Supplement 4-A

The Wentzel-Kramers-Brillouin-Jeffreys Approximation

This approximation method is particularly useful when one is dealing with slowly varying potentials. Exactly what this means will become clear later. One wants to solve the equation

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0 \tag{4A-1}$$

and to do so, it is useful to write

$$\psi(x) = R(x)e^{iS(x)/\hbar} \tag{4A-2}$$

Then

$$\frac{d^2\psi}{dx^2} = \left[\frac{d^2R}{dx^2} + \frac{2i}{\hbar}\frac{dR}{dx}\frac{dS}{dx} + \frac{i}{\hbar}R\frac{d^2S}{dx^2} - \frac{1}{\hbar^2}R\left(\frac{dS}{dx}\right)^2\right]e^{iS(x)/\hbar} \tag{4A-3}$$

so that the differential equation splits into two, by taking the real and imaginary part of (4A-1) after (4A-3) has been substituted. The imaginary part gives

$$R\frac{d^2S}{dx^2} + 2\frac{dR}{dx}\frac{dS}{dx} = 0 \tag{4A-4}$$

that is,

$$\frac{d}{dx}\left(\log\frac{dS}{dx} + 2\ \log\ R\right) = 0$$

whose solution is

$$\frac{dS}{dx} = \frac{C}{R^2} \tag{4A-5}$$

The real part reads

$$\frac{d^2R}{dx^2} - \frac{1}{\hbar^2}R\left(\frac{dS}{dx}\right)^2 + \frac{2m[E - V(x)]}{\hbar^2}R = 0$$

which, when (4A-5) is substituted, becomes

$$\frac{d^2R}{dx^2} - \frac{C^2}{\hbar^2}\frac{1}{R^3} + \frac{2m[E - V(x)]}{\hbar^2}R = 0 \tag{4A-6}$$

At this point we make the approximation that

$$\frac{1}{R}\frac{d^2R}{dx^2} \ll \frac{C^2}{\hbar^2}\frac{1}{R^4} = \frac{1}{\hbar^2}\left(\frac{dS}{dx}\right)^2 \tag{4A-7}$$

so that the equation becomes

$$\frac{C^2}{R^4} = 2m[E - V(x)] \tag{4A-8}$$

Thus

$$\frac{C}{R^2} = \frac{dS}{dx} = \sqrt{2m[E - V(x)]} \tag{4A-9}$$

and hence

$$S(x) = \int_{x_1}^{x} dy \sqrt{2m[E - V(x)]} \tag{4A-10}$$

The condition for the validity can be translated into a statement about the variation of $V(x)$. It will be satisfied if $V(x)$ varies slowly in a wavelength, which varies from point to point, but which for slowly varying $V(x)$ is defined by

$$\lambdabar(x) = \frac{\hbar}{p(x)} = \frac{\hbar}{\{2m[E - V(x)]\}^{1/2}} \tag{4A-11}$$

At the points where

$$E - V(x) = 0 \tag{4A-12}$$

special treatment is required, because in the approximate equation (4A-8) $R(x)$ appears to be singular. This cannot be, which means that the approximation (4A-7) must be poor there. The special points are called *turning points* because it is there that a classical particle would turn around: It can only move where $E - V(x) \geq 0$. The way of handling solutions near turning points is a little too technical to be presented here. The basic idea is that we have a solution to the left of the turning point [where $E > V(x)$, say], of the form

$$\psi(x) = R(x)\exp\left\{ i\int_{x_1}^{x} dy\sqrt{2m(E - V(y))/\hbar^2} \right\} \tag{4A-13}$$

and a solution to the right of the turning point [where $E < V(x)$], and what we need is a formula that interpolates between them. In the vicinity of the turning point one can approximate $\sqrt{(2m/\hbar^2)[E - V(x)]}$ by a straight line over a small interval, and solve the Schrödinger equation exactly. Since it is a second-order equation, there are two adjustable constants, one that is fixed by fitting the solution to (4A-13) and the other by fitting it to

$$\psi(x) = R(x)\exp\left\{ -\int_{x_1}^{x} dy\sqrt{2m(V(y)) - E/\hbar^2} \right\} \tag{4A-14}$$

the solution to the right of the turning point.[1] The preceding solution decreases in amplitude as x increases. The total attenuation at the next turning point, when $E \geq V(x)$ again, is

$$\frac{\psi(x_{II})}{\psi(x_I)} \simeq \exp\left\{ -\int_{x_1}^{x_{II}} dy\sqrt{2m(V(y) - E)/\hbar^2} \right\} \tag{4A-15}$$

which is just the square root of the transmission probability that we found in Chapter 4.

