THE POTENTIAL WELL

We next consider the potential (Fig. 5-2)

$$\begin{aligned} V(x) &= 0 && x < -a \\ &= -V_0 && -a < x < a \\ &= 0 && a < x \end{aligned} \tag{5-20}$$

In addition to the solutions for $E > 0$ discussed in the section on the potential **well** there are, remarkably, also solutions for $E < 0$ provided the potential is nega**tive,** that is, $V_0 > 0$ in (5-20). They will turn out to be discrete. Let us write

$$\frac{2mE}{\hbar^2} = -\kappa^2 \tag{5-57}$$

The solutions outside the well that are bounded at infinity are

$$\begin{aligned} u(x) &= C_1\, e^{\kappa x} && x < -a \\ u(x) &= C_2\, e^{-\kappa x} && a < x \end{aligned} \tag{5-58}$$

Since we are dealing with real functions, it is more convenient to write the solution inside the well in the form

$$u(x) = A\cos qx + B\sin qx \qquad -a < x < a \tag{5-59}$$

Note that

$$q^2 = \frac{2m}{\hbar^2}(V_0 - |E|) > 0 \tag{5-60}$$

Matching solutions and derivatives at the edges $x = \pm a$ yields

$$\begin{aligned} C_1 e^{-\kappa a} &= A\cos qa - B\sin qa \\ \kappa C_1 e^{-\kappa a} &= q(A\sin qa + B\cos qa) \\ C_2 e^{-\kappa a} &= A\cos qa + B\sin qa \\ -\kappa C_2 e^{-\kappa a} &= -q(A\sin qa - B\cos qa) \end{aligned} \tag{5-61}$$

These may be combined to yield

$$\begin{aligned} \kappa &= q\,\frac{A\sin qa - B\cos qa}{A\cos qa + B\sin qa} \\ &= q\,\frac{A\sin qa + B\cos qa}{A\cos qa - B\sin qa} \end{aligned} \tag{5-62}$$

Together these imply that $AB = 0$, that is, the solutions are either even in x ($B = 0$) or odd in x ($A = 0$). The wave functions are roughly of the shape shown in Fig. 5-10. The ground state, with no nodes, is even. This is a general property of simple systems. The conditions that determine the energy are from (5-62)

$$\begin{aligned} \kappa &= q\tan qa && \text{even solutions} \\ \kappa &= -q\cot qa && \text{odd solutions} \end{aligned} \tag{5-63}$$

Let us examine these separately.

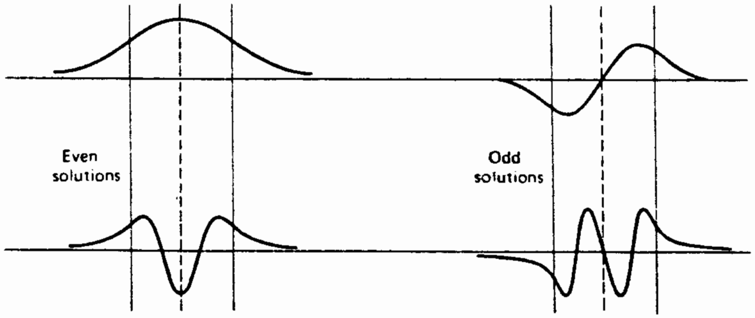


Figure 5-10. Solutions for discrete spectrum in attractive potential well.

(a) The even solutions:

With the notation

$$\begin{aligned} \lambda &= \frac{2mV_0a^2}{\hbar^2} \\ y &= qa \end{aligned} \tag{5-64}$$

the first of the relations (5-63) reads

$$\frac{\sqrt{\lambda - y^2}}{y} = \tan y \tag{5-65}$$

If we plot $\tan y$ and $\sqrt{\lambda - y^2}/y$ as functions of y (Fig. 5-11), the points of intersection determine the eigenvalues. These form a discrete set. The larger λ is, the further the curves for $\sqrt{\lambda - y^2}/y$ go, that is, *when the potential is deeper and/or broader, there are more bound states.* The figure also shows that no matter how small λ is, there will always be at least one bound state. This is characteristic of one-dimensional attractive potentials, and is *not* true for three-dimensional potentials, which behave much more like the odd-solution problem that we will discuss later. As λ becomes large, the eigenvalues tend to become equally spaced in y, with the intersection points given approximately by

$$y \simeq (n + \tfrac{1}{2})\pi \qquad n = 0, 1, 2, \ldots \tag{5-66}$$

This is just the eigenvalue condition for the even solutions of the infinite box centered at the origin (eigenfunctions given in (4-48)). This is as might be expected,

