Intro to QM due: November 26, 2018

Problem Set 9

Consider a particle of mass m in a 1-dimensional square well potential:

$$V(x) = \begin{cases} 0, & |x| \le a \\ V_0, & |x| \ge a \end{cases}$$

for $V_0 > 0$ positive. We are interested in the bound state energy eigenvalues and eigenstates, i.e., those with energy eigenvalues $0 \le E \le V_0$. As in the infinite square well potential, the eigenstate wave functions $\phi(x)$ will be either even: $\phi(-x) = \phi(x)$, or odd: $\phi(-x) = -\phi(x)$.

Problem 1: Show that the energy eigenvalues satisfy the equations

$$\begin{aligned} k\tan(ka) &= +\kappa && \text{for even eigenstates} \\ k\cot(ka) &= -\kappa && \text{for odd eigenstates} \end{aligned} \tag{1}$$

where k and $i\kappa$ are the real and complex wave numbers inside and outside the well, respectively. Show also that k and κ are related by

$$k^2 + \kappa^2 = 2mV_0/\hbar^2. \tag{2}$$

Solution: Call $x < -a$ region I, $-a < x < a$ region II, and $x > a$ region III. Then solving for the energy eigenstates, $-\hbar^2\psi'' = 2m(E - V(x))\psi$, of energy $E \le V_0$ in each region gives $\psi_I = Ae^{-\kappa x} + Be^{\kappa x}$, $\psi_{II} = Ce^{ikx} + De^{-ikx}$, and $\psi_{III} = Ee^{-\kappa x} + Fe^{\kappa x}$, with $\hbar\kappa = \sqrt{2m(V_0 - E)}$ and $\hbar k = \sqrt{2mE}$. We must have $A = F = 0$ so that the wave function does not grow exponentially as $x \to \pm\infty$. The boundary conditions at $x = \pm a$ are that ψ and ψ' are continuous, implying

$$\begin{aligned} Be^{-\kappa a} &= Ce^{-ika} + De^{ika}, \\ \kappa Be^{-\kappa a} &= ikCe^{-ika} - ikDe^{ika}, \\ Ee^{-\kappa a} &= Ce^{ika} + De^{-ika}, \\ -\kappa Ee^{-\kappa a} &= ikCe^{ika} - ikDe^{-ika}, \end{aligned}$$

Taking the suggestion of the problem, let's look for even and odd solutions, that is, those satisfying $\psi(-x) = \psi(x)$ and $\psi(-x) = -\psi(x)$, respectively.

Even solutions: For ψ to be even, we need $B = E$ and $C = D$. The above boundary conditions then become

$$\begin{aligned} Be^{-\kappa a} &= Ce^{-ika} + Ce^{ika}, \\ \kappa Be^{-\kappa a} &= ikCe^{-ika} - ikCe^{ika}, \end{aligned}$$

which can be rewritten as

$$\begin{pmatrix} e^{-\kappa a} & -2\cos(ka) \\ \kappa e^{-\kappa a} & -2k\sin(ka) \end{pmatrix} \begin{pmatrix} B \\ C \end{pmatrix} = 0,$$

which has a solution for nonzero $(B\ C)$ only if the determinant of the matrix vansihes, implying $k\sin(ka)=\kappa\cos(ka)$, which is the result we wanted.

Odd solutions: For ψ to be even, we need $B=-E$ and $C=-D$. The above boundary conditions then become just two independent equations which can be rewritten as

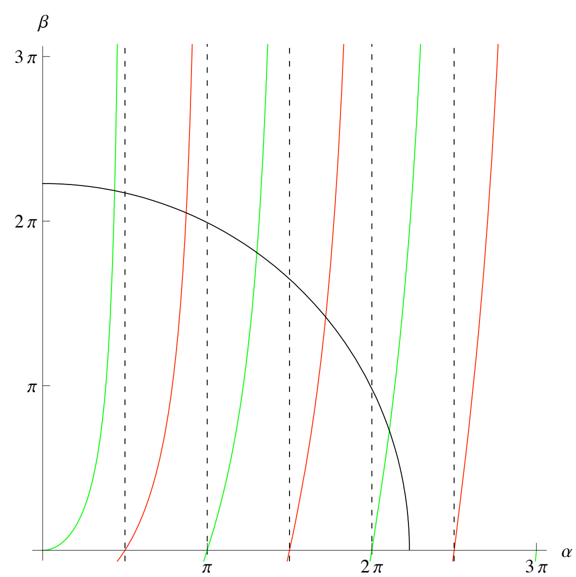
$$\begin{pmatrix} e^{-\kappa a} & 2i\sin(ka) \\ \kappa e^{-\kappa a} & -2ik\cos(ka) \end{pmatrix} \begin{pmatrix} B \\ C \end{pmatrix} = 0.$$

The determinant of the matrix vansihes when $-k\cos(ka)=\kappa\sin(ka)$, which is the result we wanted.