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[1]For more details, see almost any of the more advanced books on quantum mechanics—for example, J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesley, Reading, Mass., 1961; L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1968.

Tunneling in Nuclear Physics

Tunneling is important in nuclear physics. Nuclei are very complicated objects, but under certain circumstances it is appropriate to view nucleons as independent particles occupying levels in a potential well. With this picture in mind, the decay of a nucleus into an α-particle (a He nucleus with $Z = 2$) and a daughter nucleus can be described as the tunneling of an α-particle through a barrier caused by the Coulomb potential between the daughter and the α-particle (Fig. 4B-1). The α-particle is not viewed as being in a bound state: if it were, the nucleus could not decay. Rather, the α-particle is taken to have positive energy, and its escape is only inhibited by the existence of the barrier.[1]

If we write

$$|T|^2 = e^{-G} \tag{4B-1}$$

then

$$G = 2\left(\frac{2m}{\hbar^2}\right)^{1/2} \int_R^b dr \sqrt{\frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r} - E} \tag{4B-2}$$

where R is the nuclear radius[2] and b is the turning point, determined by the vanishing of the integrand (4B-2); Z_1 is the charge of the daughter nucleus, and Z_2 ($= 2$ here) is the charge of the particle being emitted. The integral can be done exactly

$$\int_R^b dr \left(\frac{1}{r} - \frac{1}{b}\right)^{1/2} = \sqrt{b}\left[\cos^{-1}\left(\frac{R}{b}\right)^{1/2} - \left(\frac{R}{b} - \frac{R^2}{b^2}\right)^{1/2}\right] \tag{4B-3}$$

At low energies (relative to the height of the Coulomb barrier at $r = R$), we have $b \gg R$, and then

$$G = \frac{2}{\hbar}\left(\frac{2mZ_1 Z_2 e^2 b}{4\pi\varepsilon_0}\right)^{1/2}\left[\frac{\pi}{2} - \sqrt{\frac{R}{b}}\right] \tag{4B-4}$$

with $b = Z_1 Z_2 e^2 / 4\pi\varepsilon_0 E$. If we write for the α-particle energy $E = mv^2/2$, where v is its final velocity, then

$$G = \frac{2\pi Z_1 Z_2 e^2}{4\pi\varepsilon_0 \hbar v} = 2\pi\alpha Z_1 Z_2 \left(\frac{c}{v}\right) \tag{4B-5}$$

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[1]If you find it difficult to imagine why a repulsion would keep two objects from separating, think of the inverse process, α capture. It is clear that the barrier will tend to keep the α-particle out.

[2]In fact, early estimations of the nuclear radius came from the study of α-decay. Nowadays one uses the size of the charge distribution as measured by scattering electrons off nuclei to get nuclear radii. It is not clear that the two should be expected to give exactly the same answer.
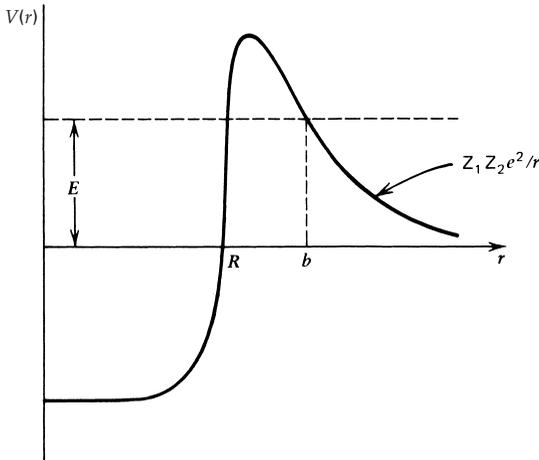
Figure 4B-1 Potential barrier for α decay.