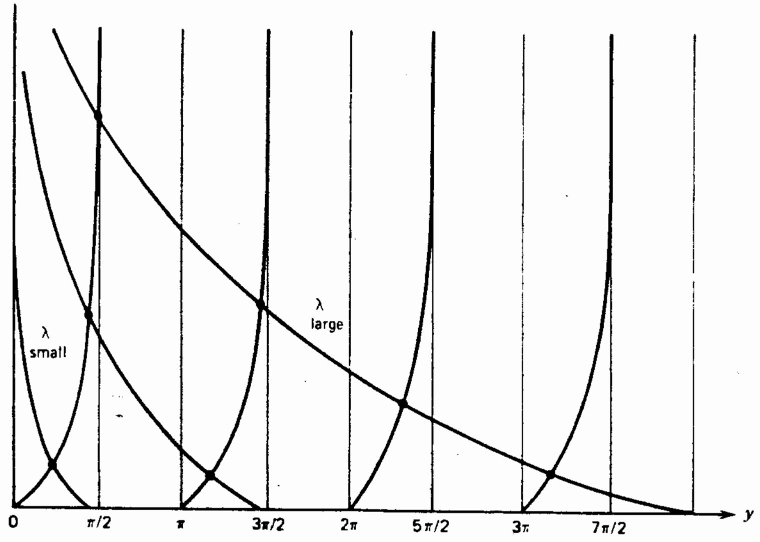


Figure 5-11. Location of discrete eigenvalues for even solutions in square well. The rising curves represent $\tan y$; the falling curves are $\sqrt{\lambda - y^2}/y$ for different values of λ.

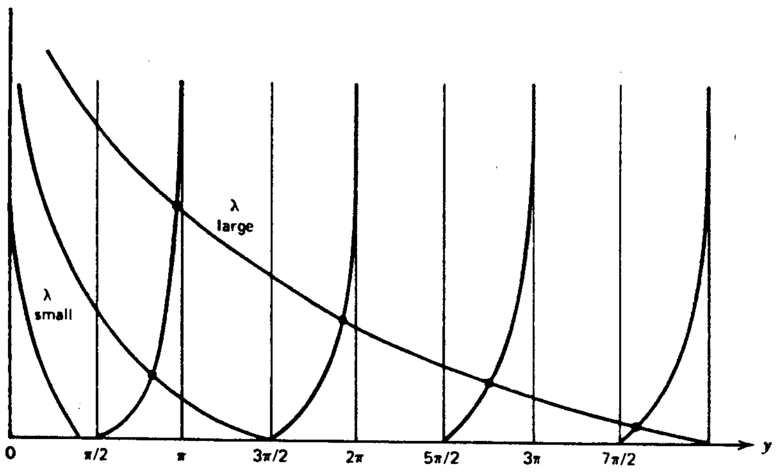


Figure 5-12. Location of discrete eigenvalues for odd solutions in square well. The rising curves represent $-\cot y$; the falling curves are $\sqrt{\lambda - y^2}/y$ for different values of λ. Note that there is no eigenvalue for $\lambda < (\pi/2)^2$.

since for the deep-lying states in the potential, the fact that it is not really infinitely deep does not matter very much.

