})T(\boldsymbol{k}, i \to \boldsymbol{k}_f, f) \, d\boldsymbol{k}. \tag{3.15}$$

We can now specify more precisely the half-width of the wave packet. We note that the main contribution of $G(\boldsymbol{k})$ to the integral on the right-hand side of (3.15) comes from the sphere $|\boldsymbol{k} - \boldsymbol{k}_i| \leqslant L^{-1}$ in momentum space (cf (3.3)). The half-width will therefore be taken sufficiently large for the variation of the transition amplitude $T(\boldsymbol{k}, i \to \boldsymbol{k}_f, f)$ over the sphere $|\boldsymbol{k} - \boldsymbol{k}_i| \leqslant L^{-1}$ to be small; this quantity may therefore be replaced by its value at $\boldsymbol{k} = \boldsymbol{k}_i$ and taken outside the integral over $\boldsymbol{k}$. We thus obtain from (3.15)

$$\langle \boldsymbol{k}_f, f|VU(0, -\tau)|0\rangle \simeq T(\boldsymbol{k}_i, i \to \boldsymbol{k}_f, f)\int G(\boldsymbol{k}) \, d\boldsymbol{k} = 2^{3/2}\pi^{3/4}L^{-3/2}T(\boldsymbol{k}_i, i \to \boldsymbol{k}_f, f) \tag{3.16}$$

on use of (3.3).

If we premultiply (3.9) by V and take the inner product with $|\boldsymbol{k}_f, f\rangle$ we get

$$\langle \boldsymbol{k}_f, f|V|0, +\rangle_u = \int\int G(\boldsymbol{k})\langle \boldsymbol{\kappa}|i\rangle\langle \boldsymbol{k}_f, f|V|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle \, dk \, d\boldsymbol{\kappa}. \tag{3.17}$$

The quantity

$$t(\boldsymbol{k}, i \to \boldsymbol{k}_f, f) = \int \langle \boldsymbol{\kappa}|i\rangle\langle \boldsymbol{k}_f, f|V|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle \, d\boldsymbol{\kappa} \tag{3.18}$$

is, by (2.22), the approximate transition amplitude according to the impulse hypothesis. If we take L sufficiently large so that $t(\boldsymbol{k}, i \to \boldsymbol{k}_f, f)$ varies little over the sphere $|\boldsymbol{k} - \boldsymbol{k}_i| \leq L^{-1}$ we obtain from (3.17) and (3.18) the result

$$\langle \boldsymbol{k}_f, f | V | 0, + \rangle_u \simeq 2^{3/2} \pi^{3/4} L^{-3/2} t(\boldsymbol{k}_i, i \to \boldsymbol{k}_f, f). \tag{3.19}$$

The evolution operator $U_u(t_1, t_2)$ for scattering by V in the absence of the binding W is obtained from (3.11) by putting W equal to zero, so that

$$U_u(t_1, t_2) = \exp(\mathrm{i} h_0 t_1/\hbar) \exp[-\mathrm{i}(h_0 + V)(t_1 - t_2)/\hbar] \exp(-\mathrm{i} h_0 t_2/\hbar). \tag{3.20}$$

Now $|0, +\rangle_u$ is the perturbed state produced at time $t = 0$ by V from the state which, if allowed to evolve under the free particles Hamiltonian h_0, would become the state $|0\rangle$. It is therefore given by

$$|0, +\rangle_u = U_u(0, -\tau)|0\rangle. \tag{3.21}$$

(This assumes that the collision of the freely moving particles begins at the same time $-\tau$, a point which will be discussed later). Substitution of (3.21) into (3.19) yields

$$\langle \boldsymbol{k}_f, f | V U_u(0, -\tau)|0\rangle \simeq 2^{3/2} \pi^{3/4} L^{-3/2} t(\boldsymbol{k}_i, i \to \boldsymbol{k}_f, f). \tag{3.22}$$

If we compare (3.16) with (3.22) we see that the assumption

$$T(\boldsymbol{k}_i, i \to \boldsymbol{k}_f, f) \simeq t(\boldsymbol{k}_i, i \to \boldsymbol{k}_f, f) \tag{3.23}$$

is logically equivalent to the assumption

$$\langle \boldsymbol{k}_f, f | V U(0, -\tau|0\rangle \simeq (\boldsymbol{k}_f, f | V U_u(0, -\tau)|0\rangle. \tag{3.24}$$

From (3.11) and (3.20) we see that the two sides of (3.24) differ only in the neglect of W in the evolution operator U_u on the right-hand side of (3.24), establishing the equivalence of assumption III and (2.22).

