CHAPTER 4.

1. The solution to the left side of the potential region is $\psi(x) = Ae^{ikx} + Be^{-ikx}$. As shown in Problem 3-15, this corresponds to a flux

$$j(x) = \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right)$$

The solution on the right side of the potential is $\psi(x) = Ce^{ikx} + De^{-ikxx}$, and as above, the flux is

$$j(x) = \frac{\hbar k}{m}\left(|C|^2 - |D|^2\right)$$

Both fluxes are independent of *x*. Flux conservation implies that the two are equal, and this leads to the relationship

$$|A|^2 + |D|^2 = |B|^2 + |C|^2$$

If we now insert

$$C = S_{11}A + S_{12}D$$
$$B = S_{21}A + S_{22}D$$

into the above relationship we get

$$|A|^2 + |D|^2 = (S_{21}A + S_{22}D)(S_{21}^*A^* + S_{22}^*D^*) + (S_{11}A + S_{12}D)(S_{11}^*A^* + S_{12}^*D^*)$$

Identifying the coefficients of $|A|^2$ and $|D|^2$, and setting the coefficient of AD^* equal to zero yields

$$|S_{21}|^2 + |S_{11}|^2 = 1$$
$$|S_{22}|^2 + |S_{12}|^2 = 1$$
$$S_{12}S_{22}^* + S_{11}S_{12}^* = 0$$

Consider now the matrix

$$S^{tr} = \begin{pmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{pmatrix}$$

The unitarity of this matrix implies that

$$\begin{pmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{pmatrix}\begin{pmatrix} S_{11}^* & S_{12}^* \\ S_{21}^* & S_{22}^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

that is,

$$|S_{11}|^2 + |S_{21}|^2 = |S_{12}|^2 + |S_{22}|^2 = 1$$
$$S_{11}S_{12}^* + S_{21}S_{22}^* = 0$$

These are just the conditions obtained above. They imply that the matrix S^{tr} is unitary, and therefore the matrix S is unitary.

2. We have solve the problem of finding R and T for this potential well in the text.We take $V_0 < 0$. We dealt with wave function of the form

$$e^{ikx} + Re^{-ikx} \qquad x < -a$$

$$Te^{ikx} \qquad x > a$$

In the notation of Problem 4-1, we have found that if $A = 1$ and $D = 0$, then $C = S_{11} = T$ and $B = S_{21} = R$.. To find the other elements of the S matrix we need to consider the same problem with $A = 0$ and $D = 1$. This can be solved explicitly by matching wave functions at the boundaries of the potential hole, but it is possible to take the solution that we have and reflect the "experiment" by the interchange $x \rightarrow -x$. We then find that $S_{12} = R$ and $S_{22} = T$. We can easily check that

$$|S_{11}|^2 + |S_{21}|^2 = |S_{12}|^2 + |S_{22}|^2 = |R|^2 + |T|^2 = 1$$

Also

$$S_{11}S_{12}^* + S_{21}S_{22}^* = TR^* + RT^* = 2\,\mathrm{Re}(TR^*)$$

If we now look at the solutions for T and R in the text we see that the product of T and R^* is of the form (-i) x (real number), so that its real part is zero. This confirms that the S matrix here is unitary.

3. Consider the wave functions on the left and on the right to have the forms

$$\psi_L(x) = Ae^{ikx} + Be^{-ikx}$$
$$\psi_R(x) = Ce^{ikx} + De^{-ikx}$$

Now, let us make the change $k \rightarrow -k$ *and* complex conjugate everything. Now the two wave functions read

$$\psi_L(x)' = A^* e^{ikx} + B^* e^{-ikx}$$
$$\psi_R(x)' = C^* e^{ikx} + D^* e^{-ikx}$$

Now complex conjugation and the transformation $k \rightarrow -k$ changes the original relations to

$$C^* = S_{11}^*(-k)A^* + S_{12}^*(-k)D^*$$
$$B^* = S_{21}^*(-k)A^* + S_{22}^*(-k)D^*$$

On the other hand, we are now relating outgoing amplitudes C^*, B^* to ingoing amplitude A^*, D^*, so that the relations of problem 1 read

$$C^* = S_{11}(k)A^* + S_{12}(k)D^*$$
$$B^* = S_{21}(k)A^* + S_{22}(k)D^*$$

This shows that $S_{11}(k) = S_{11}^*(-k);\ \ S_{22}(k) = S_{22}^*(-k);\ \ S_{12}(k) = S_{21}^*(-k)$. These result may be written in the *matrix* form $\mathbf{S}(k) = \mathbf{S}^+(-k)$.