(b) The odd solutions:

Here the eigenvalue condition reads

$$\frac{\sqrt{\lambda - y^2}}{y} = -\cot y \tag{5-67}$$

Since $-\cot y = \tan(\pi/2 + y)$, the plot in Fig. 5-12 is the same as in Fig. 5-11 with the tangent curves shifted by $\pi/2$. The large λ behavior is more or less the same, with (5-66) replaced by

$$y \simeq n\pi \qquad n = 1, 2, 3, \ldots \tag{5-68}$$

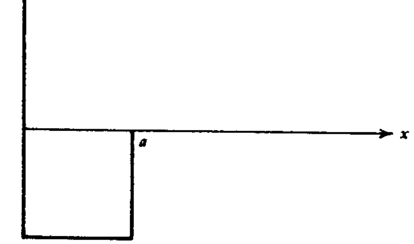


Figure 5-13. Equivalent potential for odd solutions of square well bound state problem.

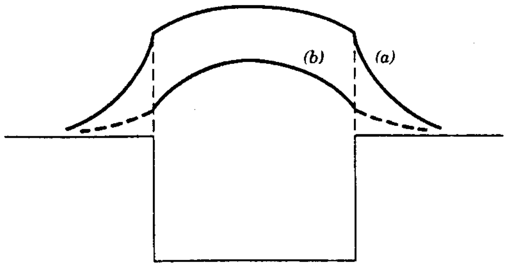


Figure 5-14. (*a*) Mismatch with E_B too large. (*b*) Mismatch with E_B too small.

In contrast to the even solutions, there will only be an intersection if $\sqrt{\lambda - \pi^2/4} > 0$, that is, if

$$\frac{2mV_0a^2}{\hbar^2} \geq \frac{\pi^2}{4} \tag{5-69}$$

The odd solutions all vanish at $x = 0$, and hence the bound-state problem for the odd solutions will be the same as for the potential well shown in Fig. 5-13, since in the latter, the condition $u(0) = 0$ would be imposed. We shall see that such conditions are imposed on wave functions in the three-dimensional world.

The detailed calculations that we have carried out support the qualitative understanding of the reason for discrete eigenvalues. These arise because we require the wave functions to vanish at infinity. We see this graphically in Fig. 5-14. The even-parity ground-state wave function inside the potential, of the form $\cos qx$, must tie on continuously to a falling exponential $e^{-\alpha|x|}$ with $\alpha^2 = 2mE_B/\hbar^2$. Large binding means a rapidly falling exponential. Since $q^2 = (2mV_0/\hbar^2 - \alpha^2)$, a large binding energy means that q^2 is small, that is, the wave function is quite flat: thus matching is impossible. As we reduce the trial E_B, the exponential falls less steeply and the wave function inside curves more, so that at some point the matching (continuous slope) becomes possible. If the value of α is lowered beyond this point, the outside curve is too flat to match the more curved inside wave function. For the first excited state, with odd parity, the wave function vanishes at the origin, so that it can only tie onto a falling exponential if it has a chance to turn over inside the potential. The condition that it turns over just enough to tie to a straight line ($\alpha = 0$) is that $\sin qa = 1$, so that $qa = \pi/2$, which corresponds to the condition expressed in (5-69).

DELTA FUNCTION POTENTIALS

We consider a potential $V(x)$ whose spatial behavior is given by $\delta(x)$. Since $\delta(x)$ has the dimensions of a reciprocal length, it is convenient to write for the attractive potential

$$V(x) = -\frac{\hbar^2\lambda}{2ma}\,\delta(x) \tag{5-70}$$

P] Use las relaciones de conmutación entre el momentum p y la posición x para obtener las ecuaciones que describen la dependencia del tiempo de $\langle x\rangle$ y $\langle p\rangle$ dados los siguientes Hamiltoneanos

(a) $H = \frac{p^2}{2m} + \frac{1}{2}m(\omega_1^2 x^2 + \omega_2 x + \epsilon)$

(b) $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - \frac{A}{x^2}$

Sol: $$\frac{d\langle A\rangle}{dt} = \frac{i}{\hbar}\langle [H, A]\rangle + \cancel{\frac{\partial\langle A\rangle}{\partial t}} \to 0$$ en estado estacionario