4. Relation to the Born approximation

If we premultiply (3.5) by V and then take the inner product with $|k_f, f\rangle$ we obtain

$$\langle k_f, f | V | 0\rangle = \int G(\boldsymbol{k}) \langle \boldsymbol{k}_f, f | V | \boldsymbol{k}, i\rangle \, \mathrm{d}\boldsymbol{k}. \tag{4.1}$$

As before, for sufficiently large L equation (4.1) becomes

$$\langle \boldsymbol{k}_f, f | V | 0\rangle \simeq \langle \boldsymbol{k}_f, f | V | \boldsymbol{k}_i, i\rangle \int G(\boldsymbol{k}) \, \mathrm{d}k = 2^{3/2} \pi^{3/4} L^{-3/2} \langle \boldsymbol{k}_f, f | V | \boldsymbol{k}_i, i\rangle. \tag{4.2}$$

Now if we assume that $U(0, -\tau)$ may be replaced by the identity operator in the matrix element on the left-hand side of (3.16) we have

$$\langle \boldsymbol{k}_f, f | V U(0, -\tau)|0\rangle \simeq \langle \boldsymbol{k}_f, f | V | 0\rangle. \tag{4.3}$$

(3.16) and (4.2) show that the approximation (4.3) is equivalent to the approximation

$$T(\boldsymbol{k}_i i \to \boldsymbol{k}_f, f) \simeq \langle \boldsymbol{k}_f, f | V | \boldsymbol{k}_i, i\rangle \tag{4.4}$$

which is the Born approximation.

5. Sufficient conditions for the neglect of binding

As we saw in the last section the approximation (4.3) is logically equivalent to the Born approximation (4.4). As can be seen from (3.11), approximation (4.3) is equivalent to the assumption that the interaction V is weak and so can be neglected in the evolution operator on the left-hand side of (4.3). We shall now investigate the conditions under which W may be neglected in the evolution operator; that is, conditions under which the approximation (3.24) holds.

Equation (3.24) is certainly satisfied if V can be treated as a small perturbation, for then (3.11) and (3.20) show that both $U(0, -\tau)$ and $U_u(0, -\tau)$ may be replaced by the identity operator. However, it may happen that the binding W can be neglected even although V may not be a weak perturbation.

To investigate (3.24) we first write it out more fully using (3.11), (3.20) and (2.14) as

$$\langle \boldsymbol{k}_f, f|V \exp[-\mathrm{i}(K_1+K_2+W+V)\tau/\hbar] \exp[\mathrm{i}(K_1+K_2+W)\tau/\hbar]|0\rangle$$
$$\simeq \langle \boldsymbol{k}_f, f|V \exp[-\mathrm{i}(K_1+K_2+V)\tau/\hbar] \exp[\mathrm{i}(K_1+K_2)\tau/\hbar]|0\rangle. \tag{5.1}$$

If we put

$$W' = W + \lambda \tag{5.2}$$

where λ is an arbitrary complex number we see that (5.1) is logically equivalent to

$$\langle \boldsymbol{k}_f, f|V \exp[-\mathrm{i}(K_1+K_2+W'+V)\tau/\hbar] \exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle$$
$$\simeq \langle \boldsymbol{k}_f, f|V \exp[-\mathrm{i}(K_1+K_2+V)\tau/\hbar] \exp[\mathrm{i}(K_1+K_2)\tau/\hbar]|0\rangle, \tag{5.3}$$

and so the problem becomes that of investigating the approximation (5.3).

We first note that the approximation

$$\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle \simeq \exp[\mathrm{i}(K_1+K_2)\tau/\hbar]|0\rangle \tag{5.4}$$

is equivalent to the neglect of the renormalised binding W' during the time interval $-\tau \leqslant t \leqslant 0$ in the absence of the interaction. Since K_1 involves only the coordinates of particle 1 and $K_2 + W'$ involves only the coordinates of particle 2 we have, from (3.5), (2.1), and (2.4),

$$\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle = \int G(\boldsymbol{k}) \exp(\mathrm{i}E_k\tau/\hbar)|\boldsymbol{k}\rangle \exp[\mathrm{i}(K_2+W')\tau/\hbar]|i\rangle \, \mathrm{d}\boldsymbol{k}, \tag{5.5}$$

while

$$\exp[\mathrm{i}(K_1+K_2)\tau/\hbar]|0\rangle = \int G(\boldsymbol{k}) \exp(\mathrm{i}E_k\tau/\hbar)|\boldsymbol{k}\rangle \exp[\mathrm{i}K_2\tau/\hbar)|i\rangle \, \mathrm{d}\boldsymbol{k}. \tag{5.6}$$

Now from (5.2) and (2.5)

$$\exp[\mathrm{i}(K_2+W')\tau/\hbar]|i\rangle = \exp[\mathrm{i}(E_i+\lambda)\tau/\hbar]|i\rangle \tag{5.7}$$

while

$$\exp(\mathrm{i}K_2\tau/\hbar)|i\rangle = \int \exp(\mathrm{i}E_\kappa\tau/\hbar)|\boldsymbol{\kappa}\rangle\langle\boldsymbol{\kappa}|i\rangle \, \mathrm{d}\boldsymbol{\kappa}. \tag{5.8}$$