4. (a) With the given flux, the wave coming in from $x = -\infty$, has the form e^{ikx}, with unit amplitude. We now write the solutions in the various regions

$x < b$	$e^{ikx} + Re^{-ikx}$	$k^2 = 2mE/\hbar^2$
$-b < x < -a$	$Ae^{\kappa x} + Be^{-\kappa x}$	$\kappa^2 = 2m(V_0 - E)/\hbar^2$
$-a < x < c$	$Ce^{ikx} + De^{-ikx}$	
$c < x < d$	$Me^{iqx} + Ne^{-iqx}$	$q^2 = 2m(E + V_1)/\hbar^2$
$d < x$	Te^{ikx}	

(b) We now have

$x < 0$	$u(x) = 0$	
$0 < x < a$	$A\sin kx$	$k^2 = 2mE/\hbar^2$
$a < x < b$	$Be^{\kappa x} + Ce^{-\kappa x}$	$\kappa^2 = 2m(V_0 - E)/\hbar^2$
$b < x$	$e^{-ikx} + Re^{ikx}$	

The fact that there is total reflection at $x = 0$ implies that $|R|^2 = 1$

5. The denominator in (4-   ) has the form

$$D = 2kq\cos 2qa - i(q^2 + k^2)\sin 2qa$$

With $k = i\kappa$ this becomes

$$D = i\left(2\kappa q\cos 2qa - (q^2 - \kappa^2)\sin 2qa\right)$$

The denominator vanishes when

$$\tan 2qa = \frac{2\tan qa}{1-\tan^2 qa} = \frac{2q\kappa}{q^2-\kappa^2}$$

This implies that

$$\tan qa = -\frac{q^2-\kappa^2}{2\kappa q} \pm \sqrt{1+\left(\frac{q^2-\kappa^2}{2\kappa q}\right)^2} = -\frac{q^2-\kappa^2}{2\kappa q} \pm \frac{q^2+\kappa^2}{2\kappa q}$$

This condition is identical with (4-   ).

The argument why this is so, is the following: When $k = i\kappa$ the wave functio on the left has the form $e^{-\kappa x} + R(i\kappa)e^{\kappa x}$. The function $e^{-\kappa x}$ blows up as $x \to -\infty$ and the wave function only make sense if this term is overpowered by the other term, that is when $R(i\kappa) = \infty$. We leave it to the student to check that the numerators are the same at $k = i\kappa$.

6. The solution is $u(x) = Ae^{ikx} + Be^{-ikx} \quad x < b$

$= Ce^{ikx} + De^{-ikx} \quad x > b$

The continuity condition at $x = b$ leads to

$$Ae^{ikb} + Be^{-ikb} = Ce^{ikb} + De^{-ikb}$$

And the derivative condition is

$$(ikAe^{ikb} - ikBe^{-ikb}) - (ikCe^{ikb} - ikDe^{-ikb}) = (\lambda/a)(Ae^{ikb} + Be^{-ikb})$$

With the notation

$$Ae^{ikb} = \alpha\ ;\ Be^{-ikb} = \beta;\ Ce^{ikb} = \gamma;\ De^{-ikb} = \delta$$

These equations read

$$\alpha + \beta = \gamma + \delta$$

$$ik(\alpha - \beta + \gamma - \delta) = (\lambda/a)(\alpha + \beta)$$

We can use these equations to write (γ,β) in terms of (α,δ) as follows

$$\gamma = \frac{2ika}{2ika - \lambda}\alpha + \frac{\lambda}{2ika - \lambda}\delta$$
$$\beta = \frac{\lambda}{2ika - \lambda}\alpha + \frac{2ika}{2ika - \lambda}\delta$$

We can now rewrite these in terms of *A,B,C,D* and we get for the S matrix

$$S = \begin{pmatrix} \frac{2ika}{2ika - \lambda} & \frac{\lambda}{2ika - \lambda} e^{-2ikb} \\ \frac{\lambda}{2ika - \lambda} e^{2ikb} & \frac{2ika}{2ika - \lambda} \end{pmatrix}$$

