# Appendix A
# Some Results in Quantum Mechanics

## A.1 Barrier Penetration

Consider the one-dimensional potential shown in Figure A.1(a). Free particles of mass $m$ and energy $E$ represented by plane waves are incident from the left and encounter the constant rectangular barrier of height $V$, where $V > E$.

In region I ($x < 0$), there is an incoming wave $e^{ikx}$, where the wave number $k$ is given by

$$\hbar^2 k^2 = 2mE, \tag{A.1}$$

and also a wave reflected at the barrier travelling from right to left of the form $e^{-ikx}$. Thus the total wavefunction in region I is

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}, \tag{A.2}$$

where $A$ and $B$ are complex constants. Within the barrier, region II ($0 < x < a$), the solution of the Schrödinger equation is a decaying exponential plus an exponential wave reflected from the boundary at $x = a$, i.e. the total wavefunction is

$$\psi_2(x) = Ce^{-\kappa x} + De^{\kappa x}, \tag{A.3}$$

where $C$ and $D$ are complex constants and $\kappa$ is given by

$$\hbar^2 \kappa^2 = 2m(V - E). \tag{A.4}$$

Finally, in region III ($x > a$) to the right of the barrier, there is only an outgoing wave of the form

$$\psi_3(x) = Fe^{ikx}, \tag{A.5}$$

where again $F$ is a complex constant.

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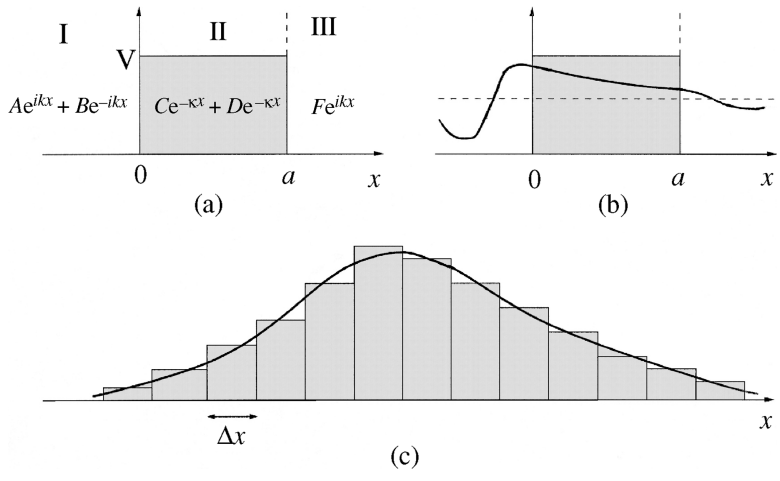


**Figure A.1** Rectangular barrier with (a) wavefunction solutions, and (b) form of the incoming and outgoing waves; (c) modelling an arbitrary smooth barrier as a series of rectangular barriers

We are interested in the *transmission coefficient* $T$, defined by

$$T \equiv |F/A|^2. \tag{A.6}$$

The values of $F$ and $A$ are found by imposing continuity of the wavefunction and its first derivative, i.e. matching the values of these quantities at the two boundaries $x = 0$ and $x = a$. The algebra may be found in any introductory book on quantum mechanics.[1] The result is

$$T = \left| \frac{2k\kappa e^{-ika}}{2k\kappa \cosh(\kappa a) - i(k^2 - \kappa^2)\sinh(\kappa a)} \right|^2. \tag{A.7}$$

The corresponding incident and transmitted waves are shown in Figure A.1(b) (the reflected waves are not shown).

For large $\kappa a$, which corresponds to small penetrations, we can make the replacement

$$\sinh(\kappa a) \approx \cosh(\kappa a) \approx \frac{1}{2} e^{\kappa a} \tag{A.8}$$

and hence

$$T \approx \left( \frac{4k\kappa}{k^2 + \kappa^2} \right)^2 e^{-2\kappa a}. \tag{A.9}$$

[1] See, for example, Chapter 6 of Me61.

The first factor is due to the reflection losses at the two boundaries $x = 0$ and $x = a$ and the decreasing exponential describes the amplitude decay within the barrier. The first factor is slowly varying with energy and is usually neglected.