At this stage we introduce the assumption that the standard deviation ΔT_i of the kinetic energy from the mean kinetic energy T_i in the state $|i\rangle$ satisfies the condition

$$\Delta T_i \tau \ll \hbar. \tag{5.9}$$

With this assumption the kinetic energy E_κ in (5.8) may be approximated by its mean value T_i, when the exponential can be taken outside the integral sign to give

$$\exp(iK_2\tau/\hbar)|i\rangle \simeq \exp(iT_i\tau/\hbar)|i\rangle. \tag{5.10}$$

Comparison of (5.7) and (5.10) shows that the right-hand sides of (5.5) and (5.6) are approximately equal if

$$|E_i + \lambda - T_i|\tau \ll \hbar. \tag{5.11}$$

If the right-hand sides of (5.5) and (5.6) are approximately equal then so are the left-hand sides, which yields (5.4). So far we have left λ as an arbitrary complex number. If we choose λ according to

$$\lambda = T_i - E_i \tag{5.12}$$

then (5.11) is automatically satisfied, leaving (5.9) as a sufficient condition for (5.4).

We now put (5.9) into a form from which its physical significance will be immediate. If $|n\rangle$ is an arbitrary bound state of particle 2 in the potential W, and ΔT_n the standard deviation of the kinetic energy in the state $|n\rangle$, then

$$\begin{aligned}(\Delta T_n)^2 &= \langle n|K_2^2|n\rangle - \langle n|K_2|n\rangle^2 \\ &= \langle n|[(K_2+W)-W]^2|n\rangle - \langle n|(K_2+W)-W|n\rangle^2 \\ &= \langle n|(K_2+W)^2|n\rangle - \langle n|(K_2+W)W|n\rangle - \langle n|W(K_2+W)|n\rangle \\ &\quad + \langle n|W^2|n\rangle - \langle n|(K_2+W)-W|n\rangle^2,\end{aligned} \tag{5.13}$$

and so using (2.5)

$$\begin{aligned}(\Delta T_n)^2 &= E_n^2 - 2E_n\langle n|W|n\rangle + \langle n|W^2|n\rangle - E_n^2 + 2E_n\langle n|W|n\rangle - \langle n|W|n\rangle^2 \\ &= \langle n|W^2|n\rangle - \langle n|W|n\rangle^2 \\ &= (\Delta W_n)^2\end{aligned} \tag{5.14}$$

where ΔW_n is the standard deviation of the potential W in the state $|n\rangle$. In particular, $\Delta T_i = \Delta W_i$ so that the condition (5.9) is logically equivalent to

$$\Delta W_i\tau \ll \hbar. \tag{5.15}$$

If d_i is of the order of the standard deviation of the component of the position vector r_2 in the state $|n\rangle$ in any direction, then dividing (5.15) by d_i and using the uncertainty principle we get

$$(\Delta W_i/d_i)\tau \ll \hbar/d_i \leqslant \Delta p_i \tag{5.16}$$

where Δp_i is of the order of the standard deviation of the momentum of particle 2 in any direction in the state $|i\rangle$. The quantity Δp_i is, in its turn, of the order of the average magnitude of the momentum $\langle p\rangle_i$ of 2 in any direction in the state $|i\rangle$, so that (5.16) is equivalent to

$$\Delta W_i\tau/d_i \ll \langle p\rangle_i. \tag{5.17}$$

Since ΔW_i is the standard deviation of the potential W in the state $|i\rangle$ the quantity $(\Delta W_i)/d_i$ is a measure of the average force on particle 2 in this state, and so the left-hand side is a measure of the impulse, or momentum generated by, the binding force in the time interval τ. The condition (5.17) then states that this must be much

smaller than the average magnitude of the momentum $\langle p\rangle_i$ of 2 in the initial state $|i\rangle$. This is precisely the classical condition for a collision to be impulsive if we do not consider possible changes in the effect of the binding force on 2 which take place during the collision.

To obtain (5.3) we investigate the conditions under which we can make the approximation

$$\langle \boldsymbol{k}_f, f|V\exp[-\mathrm{i}(K_1+K_2+W'+V)\tau/\hbar]\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle$$
$$\simeq\langle \boldsymbol{k}_f, f|V\exp[-\mathrm{i}(K_1+K_2+V)\tau/\hbar]\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle. \tag{5.18}$$

The approximation (5.4) combined with (5.18) will then yield (5.3).