The time taken for an α-particle to get out of the nucleus may be estimated as follows: the probability of getting through the barrier on a single encounter is e^{-G}. Thus the number of encounters needed to get through is $n \simeq e^{G}$. The time between encounters is of the order of $2R/v$, where R is again the nuclear radius, and v is the α velocity inside the nucleus. Thus the lifetime is

$$\tau \simeq \frac{2R}{v}\,e^{G} \tag{4B-6}$$

The velocity of the α inside the nucleus is a rather fuzzy concept, and the whole picture is very classical, so that the factor in front of the e^{G} cannot really be predicted without a much more adequate theory. Our considerations do give us an order of magnitude for it. For a 1-MeV α-particle,

$$v = \sqrt{\frac{2E}{m}} = c\sqrt{\frac{2E}{mc^2}} = 3 \times 10^8 \sqrt{\frac{2}{4 \times 940}} \simeq 7.0 \times 10^6 \text{ m/s}$$

so that one predicts, for low energy α's, the straight-line plot

$$\log_{10}\frac{1}{\tau} \simeq \text{const} - 1.73\,\frac{Z_1}{\sqrt{E(\text{MeV})}} \tag{4B-7}$$
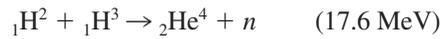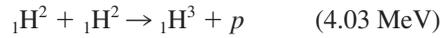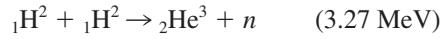
with the constant in front of the order of magnitude 27–28 when τ is measured in years instead of seconds. A large collection of data shows that a good fit to the lifetime data is obtained with the formula

$$\log_{10}\frac{1}{\tau} = C_2 - C_1\,\frac{Z_1}{\sqrt{E}} \tag{4B-8}$$

Here $C_1 = 1.61$ and C_2 lying between 55 and 62. The exponential part of the fit differs slightly from our derivation, but given the simplicity of our model, the agreement has to be rated as good.

For larger α energies, the G factor depends on R, and with $R = r_0 A^{1/3}$, one finds that r_0 is a constant—that is, that the notion of a Coulomb barrier taking over the role of the potential beyond the nuclear radius has some validity. Again, simple qualitative considerations explain the data.

The fact that the probability of a reaction (e.g., capture) between nuclei is attenuated by the factor $e^{-2(Z_1 Z_2/\sqrt{E})}$ ($Z_2 = 2$ for α's) implies that at low energies and/or for high Z's such reactions are rare. That is why all attempts to make thermonuclear reactors concentrate on the burning of hydrogen (actually heavy hydrogen–deuterium).

$$_1H^2 + {}_1H^2 \rightarrow {}_2He^3 + n \qquad (3.27 \text{ MeV})$$
$$_1H^2 + {}_1H^2 \rightarrow {}_1H^3 + p \qquad (4.03 \text{ MeV})$$
$$_1H^2 + {}_1H^3 \rightarrow {}_2He^4 + n \qquad (17.6 \text{ MeV})$$

since reactions involving higher Z elements would require much higher energies, that is, much higher temperatures, with correspondingly greater confinement problems. For the same reason, neutrons are used in nuclear reactors to fission the heavy elements. Protons, at the low energies available, would not be able to get near enough to the nuclei to react with them.

Periodic Potentials

Metals generally have a crystalline structure; that is, the ions are arranged in a way that exhibits a spatial periodicity. In our one-dimensional discussion of this topic, we will see that this periodicity has two effects on the motion of the free electrons in the metal. One is that for a perfect *lattice*—that is, for ions spaced equally—the *electron propagates without reflection*; the other is that there are restrictions on the energies allowed for the electrons; that is, *there are allowed and forbidden energy "bands."*

We begin with a discussion of the consequences of perfect periodicity.