(a) $$\frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m} + \frac{1}{2}\underbrace{m(\omega_1^2 x^2 + \omega_2 x + \epsilon)}_{\text{Conmuten con } x}, x\right]\right\rangle$$

$$\Rightarrow \frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\,\frac{1}{2m}\langle [p^2, x]\rangle \;;\; [p^2, x] = p\underbrace{[p, x]}_{-i\hbar} + \underbrace{[p, x]}_{-i\hbar}p \quad \text{(cátedra)}$$

$$\Rightarrow \frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\cdot\frac{1}{2m}\cdot(-2i\hbar)\langle p\rangle$$

$$\Rightarrow \boxed{\frac{d\langle x\rangle}{dt} = \left\langle \frac{p}{m}\right\rangle}$$

$$\frac{d\langle p\rangle}{dt} = \text{(propuesto)}$$

(b) $$\frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m} + \underbrace{\frac{1}{2}m\omega^2 x^2 - \frac{A}{x^2}}_{\text{Conmuten con } x}, x\right]\right\rangle$$

$$\Rightarrow \boxed{\frac{d\langle x\rangle}{dt} = \left\langle \frac{p}{m}\right\rangle}$$

$$\frac{d\langle p\rangle}{dt} = \frac{i}{\hbar}\left\langle\left[\underbrace{\frac{p^2}{2m}}_{\text{conmuta con } p} + \frac{1}{2}m\omega^2 x^2 - \frac{A}{x^2}, p\right]\right\rangle$$

$$\Rightarrow \frac{d\langle p\rangle}{dt} = \frac{i}{\hbar}\left(\frac{1}{2} m w^2 \langle [x^2, p] \rangle - A \langle [\tfrac{1}{x^2}, p] \rangle \right)$$

$$[x^2, p] = x \underbrace{[x, p]}_{i\hbar} + \underbrace{[x, p]}_{i\hbar} x = 2i\hbar\, x$$

$$[p, f(x)] = -i\hbar \frac{df}{dx} \Rightarrow [\tfrac{1}{x^2}, p] = - [p, \tfrac{1}{x^2}] = i\hbar \frac{d}{dx}\left(\frac{1}{x^2}\right) = -2i\hbar \frac{1}{x^3}$$

$$\Rightarrow \frac{d\langle p\rangle}{dt} = \frac{i}{\hbar}\left(\frac{1}{2} m w^2 (2i\hbar) \langle x \rangle - A(-2i\hbar) \langle \tfrac{1}{x^3} \rangle \right)$$

$$\Rightarrow \boxed{\frac{d\langle p\rangle}{dt} = -\left(m w^2 \langle x \rangle + 2A \langle \tfrac{1}{x^3} \rangle \right)}$$

Nota: $[AB, C] = A[B, C] + [A, C]B$

P1 Considere un sistema de dos electrones descrito por el Hamiltoneano $H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V(x_1) + V(x_2)$, donde $V(x) = \infty$ para $x<0$ y $x>a$; $V(x) = 0$ para $0<x<a$. Suponga que los electrones tienen el mismo spin.

(a) ¿Cuál es la energía y la función de onda del estado fundamental del sistema?

(b) ¿Cuál es la energía y la función de onda del primer estado excitado?

Sol:

(a) Este problema corresponde a un pozo potencial con dos electrones que no interactúan entre ellos.

Si el sistema fuera de una sola partícula, el resultado es conocido:

$$\underbrace{\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)}_{(*)}, \qquad E_n = \underbrace{\left(\frac{\pi^2\hbar^2}{2ma^2}\right)}_{\equiv K} n^2$$

Para el caso de 2 electrones, no es difícil concluir que la solución de la ec. de Schrödinger respectiva es:

$$\psi_{n_1 n_2}(x_1, x_2) = \psi_{n_1}(x_1)\,\psi_{n_2}(x_2), \qquad E_{n_1 n_2} = (n_1^2 + n_2^2)K$$

donde $\psi_{n_1}(x_1)$ y $\psi_{n_2}(x_2)$ están dados por $(*)$

Sin embargo, como se trata de electrones, que son fermiones, hay que antisimetrizar $\psi_{n_1 n_2}(x_1, x_2)$ con respecto al intercambio de etiquetas de las partículas: $1 \longleftrightarrow 2$.

