Phys 125
Boyda

Solutions to problems on wavefunctions in one dimension from the week of November 6.

1. A particle of mass m is in a potential well

$$V(x) = \begin{cases} 0 & 0 \le x \le 1 \\ V_0 & \text{otherwise} \end{cases},$$

with position x measured in angstroms. The wavefunction takes form

$$\psi(x) = \begin{cases} Ce^{qx} & x < 0 \\ Ae^{ikx} + Be^{-ikx} & 0 \le x < 1 \\ De^{-qx} & x \ge 1 \end{cases}.$$

We imposed conditions of continuity of the wavefunction and of the derivative at $x = \{0, 1\}$ to find two possible solutions:

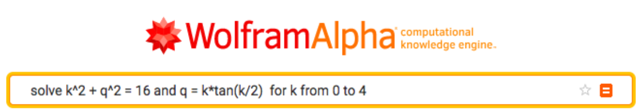
$$B = Ae^{ik} \quad \longleftrightarrow \quad q = k \tan \frac{k}{2} \tag{1}$$

$$B = -Ae^{ik} \quad \longleftrightarrow \quad q = -k \cot \frac{k}{2}, \tag{2}$$

along with the common condition

$$k^2 + q^2 = \frac{2mV_0}{\hbar^2} = 16.$$

The solution is given numerically or graphically, e.g. via Wolfram Alpha. You can enter:



and it reports (hovering the cursor over the dot on the graph)

$$k_1 = 2.060, \qquad q_1 = 3.429.$$

I've subscripted the k, q values to indicate that the solution satisfies the conditions in Eq. (1). The second solution comes from the cotangent case,

$$k_2 = 3.791, \qquad q_2 = 1.276.$$

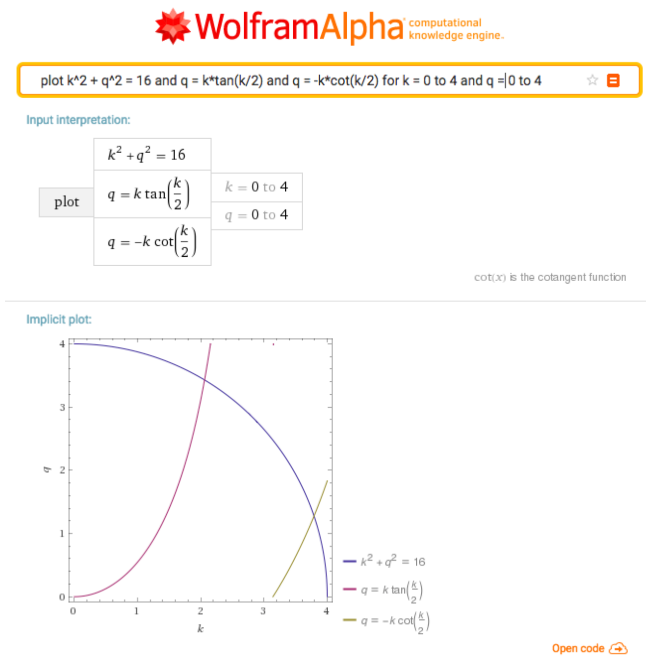


Figure 1: Bound state solutions to the finite square potential well for $2mV_0/\hbar^2 = 16$.

The two solutions are plotted together in Fig. 1.

It is easiest to find amplitudes C and D via continuity of the wavefunction at $x = \{0, 1\}$, whence

$$\text{(soln. 1)} \quad \begin{cases} C = A + B = A + Ae^{ik_1} \\ De^{-q_1} = Ae^{ik_1} + Be^{-ik_1} \longrightarrow D = e^{q_1}(Ae^{ik_1} + A) \end{cases}$$

$$\text{(soln. 2)} \quad \begin{cases} C = A + B = A - Ae^{ik_2} \\ De^{-q_2} = Ae^{ik_2} + Be^{-ik_2} \longrightarrow D = e^{q_2}(Ae^{ik_2} - A) \end{cases}$$

If you used continuity of the derivative to solve for C or D your solution will look different, but it should be equivalent to the above. Then you plug these values into the equation for $\psi(x)$ above and (optionally) normalize to determine the remaining unknown parameter A. Plots of the wavefunctions, offset by their energy relative to the well depth, are given in Fig. 2. The MATLAB code used to generate the plots is linked on our website.