The result of Equation (A.9), ignoring the first factor, may be used to find the transmission coefficient for an arbitrary smoothly-varying barrier by modelling it as a series of thin rectangular barriers. This is illustrated in Figure A.1(c). Thus by replace $2\kappa a$ by $2\sum \kappa(x)\Delta x$ and taking the limit of small $\Delta x$, the summation goes over to an integral, i.e.

$$2\kappa a \rightarrow 2\int \mathrm{d}x \left\{ \frac{2m}{\hbar^2}[V(x) - E] \right\}^{\frac{1}{2}} \tag{A.10}$$

and

$$T \approx \exp\left[ -2\int \mathrm{d}x \left\{ \frac{2m}{\hbar^2}[V(x) - E] \right\}^{\frac{1}{2}} \right]. \tag{A.11}$$

This is the essence of what is known as the WKB approximation in quantum mechanics. Equation (A.11) was used in Section 7.6 to discuss $\alpha$-decay and in Section 8.2.1 to discuss nuclear fusion.

## A.2 Density of States

Consider a spinless particle of mass $m$ confined within a cube of sides $L$ and volume $V = L^3$, oriented so that one corner is at the origin (0,0,0) and the edges are parallel to the $x$, $y$ and $z$ axes. If the potential is zero within the box, then the walls represent infinite potential barriers and the solutions of the Schrödinger equation must therefore vanish on all faces of the cube. It is straightforward to show that the solutions of the Schrödinger equation satisfying these boundary conditions are standing waves of the form

$$\psi(x, y, z) = C \sin(k_x x) \sin(k_y y) \sin(k_z z), \tag{A.12}$$

where $C$ is a constant and the components of the wave number $\mathbf{k} = (k_x, k_y, k_z)$ take the values

$$k_x = \frac{n_x \pi}{2}, \quad k_y = \frac{n_y \pi}{2}, \quad k_z = \frac{n_z \pi}{2}, \quad (n_x, n_y, n_z) = 1, 2, 3.... \tag{A.13}$$

The energy of the particle is given by

$$E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2 k^2}{2m} = \frac{(\hbar\pi)^2}{8m}(n_x^2 + n_y^2 + n_z^2), \tag{A.14}$$

where $k \equiv |\mathbf{k}| = p/\hbar$ and $p$ is the particle's momentum. Negative values of the integers do not lead to new states since they merely change the sign of the wave function Equation (A.12) and phase factors have no physical significance.

The allowed values of $\mathbf{k}$ form a cubic lattice in the quadrant of '$\mathbf{k}$-space' where all the values of $(n_x, n_y, n_z)$ are positive. Since each state corresponds to one combination of $(n_x, n_y, n_z)$, the number of allowed states is equal to the number of lattice points. The spacing between the lattice points is $(L/\pi)$, so the density of points per unit volume in $\mathbf{k}$-space is $(L/\pi)^3$. The number of lattice points $n(k_0)$ with $k$ less than some fixed value $k_0$ is the number contained within a volume that for large values of $k_0$ may be well approximated by the quadrant of a sphere of radius $k_0$, i.e.

$$n(k_0) = \frac{1}{8}\frac{4}{3}\pi k_0^3 \left(\frac{L}{\pi}\right)^3 = \frac{V}{(2\pi)^3}\frac{4\pi k_0^3}{3}. \tag{A.15}$$

Hence the number of points with $k$ in the range $k_0 < k < (k_0 + \mathrm{d}k_0)$ is

$$\mathrm{d}n(k_0) = \frac{V}{(2\pi)^3} 4\pi k_0^2 \mathrm{d}k_0. \tag{A.16}$$

The *density of states* is defined as $\rho(k_0) \equiv \mathrm{d}n(k_0)/\mathrm{d}k_0$ and so is given by

$$\rho(k_0) = \frac{V}{(2\pi)^3} 4\pi k_0^2. \tag{A.17}$$

Thus $\rho(k_0)\mathrm{d}k_0$ is the number of states with $k$ between $k_0$ and $k_0 + \mathrm{d}k_0$, or equivalently

$$\rho(p)\mathrm{d}p = \frac{4\pi V}{(2\pi\hbar)^3} p^2 \mathrm{d}p \tag{A.18}$$

is the number of states with momentum between $p$ and $p + \mathrm{d}p$. This is the form used in Equation (7.1) when discussing the Fermi energy in the Fermi gas model. Equation (A.18) can also be written in terms of energy using $E = p^2/2m$, when it becomes

$$\rho(E)\mathrm{d}E = \frac{4\pi V}{(2\pi\hbar)^3} m\, p\, \mathrm{d}E \tag{A.19}$$

and this was the form used in discussing $\beta$-decay in Section 7.7.2.