$$\psi_{n_1 n_2}^{(A)}(x_1, x_2) = \frac{1}{\sqrt{2!}}\begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_1}(x_2) \\ \psi_{n_2}(x_1) & \psi_{n_2}(x_2) \end{vmatrix} \qquad \text{(determinante de Slater)}$$

$$= \frac{1}{\sqrt{2}}\left(\psi_{n_1}(x_1)\,\psi_{n_2}(x_2) - \psi_{n_1}(x_2)\,\psi_{n_2}(x_1)\right)$$

La antisimetría de $\psi_{n_1 n_2}^{(A)}(x_1, x_2)$ implica que los electrones deben estar en niveles de energía distintos, pues si $n_1 = n_2$

$$\Rightarrow \psi_{n_1 n_1}^{(A)}(x_1, x_2) = \frac{1}{\sqrt{2}}\left(\psi_{n_1}(x_1)\,\psi_{n_1}(x_2) - \psi_{n_1}(x_2)\,\psi_{n_1}(x_1)\right) = 0$$

Entonces, en el estado fundamental de este sistema, un electrón se encuentra en el nivel $n=1$, y el otro en el nivel $n=2$

$$\Rightarrow \psi_{21}^{(A)}(x_1,x_2) = \frac{\sqrt{2}}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) - \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$$

$$\text{y} \quad E_{21} = E_{12} = (2^2+1^2)K = 5K$$

(b) El primer estado excitado corresponde a $n=1$ para un electrón y $n=3$ para el otro

$$E_{13} = E_{31} = (3^2+1^2)K = 10K$$

$$\psi_{31}^{(A)}(x_1,x_2) = \frac{\sqrt{2}}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{3\pi x_2}{a}\right) - \sin\left(\frac{3\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$$

El siguiente estado excitado es $E_{23} = E_{32} = 13K$

" " " " $E_{14} = E_{41} = 17K$

Así sucesivamente, aumentando las energías del sistema.

Si el sistema fuera de 3 electrones, entonces la función de onda del sistema sería:

$$\psi_{n_1n_2n_3}^{(A)}(x_1,x_2,x_3) = \frac{1}{\sqrt{3!}}\begin{vmatrix} \psi_{n_1}(x_1) & \psi_{n_1}(x_2) & \psi_{n_1}(x_3) \\ \psi_{n_2}(x_1) & \psi_{n_2}(x_2) & \psi_{n_2}(x_3) \\ \psi_{n_3}(x_1) & \psi_{n_3}(x_2) & \psi_{n_3}(x_3) \end{vmatrix}$$

P] El mismo problema anterior, pero con spin.

Sol:

(a) El spin del electrón les agrega un grado de libertad a las funciones de onda, lo que permite que 2 electrones con distintos spin se sitúen en el mismo nivel de energía.

Sean
$$\psi_n^+(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi}{a}x\right)|\uparrow\rangle$$
$$\psi_n^-(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi}{a}x\right)|\downarrow\rangle$$

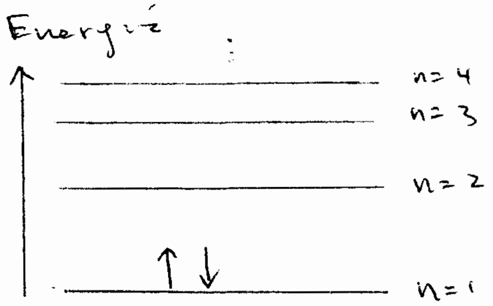
funciones de onda de un solo electrón, donde $|\uparrow\rangle$ y $|\downarrow\rangle$ son "etiquetas" para los dos estados de spin posibles.

Entonces, el estado fundamental del sistema corresponde a tener a los 2 electrones en el nivel $n=1$ con distintos spines.

$$\Psi_{\text{sistema}}(x_1, x_2) = \frac{1}{\sqrt{2!}}\begin{vmatrix} \psi_1^+(x_1) & \psi_1^+(x_2) \\ \psi_1^-(x_1) & \psi_1^-(x_2) \end{vmatrix}$$

(no olvidar que la fn. de onda del sist. debe ser antisimétrica ante permutación de las partículas)

y la energía del sistema es $E_{11} = (1^2+1^2)k = 2k$



(b) propuesto