Problem 2. We are given the momentum-space wavefunction

$$\psi(p) = \langle p|\psi\rangle = \sqrt{\frac{a}{\hbar\sqrt{\pi}}} e^{-(p-p_0)^2 a^2/2\hbar^2}.$$

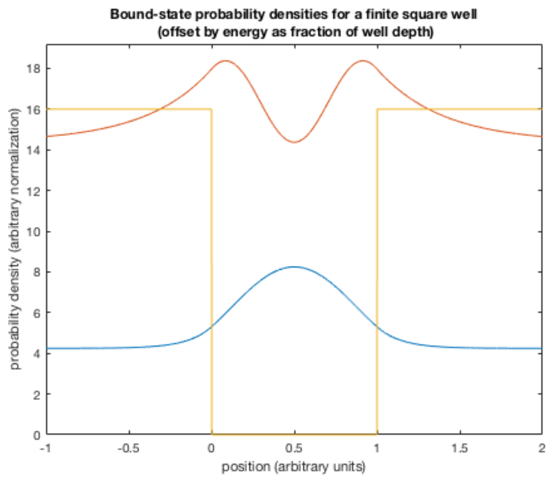


Figure 2: Bound state probability densities for the finite square potential well with $2mV_0/\hbar^2 = 16$.

This means the initial position-space wavefunction is a superposition of momentum eigenstates weighted by $\psi(p)$:

$$\psi(x,0) = \langle x|\psi\rangle = \int dp\, \langle x|p\rangle\langle p|\psi\rangle = \int dp\, \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\sqrt{\frac{a}{\hbar\sqrt{\pi}}}e^{-(p-p_0)^2a^2/2\hbar^2}.$$

We are told further that $a = \hbar/\sqrt{2}p_0$ and the average momentum p_0 is such that the average kinetic energy $p_0^2/2m = 10\,\mathrm{eV}$. Fortunately, the momentum eigenstates $|p\rangle$ are also eigenstates of $\hat{H} = \hat{p}_x^2/2m$, with eigenvalue $p^2/2m$, making it simple to apply the time evolution operator:

$$\psi(x,t) = e^{-iHt/\hbar}\psi(x,0) = \int dp\, e^{-i(p^2/2m)t/\hbar}\frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\sqrt{\frac{a}{\hbar\sqrt{\pi}}}e^{-(p-p_0)^2a^2/2\hbar^2}.$$

You might want to check the above equation by substituting the position-space representation of the $\hat{H}$ operator,

$$\hat{H} \xrightarrow[\text{x-rep}]{} H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}.$$

Do a u-substitution: $u = p - p_0$, $du = dp$. The limits of integration remain $(-\infty, \infty)$.

$$\begin{aligned}
\psi(x,t) &= \int du\, e^{-i((u+p_0)^2/2m)t/\hbar} \frac{e^{i(u+p0)x/\hbar}}{\sqrt{2\pi\hbar}} \sqrt{\frac{a}{\hbar\sqrt{\pi}}} e^{-u^2a^2/2\hbar^2} \\
&= e^{-i(p_0^2/2m)t/\hbar} e^{ip_0x/\hbar} \int du\, e^{-i(u^2+2up_0)/2m)t/\hbar} \frac{e^{iux/\hbar}}{\sqrt{2\pi\hbar}} \sqrt{\frac{a}{\hbar\sqrt{\pi}}} e^{-u^2a^2/2\hbar^2} \\
&= e^{-i(p_0^2/2m)t/\hbar} e^{ip_0x/\hbar} \int du\, e^{-i(u^2/2m)t/\hbar} \frac{e^{iu(x-(p_0t/m)/\hbar}}{\sqrt{2\pi\hbar}} \sqrt{\frac{a}{\hbar\sqrt{\pi}}} e^{-u^2a^2/2\hbar^2}.
\end{aligned}$$

The u is just a dummy variable of integration, and you can see that the integral is identical to the one derived in problem 6.4 for the time-evolution of the free-particle wavefunction in the $\langle p_x \rangle = 0$ case, with the substituion $x \to (x - p_0t/m)$. Since x is a constant with respect to the integration, we can simply carry that substitution through to the solution given to 6.4. The new overall phase drops out on taking the complex magnituded squared.

$$|\psi(x)|^2 = \frac{1}{\sqrt{\pi(a^2 + (\hbar t/ma)^2)}} e^{-(x-p_0t/m)^2/(a^2+(\hbar t/ma)^2)}.$$

The peak of the wavefunction is where $x = p_0t/m$, which is to say the particle moves rightward with mean speed $v_0 = p_0/m$, while undergoing spreading of its wavefunction. The time/distance scales suggested in the problem were better suited to a larger-spread wavepacket I had been playing with. The behavior I wanted you to see appears in Fig. 3. The corresponding MATLAB code is linked from our website.