The periodicity will be built into the potential, for which we require that

$$V(x + a) = V(x) \tag{4C-1}$$

Since the kinetic energy term $-(\hbar^2/2m)(d^2/dx^2)$ is unaltered by the change $x \rightarrow x + a$, the whole *Hamiltonian is invariant under displacements by a*. For the case of zero potential, when the solution corresponding to a given energy $E = \hbar^2 k^2/2m$ is

$$\psi(x) = e^{ikx} \tag{4C-2}$$

the displacement yields

$$\psi(x + a) = e^{ik(x+a)} = e^{ika}\psi(x) \tag{4C-3}$$

that is, the original solution multiplied by a phase factor, so that

$$|\psi(x + a)|^2 = |\psi(x)|^2 \tag{4C-4}$$

The observables will therefore be the same at x as at $x + a$; that is, we cannot tell whether we are at x or at $x + a$. In our example we shall also insist that $\psi(x)$ and $\psi(x + a)$ differ only by a phase factor, which need not, however, be of the form e^{ika}.

We digress briefly to discuss this requirement more formally. The invariance of the Hamiltonian under a displacement $x \rightarrow x + a$ can be treated formally as follows. Let D_a be an operator whose rule of operation is that

$$D_a f(x) = f(x + a) \tag{4C-5}$$

The invariance implies that

$$[H, D_a] = 0 \tag{4C-6}$$

We can find the eigenvalues of this operator by noting that

$$D_a \psi(x) = \lambda_a \psi(x) \tag{4C-7}$$

together with

$$D_{-a}D_a f(x) = D_a D_{-a} f(x) = f(x) \tag{4C-8}$$

implies that $\lambda_a \lambda_{-a} = 1$. This then implies that λ_a must be of the form e^{iqa}. Here q must be real, because if q had an imaginary part, a succession of displacements by a would make the wave function larger and larger with each displacement in one or the other direction.

Consider now a simultaneous eigenfunction of H and D_a, and define

$$u(x) = e^{-iqx}\psi(x) \tag{4C-9}$$

Then, using the fact that $\lambda_a = e^{iqa}$, we get

$$D_a u(x) = e^{-iq(x+a)}D_a\psi(x) = e^{-iq(x+a)}e^{iqa}\psi(x) = e^{-iqx}\psi(x) = u(x) \tag{4C-10}$$

This means that $u(x)$ is a periodic function obeying $u(x + a) = u(x)$. The upshot is that a function which is a simultaneous eigenfunction of H and D_a must be of the form

$$\psi(x) = e^{iqx}u(x) \tag{4C-11}$$

with $u(x)$ periodic. This result is known as *Bloch's Theorem*.

For a free particle $q = k$, the wave number corresponds to the energy E. More generally, the relation between q and k is more complicated. In any case, it is clear that (4C-4) holds, so that the net flux is unchanged as we go from x to $x + a$, and by extension to $x + na$. This means that an electron propagates without a change in flux.

Let us consider a series of ions in a line, with their centers located at $x = na$. To avoid having to deal with *end effects*, we assume that there are N ions placed on a very large ring, so that $n = 1$ and $n = N + 1$ are the same site. We will assume that the most loosely bound electrons—the ones that are viewed as "free"—are still sufficiently strongly bound to the ions that their wave functions do not overlap more than one or two nearest neighbors. We may now ask: What is the effect of this overlap on the energies of the electrons?

To answer this question, we consider first a classical analogy. We represent the electrons at the different sites by simple harmonic oscillators, all oscillating with the same angular frequency ω. In the absence of any coupling between the oscillators, we have the equation of motion

$$\frac{d^2x_n}{dt^2} = -\omega^2 x_n \qquad (n = 0, 1, 2, \ldots) \tag{4C-12}$$

If the harmonic oscillators are coupled to their nearest neighbors, then the equation is changed to

$$\frac{d^2x_n}{dt^2} = -\omega^2 x_n - K[(x_n - x_{n-1}) + (x_n - x_{n+1})] \tag{4C-13}$$