Unitarity is easily established:

$$|S_{11}|^2 + |S_{12}|^2 = \frac{4k^2a^2}{4k^2a^2 + \lambda^2} + \frac{\lambda^2}{4k^2a^2 + \lambda^2} = 1$$
$$S_{11}S_{12}^* + S_{12}S_{22}^* = \left(\frac{2ika}{2ika - \lambda}\right)\left(\frac{\lambda}{-2ika - \lambda} e^{-2ikb}\right) + \left(\frac{\lambda}{2ika - \lambda} e^{-2ikb}\right)\left(\frac{-2ika}{-2ika - \lambda}\right) = 0$$

The matrix elements become infinite when $2ika = \lambda$. In terms of $\kappa = -ik$, this condition becomes $\kappa = -\lambda/2a = |\lambda|/2a$.

7. The exponent in $T = e^{-S}$ is

$$S = \frac{2}{\hbar}\int_A^B dx\sqrt{2m(V(x) - E)}$$
$$= \frac{2}{\hbar}\int_A^B dx\sqrt{(2m(\frac{m\omega^2}{2}(x^2 - \frac{x^3}{a})) - \frac{\hbar\omega}{2}}$$

where *A* and *B* are turning points, that is, the points at which the quantity under the square root sign vanishes.
We first simplify the expression by changing to dimensionless variables:

$$x = \sqrt{\hbar/m\omega}y; \quad \eta = a/\sqrt{\hbar/m\omega} << 1$$

The integral becomes

$$2\int_{y_1}^{y_2} dy\sqrt{y^2 - \eta y^3 - 1} \qquad \text{with} \quad \eta \ll 1$$

where now y_1 and y_2 are the turning points. A sketch of the potential shows that y_2 is very large. In that region, the –1 under the square root can be neglected, and to a good approximation $y_2 = 1/\eta$. The other turning point occurs for y not particularly large, so that we can neglect the middle term under the square root, and the value of y_1 is 1. Thus we need to estimate

$$\int_1^{1/\eta} dy\sqrt{y^2 - \eta y^3 - 1}$$

The integrand has a maximum at $2y - 3\eta y^2 = 0$, that is at $y = 2\eta/3$. We estimate the contribution from that point on by neglecting the –1 term in the integrand. We thus get

$$\int_{2/3\eta}^{1/\eta} dy\, y\sqrt{1-\eta y} = \frac{2}{\eta^2}\left[\frac{(1-\eta y)^{5/2}}{5} - \frac{(1-\eta y)^{3/2}}{3}\right]_{2/3\eta}^{1/\eta} = \frac{8\sqrt{3}}{135}\frac{1}{\eta^2}$$

To estimate the integral in the region $1 < y < 2/3\eta$ is more difficult. In any case, we get a lower limit on S by just keeping the above, so that

$$S > 0.21/\eta^2$$

The factor e^S must be multiplied by a characteristic time for the particle to move back and forth inside the potential with energy $\hbar\omega/2$ which is necessarily of order $1/\omega$. Thus the estimated time is *longer* than $\frac{const.}{\omega}e^{0.2/\eta^2}$.

8. The barrier factor is e^S where

$$S = \frac{2}{\hbar}\int_{R_0}^{b} dx\sqrt{\frac{\hbar^2 l(l+1)}{x^2} - 2mE}$$

where b is given by the value of x at which the integrand vanishes, that is, with $2mE/\hbar^2 = k^2$, $b = \sqrt{l(l+1)}/k$. We have, after some algebra

$$S = 2\sqrt{l(l+1)}\int_{R_0/b}^{1}\frac{du}{u}\sqrt{1-u^2}$$
$$= 2\sqrt{l(l+1)}\left[\ln\frac{1+\sqrt{1-(R_0/b)^2}}{R_0/b} - \sqrt{1-(R_0/b)^2}\right]$$

We now introduce the variable $f = (R_0/b) \approx kR_0/l$ for large l. Then

$$e^S e^S = \left[\frac{1+\sqrt{1-f^2}}{f}\right]^{2l} e^{-2l\sqrt{1-f^2}} \approx \left(\frac{e}{2}\right)^{-2l} f^{-2l}$$

for $f << 1$. This is to be multiplied by the time of traversal inside the box. The important factor is f^{2l}. It tells us that the lifetime is proportional to $(kR_0)^{-2l}$ so that it grows as a power of l for small k. Equivalently we can say that the probability of decay falls as $(k\mathrm{R}_0)^{2l}$.