Although the above derivation is for a particle confined in a box, the same technique can be used for scattering problems. In this case we can consider a large volume $V = L^3$ and impose 'periodic' boundary conditions

$$\psi(x + L, y, z) = \psi(x, y + L, z) = \psi(x, y, z + L) = \psi(x, y, z). \tag{A.20}$$

Instead of standing waves, the solutions of the Schrödinger equation consistent with Equation (A.20) are the travelling waves

$$e^{i\mathbf{k}.\mathbf{r}} = e^{ik_x x} e^{ik_y y} e^{ik_z z} \tag{A.21}$$

where

$$k_x = \frac{2n_x\pi}{L}, \quad k_y = \frac{2n_y\pi}{L}, \quad k_z = \frac{2n_z\pi}{L}, \quad n_x, n_y, n_z = 0, \pm 1, \pm 2 \ldots. \tag{A.22}$$

The density of lattice points in **k**-space now becomes $(L/2\pi)^3$, but unlike the standing wave case, permutations of signs in Equation (A.22) *do* produce new states and the whole quadrant of lattice points has to be considered. Thus these two effects 'cancel out' and we arrive at the same result for the density of states in Equations (A.18) and (A.19). This approach was used in discussing the formal definitions of cross sections in Chapter 1.

All the above is for spinless particles. If the particle has spin then the density of states must be multiplied by the appropriate spin multiplicity factor, taking account of the Pauli principle as necessary. Thus, for example, for spin-$\frac{1}{2}$ particles, with two spin states, Equation (A.19) becomes

$$\rho(E)\mathrm{d}E = \frac{8\pi V}{(2\pi\hbar)^3} mp\, \mathrm{d}E. \tag{A.23}$$

## A.3 Perturbation Theory and the Second Golden Rule

Without detailed proof, we will outline the derivation from perturbation theory of the important relationship between the transition probability per unit time for a process and its matrix element.[2]

In perturbation theory, the Hamiltonian at time $t$ may be written in general as

$$H(t) = H_0 + V(t), \tag{A.24}$$

where $H_0$ is the unperturbed Hamiltonian and $V(t)$ is the perturbation, which we will assume is small. The solution for the eigenfunctions of $H$ starts by expanding in terms of the complete set of energy eigenfunctions $|u_n\rangle$ of $H_0$, i.e.

$$|\psi(t)\rangle = \sum_n c_n(t)|u_n\rangle e^{-iE_n t/\hbar}, \tag{A.25}$$

[2]We follow the derivation given in Chapter 9 of Ma92.

where $E_n$ are the corresponding energies. If $|\psi(t)\rangle$ is normalized to unity, then the squared coefficient $|c_n(t)|^2$ is the probability that at time $t$ the system is in a state $|u_n\rangle$. Substituting Equation (A.25) into the Schrödinger equation leads to a differential equation for the transition coefficients:

$$i\hbar \frac{\mathrm{d}c_f(t)}{\mathrm{d}t} = \sum_n V_{fn}(t)\mathrm{e}^{i\omega_{fn}t}c_n(t), \tag{A.26}$$

where the matrix element $V_{fn} \equiv \langle u_f\ |V(t)|u_n\rangle$ and the angular frequency $\omega_{fn} \equiv (E_f - E_n)/\hbar$. If we assume initially $(t = 0)$ that the system is in a state $|u_i\rangle$, then $c_n(0) = \delta_{ni}$ and the solutions for $c_f(t)$ are found by substituting this result into the right-hand side of Equation (A.22) giving, *to first-order in V*,

$$c_i(t) = 1 + \frac{1}{i\hbar}\int_0^t V_{ii}(t')\mathrm{d}t' \tag{A.27a}$$

and

$$c_f(t) = \frac{1}{i\hbar}\int_0^t V_{fi}(t')\mathrm{e}^{i\omega_{fi}(t')}\mathrm{d}t' \qquad (f \neq i). \tag{A.27b}$$

For $f \neq i$, the quantity $\left|c_f(t)\right|^2$ is the probability, in first-order perturbation theory, that the system has made a transition from state $i$ to state $f$.

The above is for a general time-dependent perturbation $V(t)$, but the results can also be used to describe other situations, for example where the perturbation is zero up to some time $t_0$ and a constant thereafter. In this case, the integrals in Equations (A.27) can be evaluated and, in particular, Equation (A.27b) gives, again to first-order in $V$,

$$c_f(t) = \frac{V_{fi}}{\hbar\omega_{fi}}\left[1 - \mathrm{e}^{i\omega_{fi}t}\right] \tag{A.28}$$

and hence the probability of the transition $i \rightarrow f$ is

$$P_{fi}(t) = \left|c_f(t)\right|^2 = \frac{4\left|V_{fi}\right|^2}{\hbar^2}\left[\frac{\sin^2(\frac{1}{2}\omega_{fi}t)}{\omega_{fi}^2}\right]. \tag{A.29}$$

The function in the square brackets in Equation (A.29) is shown in Figure A.2.

