Physics 3610H: Assignment II

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Problem 1. Consider a single particle of mass m moving in one dimension subject to the following potential:

$$V(x) = \begin{cases} \infty, & x < -c \\ 0, & -c < x < c \\ \infty, & x > c \end{cases}$$

(a) Find the eigenvalues and eigenstates of $\hat{H}$ for this system, that is the energies E and the states ψ for which $\hat{H}\psi = E\psi$.

(b) Examine the two lowest energy states:

    (i) Draw two plots showing ψ vs x for the two lowest energy states.

    (ii) This is very similar to the problem we solved in class. Comment on whether your results for the two lowest energy states (both the energies and the states) are consistent with those we found in class.

    (iii) Show that the two lowest energy states are orthogonal.

Solution 1.

(a) Here $\hat{H}$ is the operator corresponding to the total energy of the particle. Because the particle is only subject to the potential applied by the well at its edges and possesses only kinetic energy otherwise we can say

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x} + V(x)$$

where we've obtained the operator corresponding to kinetic energy by using the momentum operator in the usual expression for kinetic energy. Now that we have $\hat{H}$ we can solve the time dependent Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi(x,t)$$

which, when we substitute our $\hat{H}$ becomes

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t).$$

We will try now to find a $\Psi(x,t)$ which is separable as $\Psi(x,t) = \psi(x)\phi(t)$ this doesn't always work but from some foreknowledge of the problem we know there is a fair chance that it will and so we try it. This means that our equation is now

$$i\hbar\frac{\partial}{\partial t}\psi(x)\phi(t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x)\phi(t).$$

We can divide through on both sides by $\psi(x)\phi(t)$ being careful to note that we cannot pull functions out of derivatives that contain the variable of differentiation, e.g. on the left side ϕ will not cancel and the derivative will instead be multiplied out front by ϕ^{-1}. This makes our equation now

$$\frac{i\hbar}{\phi(t)}\frac{\partial}{\partial t}\phi(t) = \frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x)$$

which satisfies our original reason for trying to separate Ψ: to obtain two differential equations of only on variable each which makes them ODEs instead of PDEs. Another consequence of this separation while maintaining equality is that these functions must *always* be equal. The only way this can happen is if both are equal to a constant as fixing one variable and varying the other would (if they were not equal to a constant), to preserve equality, require that x and t are related in a way that makes this possible. This is obviously not the case so we can reason that regardless of values of x or t, the two must be the same and constant. This allows us to further "separate" the equation into two independent ODEs,

$$E = \frac{i\hbar}{\phi(t)} \frac{d}{dt} \phi(t) \tag{1}$$

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

We will first begin by solving 1 as it is very easy by recognizing that there is an easy function who's derivative is itself times a constant, e^x. This gives us

$$\phi = Ce^{-iEt/\hbar}$$

where A is a constant of integration that we will determine later. Now for 2 with some rearranging (and noticing the $V(x) = 0$ in the region we care about) we have

$$-\frac{2mE}{\hbar^2} \psi(x) = \frac{d^2}{dx^2} \psi(x).$$

This means we are looking now for a function whose second derivative is itself times a negative constant. This is satisfied by

$$\psi(x) = A\sin(kx) + B\cos(kx).$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$. We can now work to determine k (really E) using the implied boundary conditions given by the fact that the particle may not exist at $x = \pm c$ meaning the wavefunction must be zero there. Applying this gives

$$\psi(c) = A\sin(kc) + B\cos(kc) = 0$$

and

$$\psi(-c) = A\sin(-kc) + B\cos(-kc) = -A\sin(kc) + B\cos(kc) = 0.$$

The fact that both of these are zero is satisfied only by

$$A\sin(kc) = B\cos(kc) = 0.$$

The only way this can happen is if either $A = B = 0$ meaning the probability of the particle being found anywhere is zero and the particle therefore does not exist or the more useful case of k being some value that makes either $\sin(kc)$ or $\cos(kc)$ zero. Knowing that k must be the same for both functions this gives rise to two possible solutions. For $\sin(x)$ to be zero x must be some integer multiple of π and for $\cos(x)$ to be zero x must be some *half* integer multiple of π. The only way to satisfy this is to construct a k of the form

$$k = \frac{n\pi}{2c}$$

and use the $\sin(kx)$ function for even values of n and $\cos(kx)$ for odd values. It's also important to note that we require $n \in \mathbb{Z} > 0$ as the negative ns are just multiples of the positive ones and so give no new information and $n = 0$ is again the no-particle-exists case and also gives no information. So we now have two possible functions for $\psi_n(x)$,

$$\psi_n(x) = \begin{cases} A\sin(kx), & n = 2, 4, 6, \dots \\ B\cos(kx), & n = 1, 3, 5, \dots \end{cases}$$