Firstly we note that if τ' is a time satisfying $\tau>\tau'>0$ then the left-hand side of (5.18) can be written as

$$\langle \boldsymbol{k}_f, f|V\exp[-\mathrm{i}(K_1+K_2+W'+V)\tau'/\hbar]\sum_{\boldsymbol{k},n}|\boldsymbol{k}, n\rangle\langle \boldsymbol{k}, n|$$
$$\times\exp[-\mathrm{i}(K_1+K_2+W'+V)(\tau-\tau')]\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle. \tag{5.19}$$

Now $\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle$ is the state of the system at the beginning of the collision $t=-\tau$, and so

$$\exp[-\mathrm{i}(K_1+K_2+W'+V)(\tau-\tau')/\hbar]\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle \tag{5.20}$$

is the state of the system at a time $t=-\tau'$ at an interval $\tau-\tau'$ after the start of the collision. Thus

$$\langle \boldsymbol{k}, n|\exp[-\mathrm{i}(K_1+K_2+W'+V)(\tau-\tau')/\hbar]\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle \tag{5.21}$$

is the probability amplitude for the unperturbed state $|\boldsymbol{k}, n\rangle$ to be observed during the collision. We shall assume for simplicity that this is negligible if $|n\rangle$ lies in the continuum, so that the sum over n in (5.19) may be taken to run only over bound states of particle 2. We now note the Trotter product formula

$$\exp(A+B)=\lim_{N\to\infty}\left(\exp\left(\frac{A}{N}\right)\exp\left(\frac{B}{N}\right)\right)^N \tag{5.22}$$

where the limit is taken in the strong sense, and A, B are self-adjoint operators in Hilbert space (Reed and Simon 1972). If we put $A=K_1+V$ and $B=K_2+W'$ the left-hand side of (5.18) becomes

$$\langle \boldsymbol{k}_f, f|V\exp[-\mathrm{i}(K_1+K_2+W'+V)\tau/\hbar]\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle$$
$$\simeq\langle \boldsymbol{k}_f, f|V\left\{\exp\left[\frac{-\mathrm{i}(K_1+V)\tau}{N\hbar}\right]\exp\left[\frac{-\mathrm{i}(K_2+W')\tau}{N\hbar}\right]\right\}^N$$
$$\times\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle \tag{5.23}$$

for sufficiently large values of the positive integer N.

Now

$$\exp\left[-\frac{\mathrm{i}(K_2+W')\tau}{N\hbar}\right]=\sum_n\exp\left[-\frac{\mathrm{i}(K_2+W')\tau}{N\hbar}\right]|n\rangle\langle n| \tag{5.24}$$

where by the argument following equation (5.19) the sum need only be taken over the

bound states of particle 2. Hence from (2.5) and (5.2)

$$\exp\left[-\frac{\mathrm{i}(K_2+W')\tau}{N\hbar}\right]=\sum_n \exp\left[-\frac{\mathrm{i}(E_n+\lambda)\tau}{N\hbar}\right]|n\rangle\langle n|. \tag{5.25}$$

If the standard deviation ΔT_n of the kinetic energy in the state $|n\rangle$ satisfies

$$\Delta T_n \tau \ll \hbar, \tag{5.26}$$

we may argue as before to obtain

$$\exp\left[-\frac{\mathrm{i}K_2\tau}{N\hbar}\right]\simeq\sum_n \exp\left[-\frac{\mathrm{i}T_n\tau}{N\hbar}\right]|n\rangle\langle n| \tag{5.27}$$

where T_n is the mean kinetic energy of the state $|n\rangle$. If we recall the product of $2N$ exponentials in (5.23) we see that the condition (5.26) ensures that the error in the product of approximating each second factor without W' according to (5.27) is small, due to the term N in the denominator of the right-hand side of (5.27).

If we compare (5.25) and (5.27) we see that the left-hand sides are approximately equal, even taking account of the product of $2N$ terms in (5.23), provided

$$|E_n+\lambda-T_n|\tau \ll \hbar. \tag{5.28}$$

From (5.12) we deduce that (5.28) is equivalent to

$$|(E_n-T_n)-(E_i-T_i)|\tau \ll \hbar. \tag{5.29}$$

As before (5.26) may be shown to be equivalent to

$$\Delta W_n \tau/d_n \ll \langle p\rangle_n \tag{5.30}$$

where d_n is a measure of the spatial spread in the state $|n\rangle$ and $\langle p\rangle_n$ is the average magnitude of the momentum in this state. The physical interpretation of (5.30) is that the momentum generated by the binding force in the state $|n\rangle$—that is, the impulse due to the binding force—must be small compared with the average magnitude of the momentum of the state $|n\rangle$.