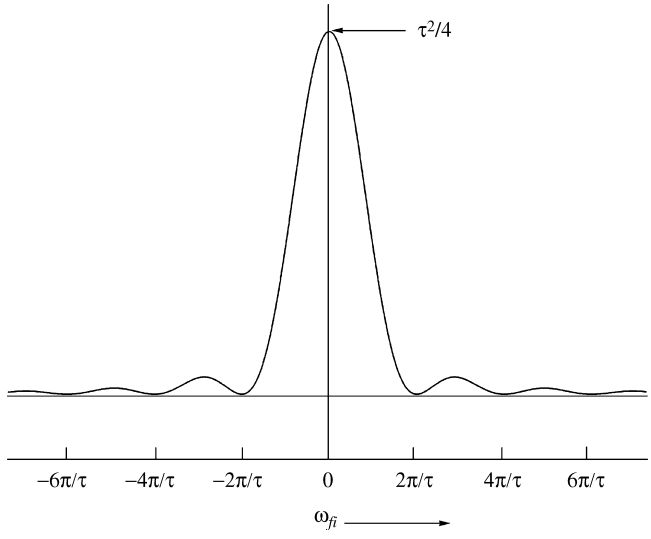


**Figure A.2** The function $\left[\dfrac{\sin^2(\frac{1}{2}\omega_{fi}t)}{\omega_{fi}^2}\right]$

For sufficiently large values of $t$, it has the form of a large central peak with much smaller side oscillations. In this case $P_{fi}$ is only appreciable if

$$\hbar\left|\omega_{fi}\right| = \left|E_f - E_i\right| \leq 2\pi\hbar/t \tag{A.30}$$

and then the square bracket can be replaced by a Dirac delta function[3], i.e.

$$\lim_{t\to\infty} \frac{\sin^2(\frac{1}{2}\omega_{fi}t)}{\omega_{fi}^2} = \frac{1}{2}\pi\hbar t\delta(E_f - E_i), \tag{A.31}$$

where the external factors are to preserve the normalization. Then

$$P_{fi}(t) = t\frac{2\pi}{\hbar}\left|V_{fi}\right|^2\delta(E_f - E_i) \tag{A.32}$$

[3]The Dirac delta function was the first so-called 'generalized function'. It is defined by the two conditions: (i) $\delta(x' - x) = 0$ if $x \neq x'$ and (ii) $\int_{-\infty}^{+\infty}\delta(x' - x)\mathrm{d}x' = 1$. It follows that if $f(x)$ is a function continuous in the interval $x_1 < x < x_2$, then $\int_{x_1}^{x_2} f(x')\delta(x' - x)\mathrm{d}x' = f(x)$ if $x_1 < x < x_2$ or $= 0$ if $x < x_1$ or $x > x_2$.

and the transition probability per unit time is

$$\frac{\mathrm{d}P_{fi}(t)}{\mathrm{d}t} = \frac{2\pi}{\hbar}\left|V_{fi}\right|^2 \delta(E_f - E_i). \tag{A.33}$$

The above assumes that the final state is discrete, but it is more common for the final states to form a continuum defined by the density of states $\rho(E)$ derived in Section A.2 above. In this case, since $\rho(E)\mathrm{d}E$ is the number of states with energy between $E$ and $E + \mathrm{d}E$, we can write the transition rate per unit time $\mathrm{d}T_{fi}/\mathrm{d}t$ to a group of states $f$ with energies in this range as

$$\frac{\mathrm{d}T_{fi}}{\mathrm{d}t} = \int \frac{\mathrm{d}P_{fi}(t)}{\mathrm{d}t}\rho(E_f)\mathrm{d}E_f = \frac{2\pi}{\hbar}\left[\left|V_{fi}\right|^2 \rho(E_f)\right]_{E_f=E_i}, \tag{A.34}$$

where the integral has been evaluated using the properties of the delta function. Equation (A.34) is called the Second Golden Rule (sometimes Fermi's Second Golden Rule, although strictly the result is not due to Fermi) and has been used in several places in this book, for example in Chapter 7 when discussing nuclear $\beta$-decay.