To solve this we write down a trial solution

$$x_n = A_n \cos \Omega t \tag{4C-14}$$

When this is substituted into (4C-13), we get

$$(\omega^2 - \Omega^2)A_n = -K(2A_n - A_{n-1} - A_{n+1}) \tag{4C-15}$$

This is known as a *difference equation*. We solve it by a trial solution. Let us assume that

$$A_n = L^n \tag{4C-16}$$

The identification of the sites at $n = 1$ and $N + 1$ implies $A_1 = A_{N+1}$ so that $L^N = 1$. This means that

$$L = e^{2\pi i r/N} \qquad r = 0, 1, 2, \ldots, (N - 1) \tag{4C-17}$$

The equation for the frequency Ω now yields

$$\omega^2 - \Omega^2 = -2K\left(1 - \cos\frac{2\pi r}{N}\right) = -4K\,\sin^2\frac{\pi r}{N}$$

The result

$$\Omega^2 = \omega^2 + 4K\,\sin^2\frac{\pi r}{N} \tag{4C-18}$$

shows that the frequencies, which, without coupling are all ω—that is, are *N-fold degenerate* (which corresponds to all the pendulums moving together)—are now spread over a range from ω to $\sqrt{\omega^2 + 4K}$. For large N there are many such frequencies, and they can be said to form a *band*. If we think of electrons as undergoing harmonic oscillations about their central locations, we can translate the above into a statement that in the absence of neighbors, all electron energies are degenerate, and the interaction with neighboring atoms spreads the energy values. We can, of course, have several fundamental frequencies $\omega_1, \omega_2, \ldots$, and different couplings to their neighbors, with strengths $K_1, K_2, \ldots$, which will then give rise to several bands that may or may not overlap.

The spreading of the frequencies is the same effect as the spreading of the energy levels of the most loosely bound electrons. For atoms far apart, with spacing larger than the exponential fall-off of the wave functions, all the energies are the same so that we have an N-fold degenerate single energy. Because the atoms are not so far apart, there is some coupling between nearest neighbors, and the energy levels spread. The classical analogy is suggestive, but not exact, since for the quantum case levels are pushed up as well as down, whereas all the frequencies above, lie above ω. Later we solve the Kronig-Penney model in which the potential takes the form

$$V(x) = \frac{\hbar^2}{2m}\frac{\lambda}{a}\sum_{-\infty}^{\infty}\delta(x - na) \tag{4C-19}$$

The solution can be shown to lead to a condition on q, which reads

$$\cos\,qa = \cos\,ka + \frac{1}{2}\lambda\,\frac{\sin\,ka}{ka} \tag{4C-20}$$

As can be seen from Figure (4C-1), this clearly shows the energy band structure.

THE KRONIG-PENNEY MODEL

To simplify the algebra, we will take a series of repulsive delta-function potentials,

$$V(x) = \frac{\hbar^2}{2m}\frac{\lambda}{a}\sum_{n=-\infty}^{\infty}\delta(x - na) \tag{4C-21}$$

Away from the points $x = na$, the solution will be that of the free-particle equation—that is, some linear combination of $\sin kx$ and $\cos kx$ (we deal with real functions for simplicity). Let us assume that in the region R_n defined by $(n - 1)\,a \le x \le na$, we have