The condition (5.29) may also be put in a form which leads to a simple physical interpretation; for

$$\begin{aligned}(E_n-T_n)-(E_i-T_i)&\\ &=\langle n|(K_2+W)-K_2|n\rangle-\langle i|(K_2+W)-K_2|i\rangle\\ &=\langle n|W|n\rangle-\langle i|W|i\rangle=W_n-W_i\end{aligned} \tag{5.31}$$

where W_n and W_i are the mean values of W in the states $|n\rangle$ and $|i\rangle$ respectively. Thus (5.29) becomes

$$|W_n-W_i|\tau \ll \hbar. \tag{5.32}$$

If d_n and d_i are the spatial spreads of the states $|n\rangle$ and $|i\rangle$ and we assume $d_n > d_i$ then $\frac{1}{2}[(d_n-d_i)+(d_n+d_i)]=d_n$ is a measure of the average 'distance' between the two states. If we divide (5.32) by d_n and use the uncertainty principle we obtain

$$\frac{|W_n-W_i|}{d_n}\tau \ll \frac{\hbar}{d_n} \leqslant \Delta p_n \sim \langle p\rangle_n \tag{5.33}$$

where Δp_n is the standard deviation of the momentum, and $\langle p\rangle_n$ is the mean magnitude of the momentum, in the state $|n\rangle$. The left-hand side of (5.33) is a measure of the average impulse due to the binding force when particle 2 changes its state from $|i\rangle$ to $|n\rangle$, and the right-hand side is a measure of the average magnitude of the momentum of 2 in the state $|n\rangle$. The quantity $\langle p\rangle_n$ will be smaller than $\langle p\rangle_i$ due to our assumption that $d_n > d_i$. Condition (5.33) says that the momentum generated on average by the binding force in taking particle 2 from state $|i\rangle$ to state $|n\rangle$ should be small compared with $\langle p\rangle_n$, and this again is reasonable on physical grounds.

Finally we consider which states $|n\rangle$ are most significant in the sum (5.24). If we assume no distortion of the initial state $|i\rangle$ during the collision and recall the argument after (5.19) we need only retain the term in i in (5.24). In this case (5.32) is automatically satisfied, while (5.26) reduces to (5.9).

If we assume that the initial state is 'frozen' during the collision, which is equivalent to the classical assumption that the target particle does not move during the collision, the sum over n in (5.24) need only be taken over states possessing significant overlap with the initial state. Alternatively we can note that the left-hand side of (5.23) may be written as

$$\sum_{\boldsymbol{k}n}\sum_{\boldsymbol{k}'n'}\langle \boldsymbol{k}_f, f|V|\boldsymbol{k}, n\rangle\langle \boldsymbol{k}, n|\exp[-\mathrm{i}(K_1+K_2+W'+V)\tau/\hbar]|\boldsymbol{k}', n'\rangle$$
$$\times\langle \boldsymbol{k}', n'|\exp[\mathrm{i}(K_1+K_2+W')\tau/\hbar]|0\rangle. \tag{5.34}$$

The Born matrix element will be largest for $n = f$, while the only contribution from the sum over n' comes from $n' = i$. This suggests that in the sum over n in (5.24) the two most significant values of n are i and f. The conditions then become (5.17), from (5.30)

$$\Delta W_f\tau/d_f \ll \langle p\rangle_f, \tag{5.35}$$

and from (5.33)

$$|W_f - W_i|\tau/d_f \ll \langle p\rangle_f. \tag{5.36}$$

The arguments which led to the physical interpretations of (5.26) and (5.32) may be put on a more precise basis as follows. From (5.14) we see that (5.26) is logically equivalent to

$$\Delta W_n\tau \ll \hbar. \tag{5.37}$$

If Δx_n is the standard deviation of the x-component of $\boldsymbol{r}_2$ in the state $|n\rangle$ (5.37) is, by the precise formulation of the position–momentum uncertainty principle, logically equivalent to

$$\frac{\Delta W_n}{\Delta x_n}\tau \ll \frac{\hbar}{\Delta x_n} \leqslant 2(\Delta p_x)_n \tag{5.38}$$

where $(\Delta p_x)_n$ is the standard deviation of the x-component of momentum in the state $|n\rangle$. The standard deviation $(\Delta p_x)_n$ is given by

$$[(\Delta p_x)_n]^2 = \langle p_x^2\rangle_n - (\langle p_x\rangle_n)^2 \tag{5.39}$$

where $\langle p_x^2\rangle_n$ and $\langle p_x\rangle_n$ are the expectation values of p_x^2 and p_x in the state $|n\rangle$. Now

$$\begin{aligned}\langle n|p_x|n\rangle &= \int\int \langle n|\boldsymbol{\kappa}\rangle\langle\boldsymbol{\kappa}|p_x|\boldsymbol{\kappa}'\rangle\langle\boldsymbol{\kappa}'|n\rangle \,\mathrm{d}\boldsymbol{\kappa}\,\mathrm{d}\boldsymbol{\kappa}' \\ &= \hbar\int\int \langle n|\boldsymbol{\kappa}\rangle\kappa_x'\langle\boldsymbol{\kappa}|\boldsymbol{\kappa}'\rangle\langle\boldsymbol{\kappa}'|n\rangle \,\mathrm{d}\boldsymbol{\kappa}\,\mathrm{d}\boldsymbol{\kappa}' = \hbar\int\int \langle n|\boldsymbol{\kappa}\rangle\kappa_x'\delta(\boldsymbol{\kappa}-\boldsymbol{\kappa}')\langle\boldsymbol{\kappa}'|n\rangle \,\mathrm{d}\boldsymbol{\kappa}\,\mathrm{d}\boldsymbol{\kappa}' \\ &= \hbar\int |\langle\boldsymbol{\kappa}|n\rangle|^2\kappa_x \,\mathrm{d}\boldsymbol{\kappa} = 0 \end{aligned} \tag{5.40}$$