9. The argument fails because the electron is not localized inside the potential. In fact, for weak binding, the electron wave function extends over a region $R = 1/\alpha = \hbar\sqrt{2mE_B}$, which, for weak binding is much larger than a.

10. For a bound state, the solution for $x > a$ must be of the form $u(x) = Ae^{-\alpha x}$, where $\alpha = \sqrt{2mE_B}/\hbar$. Matching $\frac{1}{u}\frac{du}{dx}$ at $x = a$

yields $-\alpha = f(E_B)$. If $f(E)$ is a constant, then we immediately know α.. Even if $f(E)$ varies only slightly over the energy range that overlaps small positive E, we can determine the binding energy in terms of the reflection coefficient. For positive energies the wave function $u(x)$ for $x > a$ has the form $e^{-ikx} + R(k)e^{ikx}$, and matching yields

$$f(E) \approx -\alpha = -ik\frac{e^{-ika} - Re^{ika}}{e^{-ika} + Re^{ika}} = -ik\frac{1 - Re^{2ika}}{1 + Re^{2ika}}$$

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so that

$$R = e^{-2ika}\frac{k + i\alpha}{k - i\alpha}$$

We see that $|R|^2 = 1$.

11. Since the well is symmetric about $x = 0$, we need only match wave functions at $x = b$ and a. We look at $E < 0$, so that we introduce and $\alpha^2 = 2m|E|/\hbar^2$ and $q^2 = 2m(V_0-|E|)/\hbar^2$. We now write down

Even solutions:

$$\begin{aligned} u(x) &= \cosh\alpha x & 0 < x < b \\ &= A\sin qx + B\cos qx & b < x < a \\ &= C\,e^{-\alpha x} & a < x \end{aligned}$$

Matching $\frac{1}{u(x)}\frac{du(x)}{dx}$ at $x = b$ and at $x = a$ leads to the equations

$$\alpha \tanh \alpha b = q\frac{A\cos qb - B\sin qb}{A\sin qb + B\cos qb}$$

$$-\alpha = q\frac{A\cos qa - Bsnqa}{A\sin qa + B\cos qa}$$

From the first equation we get

$$\frac{B}{A} = \frac{q\cos qb - \alpha \tanh \alpha b \sin qb}{q\sin qb + \alpha \tanh \alpha b \cos qb}$$

and from the second

$$\frac{B}{A} = \frac{q\cos qa + \alpha \sin qa}{q\sin qa - \alpha \cos qa}$$

Equating these, cross-multiplying, we get after a little algebra

$$q^2 \sin q(a-b) - \alpha \cos q(a-b) = \alpha \tanh \alpha b[\alpha \sin q(a-b) + q\cos q(a-b)]$$

from which it immediately follows that

$$\frac{\sin q(a-b)}{\cos q(a-b)} = \frac{\alpha q(\tanh \alpha b + 1)}{q^2 - \alpha^2 \tanh \alpha b}$$

Odd Solution

Here the only difference is that the form for $u(x)$ for $0 < x < b$ is $\sinh \alpha x$. The result of this is that we get the same expresion as above, with $\tanh \alpha b$ replaced by $\coth \alpha b$.

11. (a) The condition that there are at most two bound states is equivalent to stating that there is at most one *odd* bound state. The relevant figure is Fig. 4-8, and we ask for the condition that there be no intersection point with the tangent curve that starts up at $3\pi/2$. This means that

$$\frac{\sqrt{\lambda - y^2}}{y} = 0$$

for $y \le 3\pi/2$. This translates into $\lambda = y^2$ with $y < 3\pi/2$, i.e. $\lambda < 9\pi^2/4$.
(b) The condition that there be at most three bound states implies that there be at most two *even* bound states, and the relevant figure is 4-7. Here the conditon is that $y < 2\pi$ so that $\lambda < 4\pi^2$.

(c) We have $y = \pi$ so that the second *even* bound state have zero binding energy. This means that $\lambda = \pi^2$. What does this tell us about the first bound state? All we know is that y is a solution of Eq. (4-54) with $\lambda = \pi^2$. Eq.(4-54) can be rewritten as follows:

$$\tan^2 y = \frac{1-\cos^2 y}{\cos^2 y} = \frac{\lambda - y^2}{y^2} = \frac{1-(y^2/\lambda)}{(y^2/\lambda)}$$

so that the *even* condition is $\cos y = y/\sqrt{\lambda}$, and in the same way, the *odd* conditin is $\sin y = y/\sqrt{\lambda}$. Setting $\sqrt{\lambda} = \pi$ still leaves us with a transcendental equation. All we can say is that the binding energy f the even state will be larger than that of the odd one.