Working out E now as it is the only thing inside k which we can set to force k to adopt our constructed value,

$$k = \frac{n\pi}{2c} = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\implies \frac{n^2\pi^2}{4c^2} = \frac{2mE}{\hbar^2}$$

$$\implies \frac{n^2\pi^2\hbar^2}{8mc^2} = E_n$$

Now using our last available bit of information, the requirement that the probability of finding the particle anywhere must be 1, we integrate our wavefunction (either one! both have the same amplitude and will therefore have the same constant) over all space and force it to be 1 using the constants. We can also note that helpfully the particle is guaranteed to only exist within the well so we can narrow down our bounds of integration,

$$
\begin{aligned}
1 &= \int_{-c}^{c} \psi(x)\psi^*(x)dx \\
&= \int_{-c}^{c} |A| \sin\left(\frac{n\pi}{2c}x\right) |A| \sin\left(\frac{n\pi}{2c}x\right) dx \\
&= |A|^2 \int_{-c}^{c} \sin^2\left(\frac{n\pi}{2c}x\right) dx \\
&= \frac{|A|^2}{2}\left[\int_{-c}^{c} 1\, dx - \int_{-c}^{c} \cos\left(\frac{n\pi}{c}x\right) dx\right] \\
&= \frac{|A|^2}{2}\left[2c - \int_{-c}^{c} \cos\left(\frac{n\pi}{c}x\right) dx\right] \\
&= \frac{|A|^2}{2}\left[2c - \frac{2c}{n\pi}\sin(\pi n)\right]_{}^{0} \qquad\qquad \implies c|A|^2 = 1 \implies |A| = \sqrt{\frac{1}{c}}
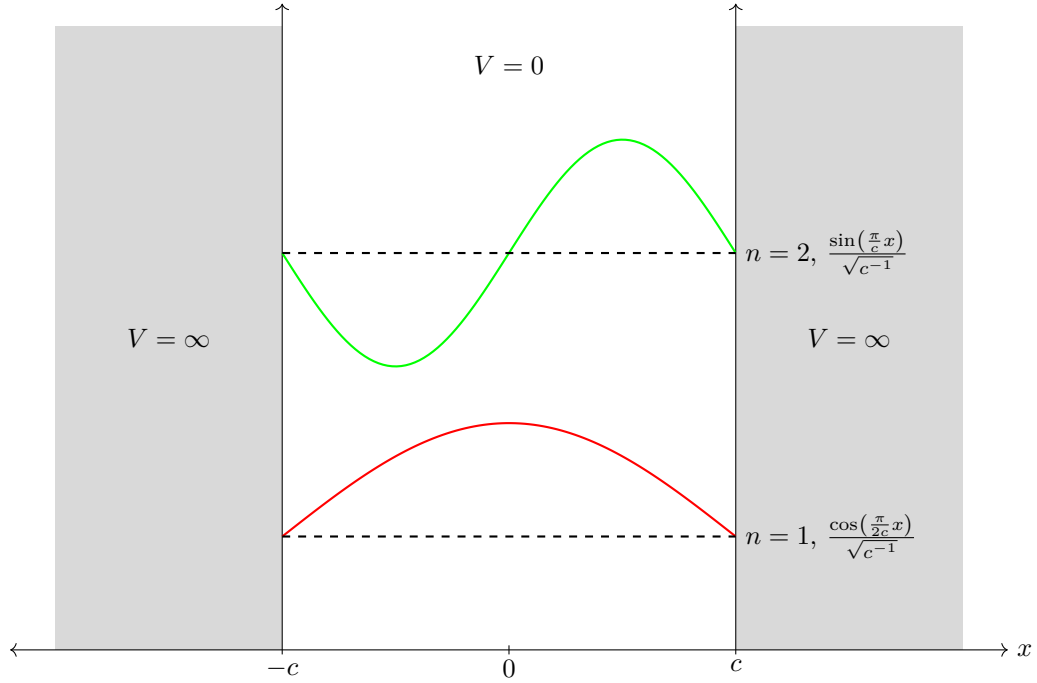\end{aligned}
$$