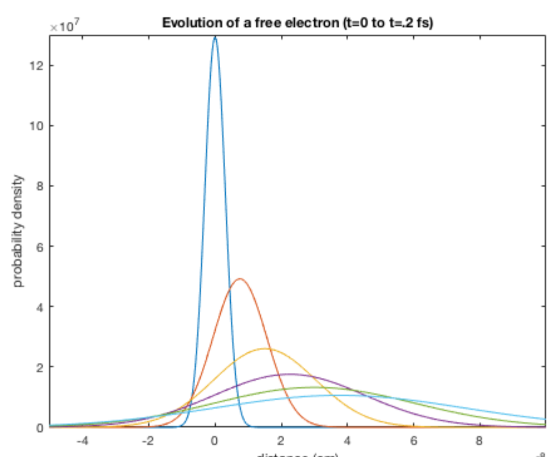


Figure 3: Six even time steps in the evolution of a free electron with mean energy 10 eV.

Problem 7.5. This problem asks you to derive eqns. 7.56 and 7.57. In the exicited states we still have $\langle x\rangle = 0$, $\langle p_x\rangle = 0$, because creation and annihilation operators turn $|n\rangle$ into $|n\pm 1\rangle$, which are orthogonal to $|n\rangle$. However,

$$\begin{aligned}
\langle p_x^2\rangle &= -\frac{m\omega\hbar}{2}\langle n|(\hat{a}-\hat{a}^\dagger)^2|n\rangle \\
&= -\frac{m\omega\hbar}{2}\langle n|(\hat{a}^2-\hat{a}\hat{a}^\dagger-\hat{a}^\dagger\hat{a}+\hat{(}a^\dagger)^2)|n\rangle \\
&= \frac{m\omega\hbar}{2}\langle n|(\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a})|n\rangle \\
&= \frac{m\omega\hbar}{2}\langle n|(2\hat{a}^\dagger\hat{a}+[\hat{a},\hat{a}^\dagger])|n\rangle \\
&= \frac{m\omega\hbar}{2}\langle n|(2n+1)|n\rangle \\
&= \frac{m\omega\hbar}{2}(2n+1) \qquad \Longrightarrow \\
\Delta p_x &= \sqrt{\langle p_x^2\rangle - \langle p_x\rangle^2} = \sqrt{(n+\frac{1}{2})m\omega\hbar}.
\end{aligned}$$

The computation for Δx is similar.

Problem 7.7. The energies of the ground and first excited state are equally probable, meaning each has weight $\frac{1}{\sqrt{2}}$ in the superposition, and choosing the overall phase so that the $|0\rangle$ term has real, positive coefficient,

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i\phi}}{\sqrt{2}}|1\rangle.$$

Further, we are given $\langle p_x\rangle = \sqrt{m\omega\hbar/2}$ at $t=0$:

$$\begin{aligned}
\sqrt{\frac{m\omega\hbar}{2}} = \langle p_x\rangle &= (\frac{1}{\sqrt{2}}\langle 0| + \frac{e^{-i\phi}}{\sqrt{2}}\langle 1|)(-i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}-\hat{a}^\dagger)(\frac{1}{\sqrt{2}}|0\rangle + \frac{e^{i\phi}}{\sqrt{2}}|1\rangle) \\
&= -\frac{i}{2}\sqrt{\frac{m\omega\hbar}{2}}\left(e^{i\phi}\langle 0|\hat{a}|1\rangle - e^{-i\phi}\langle 1|\hat{a}^\dagger|0\rangle\right) \\
&= -\frac{i}{2}\sqrt{\frac{m\omega\hbar}{2}}\left(e^{i\phi}\langle 0|\hat{a}|0\rangle - e^{-i\phi}\langle 1|1\rangle\right) \\
&= -\frac{i}{2}\sqrt{\frac{m\omega\hbar}{2}}\left(e^{i\phi} - e^{-i\phi}\right) \\
&= \sqrt{\frac{m\omega\hbar}{2}}\sin\phi.
\end{aligned}$$

Therefore $\phi = \pi/2$, and

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{i}{\sqrt{2}}|1\rangle.$$

At later times

$$|\psi(t)\rangle = \frac{e^{-i\omega t/2}}{\sqrt{2}}|0\rangle + \frac{ie^{-3i\omega t/2}}{\sqrt{2}}|1\rangle = e^{-i\omega t/2}\left(\frac{1}{\sqrt{2}}|0\rangle + \frac{ie^{-i\omega t}}{\sqrt{2}}|1\rangle\right).$$

You can see that the relative phase on $|1\rangle$, which was $e^{i\phi} = e^{i\pi/2} = i$, has become $ie^{-i\omega t} = e^{i\pi/2 - i\omega t}$. The previous calculation goes through with $\phi \to \pi/2 - \omega t$, and so

$$\langle p_x\rangle_{t\geq 0} = \sqrt{\frac{m\omega\hbar}{2}}\sin(\frac{\pi}{2} - \omega t) = \sqrt{\frac{m\omega\hbar}{2}}\cos\omega t.$$