Finally, from the defnitions of k and κ, the relation (2) follows immediately.

Problem 2: Equations (1) must be solved graphically. In the ($\alpha = ka$, $\beta = \kappa a$)-plane, imagine a circle that obeys equation (2). The bound states are then given by the curve $\alpha\tan\alpha=\beta$ or $\alpha\cot\alpha=-\beta$ with the circle. (Remember α and β are positive.) Plot these functions to solve for α and β (or, k and κ) graphically.

Solution: This part of the problem is just a plot. In the variables α and β defined in the problem, (2) becomes the curve of the circle $\alpha^2+\beta^2=2ma^2V_0/\hbar^2$. Plotting the circle and the $\beta=\alpha\tan\alpha$ (even states) or $\beta=-\alpha\cot\alpha$ (odd states) then gives the plot shown below. The red (darker) curves are the odd states and the green (lighter) ones are the even ones, and the quarter-circle is plotted for the value $2ma^2V_0^2/\hbar^2 = 49$. (The dotted lines just indicate the asymptotes to the red and green curves.) Each intersection of the circle with a red or green line is a solution, and therefore an energy eigenstate. For the value plotted in the figure, we thus see that there are five eigenstates.



Problem 3: Verify from the above graphical solution that as $V_0\to\infty$ we regain the energy levels of the infinite well potential.

Solution: As $V_0\to\infty$, the radius of the circle in the figure goes to infinity, so it intersects the colored curves at their asymptotes (the dashed lines), which are at $\alpha = n\pi/2$ for $n=1,2,3,\ldots$. From the definition of α this means that $k=n\pi/(2a)$, and from the definition of k, this means that $E = (\hbar k)^2/(2m) = (\hbar n\pi)^2/(8a^2 m)$, which are the energy eigenvalues of an infinite square well of width $2a$.

Problem 4: Show that there is always one even solution and that there is no odd solution unless $V_0 \geq \hbar^2\pi^2/8ma^2$. What is E when V_0 just meets this requirement?
Solution: As $V_0 \to 0$, the radius of the circle decreases. When it gets less than $\pi/2$ it can only intersect the leftmost green curve. Since that curve goes to the origin, no matter how small V_0, the circle will always intersect it, and so there will always be at least one even solution.

When the radius equals $\pi/2$, then $V_0 = \hbar^2\pi^2/8ma^2$, and the circle intersects the $\alpha\tan(\alpha)$ curve at $\alpha \approx 0.934014$ (found numerically). Since $\alpha := ka$ and $\hbar k = \sqrt{2mE}$, this implies $E = \hbar^2\alpha^2/2ma^2 \approx 0.46191\,\hbar^2/ma^2$.

Consider the case of a particle of mass m moving in one dimension in a *complex* potential $V(x) = V_r(x) + iV_i$, where the imaginary part V_i is a constant.

Problem 5: What is the Hamiltonian? Is the Hamiltontian hermitian?
Solution: The Hamiltonian is

$$H = \frac{1}{2m}P^2 + V_r(X) - iV_i$$

where V_r is a real function and V_i a real constant. Therefore

$$H^\dagger = \frac{1}{2m}(P^\dagger)^2 + V_r(X^\dagger) - (i)^* V_i = \frac{1}{2m}P^2 + V_r(X) + iV_i \neq H,$$

so H is *not* Hermitian.

Problem 6: Repeat the derivation of the probability conservation equation (6.123) of the text in this case. Show that the total probability for finding the particle decreases exponentially as $\exp\{-2V_i t/\hbar\}$. Such complex potentials are used to described processes in which particle number is not conserved, e.g., when the particles can leave the system or decay in some way.
Solution: Schrodinger's equation and its complex conjugate in this case read

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V_r\psi - iV_i\psi, \\ -i\hbar\frac{\partial\psi^*}{\partial t} &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi^* + V_r\psi^* + iV_i\psi^*. \end{aligned}$$