By example of the text we pick the positive real value of $|A|$ and so obtain

$$
\psi_n(x) = \begin{cases} \sqrt{\frac{1}{c}}\sin\left(\frac{n\pi}{2c}x\right), & n = 2,4,6,\ldots \\ \sqrt{\frac{1}{c}}\cos\left(\frac{n\pi}{2c}x\right), & n = 1,3,5,\ldots \end{cases}
$$

We can now say that the above $\psi_n(x)$s are our eigenstates and $E_n = \dfrac{n^2\pi^2\hbar^2}{8mc^2}$ our eigenvalues.

(b)

(i)

(ii) Yes, the results obtained here are consistent with those in class. In class we had a well with width a and here we have a well with width $2c$. This means we'd see a doubling everywhere there is width dependent term. For the energy eigenvalues acting as if we are now in a well of half the width we obtain $\dfrac{n^2\pi^2\hbar^2}{8m(c/2)^2} = \dfrac{n^2\pi^2\hbar^2}{2mc^2}$ which is what we same in class. For the eigenstates we see

$$\psi_n(x) = \begin{cases} \sqrt{\frac{1}{c/2}}\sin\left(\frac{n\pi}{2(c/2)}x\right), & n = 2,4,6,\ldots \\ \sqrt{\frac{1}{c/2}}\cos\left(\frac{n\pi}{2(c/2)}x\right), & n = 1,3,5,\ldots \end{cases}$$

Which simplifies down to

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{c}}\sin\left(\frac{n\pi}{c}x\right), & n = 2,4,6,\ldots \\ \sqrt{\frac{2}{c}}\cos\left(\frac{n\pi}{c}x\right), & n = 1,3,5,\ldots \end{cases}$$

which is similar to what we had in class, the only difference coming from the fact that we have assumed that the origin is in the middle of our bounds. If we followed the previous math used to obtain these ψ values but assumed the origin was at the left bound of a well with width $c/2$ we would obtain the in class solution as we would expect.

(iii) Orthogonality on functions is defined using the inner product of functions,

$$\int_{-c}^{c} f(x)g(x)\,dx$$

4

with the typical definition of orthogonality (0 means orthogonal). So,

$$= \int_{-c}^{c} \psi_1(x)\psi_2(x)\, dx$$

$$= \int_{-c}^{c} \sqrt{\frac{1}{c}} \cos\left(\frac{\pi}{2c}x\right) \sqrt{\frac{1}{c}} \sin\left(\frac{\pi}{c}x\right) dx$$

$$= c^{-1} \int_{-c}^{c} \cos\left(\frac{\pi}{2c}x\right) \sin\left(\frac{\pi}{c}x\right) dx \rightsquigarrow u = \frac{\pi}{2c}x \implies du = \frac{\pi}{2c}dx$$

$$= \frac{2}{\pi} \int_{-c}^{c} \cos(u) \sin(2u)\, du \rightsquigarrow \sin(2u) = 2\sin(u)\cos(u)$$

$$= \frac{2}{\pi} \int_{-c}^{c} 2\cos^2(u) \sin(u)\, du \rightsquigarrow s = \cos(u) \implies ds = -\sin(u)du$$

$$= -\frac{4}{\pi} \int_{-c}^{c} s^2\, ds$$

$$= -\frac{4}{3\pi} s^3 \Big|_{-c}^{c} = -\frac{4}{3\pi} \cos^3(u) \Big|_{-c}^{c} = -\frac{4}{3\pi} \cos^3\left(\frac{\pi}{2c}x\right) \Big|_{-c}^{c}$$

$$= -\frac{4}{3\pi} \left[\cos^3\left(\frac{\pi}{2c}c\right) - \cos^3\left(-\frac{\pi}{2c}c\right)\right] = 0$$