$$\psi(x) = A_n\,\sin\,k(x - na) + B_n\,\cos\,k(x - na) \tag{4C-22}$$

and in the region R_{n+1} defined by $na \le x \le (n + 1)\,a$ we have

$$\psi(x) = A_{n+1}\,\sin\,k[x - (n + 1)\,a] + B_{n+1}\,\cos\,k[x - (n + 1)\,a] \tag{4C-23}$$
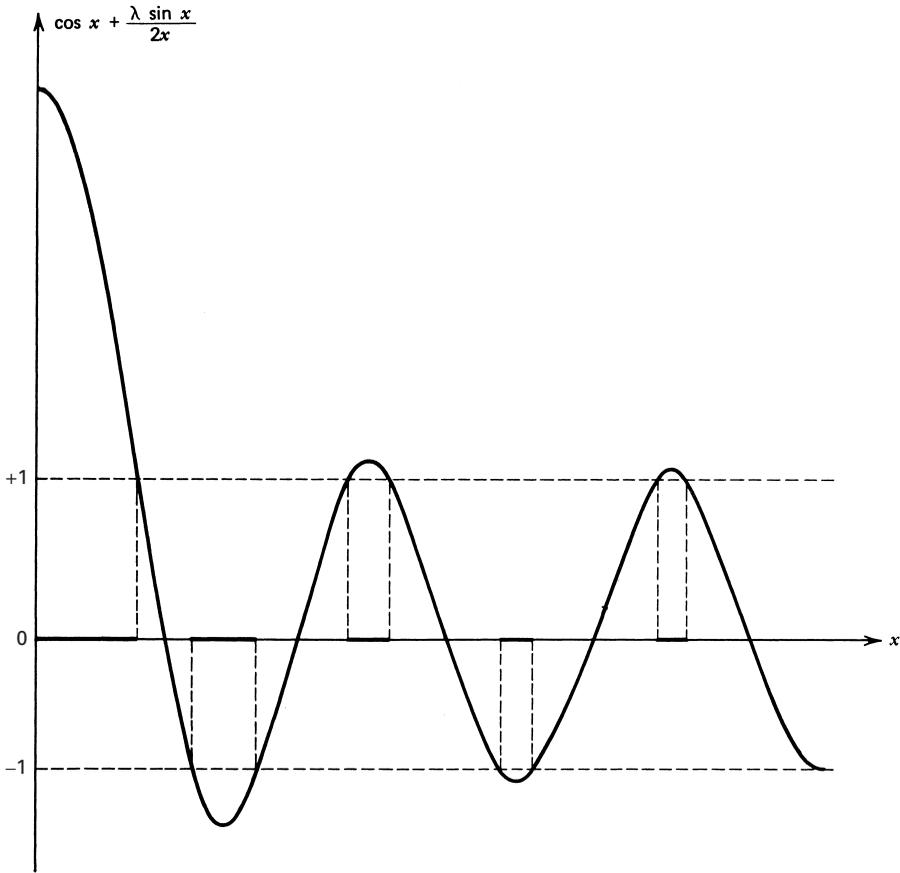
Figure 4C-1 Plot of $\cos x + (\lambda/2)(\sin x/x)$ as a function of x. The horizontal lines represent the bounds ± 1. The regions of x for which the curve lines outside the strip are forbidden.

Continuity of the wave function implies that $(x = na)$

$$-A_{n+1} \sin ka + B_{n+1} \cos ka = B_n \tag{4C-24}$$

and the discontinuity condition (4-68) here reads

$$kA_{n+1} \cos ka + kB_{n+1} \sin ka - kA_n = \frac{\lambda}{a} B_n \tag{4C-25}$$

A little manipulation yields

$$A_{n+1} = A_n \cos ka + (g \cos ka - \sin ka) B_n$$
$$B_{n+1} = (g \sin ka + \cos ka) B_n + A_n \sin ka \tag{4C-26}$$

where $g = \lambda/ka$.

The requirement from Bloch's theorem that

$$\psi(x + a) = e^{iq(x+a)}u(x + a) = e^{iq(x+a)} u(x) = e^{iqa}\psi(x) \tag{4C-27}$$

implies that the wave functions in the adjacent regions R_n and R_{n+1} are related, since the wave function in (4C-22) may be written as

$$\psi(x) = A_n\sin[k((x+a)-(n+1)a]+B_n\cos k[k((x+a)-(n+1)a]$$

which is identical to that in (4C-23), provided

$$A_{n+1} = e^{iqa} A_n$$
$$B_{n+1} = e^{iqa} B_n \qquad \text{(4C-28)}$$

When this is inserted into the (4C-26), that is, into the conditions that the wave equation obeys the Schrödinger equation with the delta function potential, we get

$$A_n(e^{iqa} - \cos ka) = B_n(g \cos ka - \sin ka)$$
$$B_n(e^{iqa} - (g \sin ka + \cos ka)) = A_n \sin ka \qquad \text{(4C-29)}$$