since $|\langle\boldsymbol{\kappa}|n\rangle|^2\kappa_x$ is an odd function of κ_x by parity arguments. Thus $\langle p_x\rangle_n = 0$, a result which is also seen on physical grounds. For if $\langle p_x\rangle_n$ were not zero then the particle 2 would drift from the origin in the x-direction in the state $|n\rangle$, contradicting the fact that this is a bound state. Thus (5.39) yields $[(\Delta p_x)_n]^2 = \langle p_x^2\rangle_n$ so that (5.38) implies

$$\frac{\Delta W_n}{\Delta x_n}\tau \ll \langle p_x^2\rangle_n^{1/2}. \tag{5.41}$$

Since $\langle p_x^2\rangle_n^{1/2}$ is a measure of the mean magnitude of the momentum in the x-direction we see that under the first condition (5.26) for the impulse hypothesis to be valid the average impulse due to the binding force during the collision is small compared with the mean magnitude of the momentum. A similar argument applies to condition (5.32).

It should be noted that the precise argument only shows that the classical conditions are implied by the quantum mechanical ones. The equivalence deduced earlier depended on the assumption that $(\Delta p_x)_n\Delta x_n$ is of the order of $\hbar$. In practice this is often the case.

6. The collision time τ

So far we have not said anything about the order of magnitude of the 'collision time' τ. To do this we need to say a little more about the choice of the half-width L.

The half-width L is chosen so that the relevant transition amplitudes vary little over the sphere $|\boldsymbol{k}-\boldsymbol{k}_i| \leqslant L^{-1}$. Now the transition amplitude $T(\boldsymbol{k}, i\to\boldsymbol{k}_f, f)$ is given by

$$T(\boldsymbol{k}, i\to\boldsymbol{k}_f, f) = \langle\boldsymbol{k}_f, f|V|\boldsymbol{k}, i, +\rangle = \langle\boldsymbol{k}_f, f, -|V|\boldsymbol{k}, i\rangle. \tag{6.1}$$

The second form of the transition amplitude in (6.1) suggests that the variation of T is small for $|\boldsymbol{k}-\boldsymbol{k}_i| \leqslant L^{-1}$ if $L^{-1}R \ll 1$, where R is the range of the interaction of 2 with 1 in the state $|i\rangle$; that is, $L \gg R$. For example, this is certainly the case for the Born approximation to the transition amplitude for the elastic scattering of an electron by a hydrogen atom in its ground state.

The condition $L \gg R$ means that the wave packet is large compared with the region of interaction. The time $t = -\tau$, when the collision begins, is the time when the wave packet first begins to overlap the region of interaction. Since the region of interaction is small compared with the half-width of the packet we can take τ as of the order of L/v. This assumes that the rate of expansion $\hbar/m_1L$ is small compared with v; that is, $k_iL \gg 1$, so we require L to satisfy this condition also. Support for this is given by detailed numerical calculations of the scattering of a particle by a square well potential (Goldberg *et al* 1967) and of $H+H_2$ reactions employing a Porter–Karplus potential energy surface (McCullough and Watt 1971).

The condition $k_i L \gg 1$ is equivalent to

$$\tau = \frac{L}{v} \gg \frac{1}{k_i v} = \frac{\hbar}{m_1 v^2} = \frac{\hbar}{2T_1} \tag{6.2}$$

where T_1 is the kinetic energy of the incident particle 1. Our requirements on the collision time τ are therefore:

$$\tau \gg R/v, \tag{6.3}$$

$$\tau \gg \hbar/2T_1. \tag{6.4}$$

An interesting special case is that of resonance scattering. During such a process the incident particle 1 is temporarily captured by the target particle 2 to form an unstable bound state which then subsequently decays with the emission of 1. This is precisely opposite to the conditions under which we would expect the impulse hypothesis to be valid, and we shall now confirm this.