Multiplying the first by ψ^* and the second by ψ and taking the difference, then dividing by $i\hbar$ gives

$$\frac{\partial\rho}{\partial t} = -\frac{\partial}{\partial x}j_x - \frac{2}{\hbar}V_i P,$$

where $\rho := |\psi|^2$ and $j_x := \hbar(\psi^*\frac{\partial}{\partial x}\psi - \psi\frac{\partial}{\partial x}\psi^*)/(2mi)$ are the probability density and current, respectively. Integrating this over all space, the $\frac{\partial}{\partial x}j_x$ term vanishes since we assume $j_x \to 0$ at infinity, giving

$$\frac{d\mathcal{P}}{dt} = -\frac{2}{\hbar}V_i\,\mathcal{P},$$

where $\mathcal{P} = \int_{-\infty}^{\infty} dx\, \rho$ is the total probability. (I can pull V_i out of the integral since it is assumed constant in the problem.) Integrating this differential equation gives

$$\mathcal{P}(t) = \mathcal{P}(0)\, e^{-2V_i t/\hbar}.$$

Consider a particle of mass m moving in two dimensions. Its position is then measured by two commuting hermitean operators $\widehat{x}$, $\widehat{y}$, so has position eigenstates $|x, y\rangle$ satisfying

$$\begin{aligned} \widehat{x}|x,y\rangle &= x|x,y\rangle, & \langle x,y|x',y'\rangle &= \delta(x-x')\delta(y-y'), \\ \widehat{y}|x,y\rangle &= y|x,y\rangle, & 1 &= \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\ |x,y\rangle\langle x,y|. \end{aligned}$$

Likewise, its momentum is measured by two commuting hermitean operators $\widehat{p}_x$, $\widehat{p}_y$, so has momentum eigenstates $|p_x, p_y\rangle$ satisfying

$$\begin{aligned} \widehat{p}_x|p_x,p_y\rangle &= p_x|p_x,p_y\rangle, & \langle p_x,p_y|p'_x,p'_y\rangle &= \delta(p_x-p'_x)\delta(p_y-p'_y), \\ \widehat{p}_y|p_x,p_y\rangle &= p_y|p_x,p_y\rangle, & 1 &= \int_{-\infty}^{\infty} dp_x \int_{-\infty}^{\infty} dp_y\ |p_x,p_y\rangle\langle p_x,p_y|. \end{aligned}$$

Finally, these operators obey the commutation relations

$$[\widehat{x}, \widehat{p}_x] = [\widehat{y}, \widehat{p}_y] = i\hbar,$$

and all other commutators vanish.

Problem 7: What is the wave function, $\langle x, y|p_x, p_y\rangle$, of the momentum eigenstate $|p_x, p_y\rangle$ in the position basis?

Solution: The Hilbert space for a particle moving in 2 dimensions is the tensor product of two copies of that of a particle moving in one dimension: $\mathcal{H}_{(x,y)\text{-plane}} = \mathcal{H}_{x\text{-axis}} \otimes \mathcal{H}_{y\text{-axis}}$. This follows because the position eignebasis $|x,y\rangle = |x\rangle \otimes |y\rangle$ is simply the tensor product of two 1-dimensional position bases. It then follows that

$$\begin{aligned} \langle x,y|p_x,p_y\rangle &= \langle x|p_x\rangle \cdot \langle y|p_y\rangle = (2\pi\hbar)^{-1/2} \exp\{ixp_x/\hbar\} \cdot (2\pi\hbar)^{-1/2} \exp\{iyp_y/\hbar\} \\ &= (2\pi\hbar)^{-1} \exp\{i(xp_x + yp_y)/\hbar\}, \end{aligned}$$

where I have used the 1-dimensional results for $\langle x|p_x\rangle$, etc.

Problem 8: Write down the Hamiltonian, $\widehat{H}$, for this particle if it is moving in a potential $V(x, y)$ in terms of the $\widehat{x}$, $\widehat{y}$, $\widehat{p}_x$, and $\widehat{p}_y$ operators.

Solution: $\widehat{H} = (\widehat{p}_x^2 + \widehat{p}_y^2)/(2m) + V(\widehat{x}, \widehat{y})$.

Problem 9: In case $V(x, y) \equiv 0$ (i.e., the particle is free), what are the energy eigenvalues and eigenstates of $\widehat{H}$?

Solution: If $V \equiv 0$, then $\widehat{H} = (2m)^{-1}(\widehat{p}_x^2 + \widehat{p}_y^2)$, which commutes with both $\widehat{p}_x$ and $\widehat{p}_y$. So the momentum eigenstates $|p_x, p_y\rangle$ are also the energy eigenstates. Indeed, $\widehat{H}|p_x, p_y\rangle = (2m)^{-1}(p_x^2 + p_y^2)|p_x, p_y\rangle$, so the energy eigenvalues are simply $E = (2m)^{-1}(p_x^2 + p_y^2)$ for all $-\infty < p_x, p_y < \infty$.