This leads to the condition

$$(e^{iqa} - \cos ka)(e^{iqa} - (g \sin ka + \cos ka)) = \sin ka(g \cos ka - \sin ka) \quad \text{(4C-30)}$$

This may be rewritten in the form

$$e^{2iqa} - 2(\cos ka + \frac{g}{2} \sin ka)e^{iqa} + 1 = 0 \qquad \text{(4C-31)}$$

This quadratic equation can be solved, and both real and imaginary parts lead to the condition

$$\cos\ qa = \cos ka + \frac{\lambda}{2} \frac{\sin ka}{ka} \qquad \text{(4C-32)}$$

This is a very interesting result, because the left side is always bounded by 1; that is, there are restrictions on the possible ranges of the energy $E = \hbar^2k^2/2m$ that depend on the parameters of our "crystal." Figure 4C-1 shows a plot of the function $\cos x + \lambda \sin x/2x$ as a function of $x = ka$. The horizontal line represents the bounds on $\cos qa$, and the regions of x, for which the curve lies outside the strip, are forbidden regions. Thus there are *allowed energy bands* separated by regions that are forbidden. Note that the onset of a forbidden band corresponds to the condition

$$qa = n\pi \qquad n = \pm 1, \pm 2, \pm 3, \ldots \qquad \text{(4C-33)}$$

This, however, is just the condition for Bragg reflection with normal incidence. The existence of energy gaps can be understood qualitatively. In first approximation the electrons are free, except that there will be Bragg reflection when the waves reflected from successive atoms differ in phase by an integral number of 2π—that is, when (4C-33) is satisfied. These reflections give rise to standing waves, with even and odd waves of the form $\cos \pi x/a$ and $\sin \pi x/a$, respectively. The energy levels corresponding to these standing waves are degenerate. Once the attractive interaction between the electrons and the positively charged ions at $x = ma$ (m integer) is taken into account, the even states, peaked in between, will move up in energy. Thus the energy degeneracy is split at $q = n\pi/a$, and this leads to energy gaps, as shown in Fig. 4C-1.

The Kronig-Penney model has some relevance to the theory of metals, insulators, and semiconductors if we take into account the fact (to be studied later) that energy levels

occupied by electrons cannot accept more electrons. Thus a metal may have an energy band partially filled. If an external field is applied, the electrons are accelerated, and if there are momentum states available to them, the electrons will occupy the momentum states under the influence of the electric field. Insulators have completely filled bands, and an electric field cannot accelerate electrons, since there are no neighboring empty states. If the electric field is strong enough, the electrons can "jump" across a forbidden energy gap and go into an empty allowed energy band. This corresponds to the breakdown of an insulator. The semiconductor is an insulator with a very narrow forbidden gap. There, small changes of conditions, such as a rise in temperature, can produce the "jump" and the insulator becomes a conductor.

The band structure is of great relevance in solid state physics. Fig. 4C-2 shows three situations that can arise when energy levels are filled with electrons. We shall learn in Chapter 13 that only two electrons are allowed per energy level. In case (*a*) the electrons fill all the energy levels below the edge of the energy gap. The application of a weak electric field will have no effect on the material. The electrons near the top of the filled band cannot be accelerated. There are no levels with higher energy available to them. Materials in which this occurs are *insulators*; that is, they do not carry currents when electric fields are applied. In case (*b*) the energy levels are only partly filled. In this case the application of an electric field accelerates the electrons at the top of the stack of levels. These electrons have empty energy levels to move into, and they would accelerate indefinitely in a perfect lattice, as stated in the previous section. What keeps them from doing that is *dissipation*. The lattice is not perfect for two reasons: one is the presence of impurities, which destroys the perfect periodicity; the other is the effect of thermal agitation on the position of the ions forming the lattice, which has the same effect of destroying perfect periodicity. Materials in which the energy levels below the gaps are only partially filled are *conductors*.