13.(*a*) As $b \to 0$, $\tan q(a-b) \to \tan qa$ and the r.h.s. reduces to α/q. Thus we get, for the even solution

$$\tan qa = \alpha/q$$

and, for the odd solution,

$$\tan qa = -q/\alpha.$$

These are just the single well conditions.

(b) This part is more complicated. We introduce notation $c = (a-b)$, which will be held fixed. We will also use the notation $z = \alpha b$. We will also use the subscript "1" for the even solutions, and "2" for the odd solutions. For b large,

$$\tanh z = \frac{e^z - e^{-z}}{e^z + e^{-z}} = \frac{1-e^{-2z}}{1+e^{-2z}} \approx 1 - 2e^{-2z}$$
$$\coth z \approx 1 = 2e^{-2z}$$

The eigenvalue condition for the even solution now reads

$$\tan q_1 c = \frac{q_1\alpha_1(1+1-2e^{-2z_1})}{q_1^2 - \alpha_1^2(1-2e^{-2z_1})} \approx \frac{2q_1\alpha_1}{q_1^2-\alpha_1^2}(1 - \frac{q_1^2+\alpha_1^2}{q_1^2-\alpha_1^2}e^{-2z_1})$$

The condition for the odd solution is obtained by just changing the sign of the e^{-2z} term, so that

$$\tan q_2 c = \frac{q_2\alpha_2(1+1+2e^{-2z_2})}{q_2^2\alpha_2^2(1+2e^{-2z_2})} \approx \frac{2q_2\alpha_2}{q_2^2-\alpha_2^2}(1 + \frac{q_2^2+\alpha_2^2}{q_2^2-\alpha_2^2}e^{-2z_2})$$

In both cases $q^2 + \alpha^2 = 2mV_0/\hbar^2$ is fixed. The two eigenvalue conditions only differ in the e^{-2z} terms, and the difference in the eigenvalues is therefore proportional to e^{-2z} , where z here is some mean value between $\alpha_1 b$ and $\alpha_2 b$.
This can be worked out in more detail, but this becomes an exercise in Taylor expansions with no new physical insights.

14. We write

$$\langle x\frac{dV(x)}{dx}\rangle = \int_{-\infty}^{\infty} dx\, \psi(x) x \frac{dV(x)}{dx}\psi(x)$$
$$= \int_{-\infty}^{\infty} dx\left[\frac{d}{dx}\left(\psi^2 xV\right) - 2\psi\frac{d\psi}{dx}xV - \psi^2 V\right]$$

The first term vanishes because ψ goes to zero rapidly. We next rewrite

$$-2\int_{-\infty}^{\infty} dx\frac{d\psi}{dx}xV\psi = -2\int_{-\infty}^{\infty} dx\frac{d\psi}{dx}x(E + \frac{\hbar^2}{2m}\frac{d^2}{dx^2})\psi$$
$$= -E\int_{-\infty}^{\infty} dxx\frac{d\psi^2}{dx} - \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dxx\frac{d}{dx}\left(\frac{d\psi}{dx}\right)^2$$

Now

$$\int_{-\infty}^{\infty} dxx\frac{d\psi^2}{dx} = \int_{-\infty}^{\infty} dx\frac{d}{dx}\left(x\psi^2\right) - \int_{-\infty}^{\infty} dx\psi^2$$

The first term vanishes, and the second term is unity. We do the same with the second term, in which only the second integral

$$\int_{-\infty}^{\infty} dx\left(\frac{d\psi}{dx}\right)^2$$

remains. Putting all this together we get

$$\langle x\frac{dV}{dx}\rangle + \langle V\rangle = \frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\left(\frac{d\psi}{dx}\right)^2 + E\int_{-\infty}^{\infty} dx\psi^2 = \langle\frac{p^2}{2m}\rangle + E$$

so that

$$\frac{1}{2}\langle x\frac{dV}{dx}\rangle = \langle\frac{p^2}{2m}\rangle$$