Since by (5.14) $\Delta W_n = \Delta T_n$ it follows from the fact $\tau = L/v$ that the condition (5.26) for the impulse hypothesis to be valid may be written

$$(L/v)\Delta W_n \ll \hbar \tag{6.5}$$

where $|n\rangle$ is a state of particle 2 likely to be excited during the collision. Now if Δk is the half-width of the resonance in terms of wave numbers the condition that the transition amplitude does not vary much over the wave packet is

$$L^{-1} \ll \Delta k. \tag{6.6}$$

If Γ is the half-width of the resonance in terms of energy

$$\Gamma = m_1 v \Delta v = v\hbar\Delta k \tag{6.7}$$

so that (6.6) is equivalent to

$$L^{-1} \ll \Gamma/\hbar v; \tag{6.8}$$

that is,

$$(L/v)\Gamma \gg \hbar. \tag{6.9}$$

Since Γ is small compared with the energy differences between adjacent states of 2 we have

$$\Gamma \ll \Delta W_n, \tag{6.10}$$

and so (6.5) implies

$$(L/v)\Gamma \ll \hbar. \tag{6.11}$$

Conditions (6.9) and (6.11) are opposite, as we should expect on physical grounds.

One further point should be added. In (3.21) we have taken τ to have the same value as in (3.13). In (3.21) $|0\rangle$ is the state into which a state of motion in which both particles are free would evolve. In order that τ in (3.21) should have the same value L/v the spatial change in the state $|i\rangle$ between $t = -\tau$ and $t = 0$ when 2 moves freely should be small compared with L. This, however, is ensured by (5.10), which ensures that the spatial change in $|i\rangle$ is very much less than R, and so therefore very much less than L. The approximation (5.10) is, in its turn, ensured by (5.9).

We can also partially see this directly from (5.9). ΔT_i is the energy uncertainty in the state of free motion of 2 which coincides with $|i\rangle$ at $t=0$. It follows from the time–energy uncertainty principle (McWeeny 1972) that the time τ_i for the mean value of r_2 in any direction to change by an amount equal to the position uncertainty in that direction satisfies

$$\tau_i \geqslant \hbar/2\Delta T_i. \tag{6.12}$$

(5.9) and (6.12) imply that

$$\tau_i \gg \tau \tag{6.13}$$

so that in the interval $0 \geqslant t \geqslant -\tau$ the mean value of r_2 does not change significantly. This suggests (but does not necessarily imply) that the spatial distribution of $|i\rangle$ when 2 is allowed to move freely does not alter much in the interval $0 \geqslant t \geqslant -\tau$.

Before leaving this section something ought to be said about the smallness of the variation of $t(\boldsymbol{k}, i \to \boldsymbol{k}_f, f)$ over the sphere $|\boldsymbol{k}-\boldsymbol{k}_i| \leqslant L^{-1}$. We note that (3.18) can be written

$$t(\boldsymbol{k}, i) \to \boldsymbol{k}_f, f) = \int\int \langle f|\boldsymbol{\kappa}'\rangle\langle \boldsymbol{k}_f, \boldsymbol{\kappa}'|V|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle\langle\boldsymbol{\kappa}|i\rangle \, \mathrm{d}\boldsymbol{\kappa} \, \mathrm{d}\boldsymbol{\kappa}'. \tag{6.14}$$

If the energy of the incident particle 1 is large compared with the mean kinetic energy of particle 2 in the bound states $|i\rangle$ and $|f\rangle$ we can assume that

$$\langle \boldsymbol{k}_f, \boldsymbol{\kappa}'|V|\boldsymbol{k}, \boldsymbol{\kappa}, +\rangle \simeq \langle \boldsymbol{k}_f, \boldsymbol{\kappa}', -|V|k, \boldsymbol{\kappa}\rangle \tag{6.15}$$

when (6.14) becomes

$$t(\boldsymbol{k}, i \to \boldsymbol{k}_f, f) \simeq \int \langle f|\boldsymbol{\kappa}\rangle\langle \boldsymbol{k}_f, \boldsymbol{\kappa}, -|V|\boldsymbol{k}, i\rangle \, \mathrm{d}\boldsymbol{\kappa}. \tag{6.16}$$

(Equation (6.15) is only exact, of course, if the energies of the initial and final states $|\boldsymbol{k}, \boldsymbol{\kappa}\rangle$ and $|\boldsymbol{k}_f, \boldsymbol{\kappa}'\rangle$ are the same.) This form suggests that it is reasonable to assume that $t(\boldsymbol{k}, i \to \boldsymbol{k}_f, f)$ does not vary much for $|\boldsymbol{k}-\boldsymbol{k}_i| \leqslant L^{-1}$ if $RL^{-1} \ll 1$; that is, $L \gg R$. The same is obviously true for the Born matrix element in (4.1).

7. Generalisation

Suppose a particle 1 collides with a target system consisting of two particles 2 and 3 bound together in a state $|i\rangle$. If V_{jk} is the interaction between particles j and k the binding is $W = V_{23}$ and the interaction is $V = V_{12} + V_{13}$. The arguments of the previous sections for the impulse hypothesis (assumption III of § 1) go through with obvious modifications. If assumptions I and II are also made the impulse approximation can be obtained in the form

$$T \simeq t_{12} + t_{13} \tag{7.1}$$

where T is the transition operator for the collision, while t_{12} and t_{13} are the transition operators for collisions between 1 and 2, and 1 and 3, respectively (cf Chew and Goldberger 1952).