The width of the gaps in the energy spectrum depends on the materials. For some insulators the gaps are quite narrow. When this happens, then at finite temperatures T, there is a calculable probability that some of the electrons are excited to the bottom of the set of energy levels above the gap. (To good approximation the probability is proportional to the Boltzmann factor $e^{-E/kT}$). These electrons can be accelerated as in a conductor, so that the application of an electric field will give rise to a current. The current is augmented by another effect: the energy levels that had been occupied by the electrons promoted to the higher energy band (called the *conduction band*) are now empty. They provide vacancies into which electrons in the lower band (called the *valence band*) can be accelerated into,
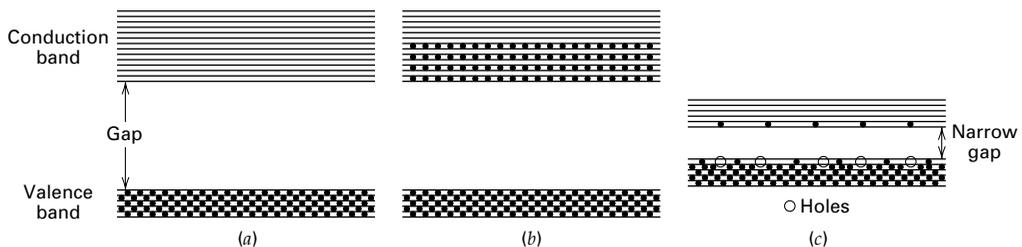

Figure 4C-2 Occupation of levels in the lowest two energy bands, separated by a gap. (*a*) Insulator has a completely filled band. Electrons cannot be accelerated into a nearby energy level. (*b*) Conductor has a half-filled band, allowing electrons to be accelerated into nearby energy levels. (*c*) In a semiconductor, thermal effects promote some electrons into a second band. These electrons can conduct electricity. The electrons leave behind them *holes* that act as positively charged particles and also conduct electricity.
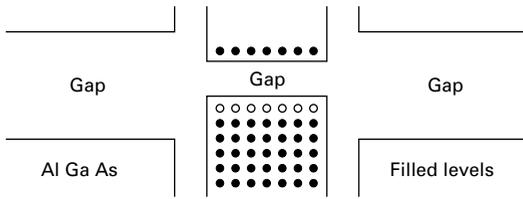
Figure 4C-3 Schematic picture of electrons and holes trapped in a well created by adjacent semiconductors with a wider gap. An example of such a heterostructure is provided by a layer of GaAs sandwiched between two layers of AlGaAs.

when an electric field is applied. These vacancies, called *holes*, propagate in the direction opposite to that of the electrons and thus add to the electric current. This is the situation shown in Fig. 4C-2(*c*).

The technology of making very thin layers of compounds of materials has improved in recent decades to such an extent that it is possible to create the analog of the infinite wells discussed in Chapter 3. Consider a "sandwich" created by two materials. The outer one has a larger energy gap than the inner one, as shown in Fig. 4C-3. The midpoints of the gaps must coincide[1] (for equilibrium reasons). The result is that both electrons and holes in the interior semiconductor cannot move out of the region between the outer semiconductors, because there are no energy levels that they can move to. Such confined regions may occur in one, two, or three dimensions. In the last case we deal with *quantum dots*. The study of the behavior of electrons in such confined regions is a very active field of research in the study of materials.

In summary, one-dimensional problems give us a very important glimpse into the physics of quantum systems in the real world of three dimensions.

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[1]A brief, semiquantitative discussion of this material may be found in *Modern Physics* by J. Bernstein, P. M. Fishbane, and S. Gasiorowicz (Prentice Hall, 2000). See also Chapter 44 in *Physics for Scientists and Engineers*, (2nd Edition) by P. M. Fishbane, S. Gasiorowicz and S. T. Thornton (Prentice Hall, 1996). There are, of course, many textbooks on semiconductors, which discuss the many devices that use *bandgap engineering* in great quantitative detail. See in particular L. Solymar and D. Walsh, *Lectures on the Electrical Properties of Materials*, Oxford University Press, New York (1998).