8. Examples

8.1. Square well potential

If W is the square well potential

$$W = \begin{cases} -V_0, & (r_2 \leqslant R,\ V_0 > 0) \\ 0, & (r_2 > R) \end{cases} \tag{8.1}$$

then for any bound state $|n>$ we have

$$0 \leqslant \Delta V_n \leqslant V_0 \tag{8.2}$$

$$0 \leqslant |W_n - W_i| \leqslant V_0 \tag{8.3}$$

and so the impulse hypothesis will be valid if

$$V_0 \tau \ll \hbar. \tag{8.4}$$

8.2. Electron–hydrogen scattering

In this case, if $|i\rangle$ is the ground state of the hydrogen atom, a simple calculation shows that ΔW_i is one atomic unit. Since the range is of the order of one atomic unit the condition $\Delta W_i \tau \ll \hbar$ leads to the requirement that the energy of the incident electron should be very much greater than one atomic unit. We therefore cannot expect the impulse hypothesis to be much better than the Born approximation in this case.

8.3. Molecular binding

Suppose 2 and 3 are atomic nuclei which are initially bound to form a molecule, and that the initial vibrational state of the molecule is the ground state. The only states of the molecule which have significant overlap with the ground state are the first few excited states and the ground state itself. It is an elementary exercise to calculate ΔW_n and $W_n - W_i$, and these quantities are in fact of the same order as the vibrational energy. If we assume that the relevant vibrational energies are less than or equal to one electron volt and R is of the order of one atomic unit the conditions

$$\Delta W_n \tau \ll \hbar \tag{8.5}$$

$$|W_n - W_i| \tau \ll \hbar \tag{8.6}$$

both become

$$(27{\cdot}07)^{-1} \tau \ll 1. \tag{8.7}$$

The conditions (6.3) and (6.4) on τ combined with (8.7) yield

$$(27{\cdot}07)^{-1} \frac{1}{v} \ll 1 \tag{8.8}$$

and

$$(27{\cdot}07)^{-1} \frac{1}{2T_1} \ll 1. \tag{8.9}$$

Condition (8.9) is equivalent to requiring that the energy of 1 is very much greater

than $\frac{1}{2}$ eV, irrespective of its mass. Condition (8.8) is equivalent to

$$T_1 = \tfrac{1}{2}\mu v^2 \gg \tfrac{1}{2}\mu(27{\cdot}07)^{-2} \tag{8.10}$$

where μ is the reduced mass of 1 and the target system, and has the role previously played by m_1.

If 1 is an electron this requires that the incident particle energy be very much greater than 0·02 eV, and so combining this with (8.9) we see that the impulse hypothesis should be valid at energies of a few eV, where the Born approximation breaks down.

If 1 is a heavy particle we can take $\mu \sim 1000$ in atomic units. Condition (8.10) shows that the incident particle energy should be much greater than 20 eV, which then automatically satisfies (8.9). Thus for heavy particle collisions the impulse hypothesis should also be valid.

9. Summary and conclusions

Part of the impulse approximation involves the neglect of binding during the collision. It is natural to investigate this by time-dependent collision theory, and we have chosen to follow the scattering of a Gaussian wave packet of half-width L. By choosing L sufficiently large for the transition amplitude to vary little over the half-width L^{-1} of the corresponding momentum distribution it is possible to confirm the equivalence of the two forms, *viz* assumption III and (2.22), of the impulse hypothesis.

The impulse hypothesis is obviously true if the unitary operators U and U_u can be replaced by the identity operator, which is the Born approximation. We investigated in § 5 the possibility of the impulse hypothesis still being true even in the case when replacement of U and U_u by the identity is too crude. We found that the impulse hypothesis held if the criteria $|W_n - W_i|\tau \ll \hbar$ and $\Delta W_n \tau \ll \hbar$ are valid for any bound states $|n\rangle$ of the target system likely to be excited during the collision, provided that the excitement of continuum states of the target system during the collision is unlikely. These conditions closely resemble the classical conditions. If it is assumed that the position probability distribution of the target particle remains unchanged during the collision the states $|n\rangle$ likely to be excited during the collision are those with significant overlap with $|i\rangle$.

The collision time τ in the conditions $|W_n - W_i|\tau \ll \hbar$ and $\Delta W_n \tau \ll \hbar$ should satisfy (6.3) and (6.4). This ensures that the variation in the transition amplitude is sufficiently small and the expansion or contraction of the incident wave packet is unimportant.

Finally we found that the impulse hypothesis is unlikely to be an improvement on the Born approximation in the case of electron collisions with ground state hydrogen, but should be applicable at intermediate energies for scattering of diatomic molecules.

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