1. a) First we need to normalize:

$$\left|\psi(t=0)\right\rangle = A\left[\left|0\right\rangle + 2e^{i\pi/2}\left|1\right\rangle\right]$$

$$1 = \left\langle \psi \middle| \psi \right\rangle = A^*\left(\left\langle 0\right| + 2e^{-i\pi/2}\left\langle 1\right|\right)A\left(\left|0\right\rangle + 2e^{i\pi/2}\left|1\right\rangle\right)$$

$$= |A|^2(1+4) = |A|^2\, 5$$

$$\Rightarrow A = \tfrac{1}{\sqrt{5}}$$

Then determine time-evolved state. We are in the energy basis, so include phase term:

$$\left|\psi(t)\right\rangle = \tfrac{1}{\sqrt{5}}\left(e^{-iE_0 t/\hbar}\left|0\right\rangle + 2e^{i\pi/2}e^{-iE_1 t/\hbar}\left|1\right\rangle\right)$$

$$= e^{-i\omega t/2}\,\tfrac{1}{\sqrt{5}}\left(\left|0\right\rangle + 2e^{i\pi/2}e^{-i\omega t}\left|1\right\rangle\right)$$

Find expectation values with ladder operators:

$$\langle x\rangle = \left\langle \psi(t)\middle| x \middle| \psi(t)\right\rangle = \sqrt{\tfrac{\hbar}{2m\omega}}\left\langle \psi(t)\middle| a^\dagger + a \middle|\psi(t)\right\rangle$$

$$= \sqrt{\tfrac{\hbar}{2m\omega}}e^{+i\omega t/2}\,\tfrac{1}{\sqrt{5}}\left(\left\langle 0\right| + 2e^{-i\pi/2}e^{+i\omega t}\left\langle 1\right|\right)\left(a^\dagger + a\right)e^{-i\omega t/2}\,\tfrac{1}{\sqrt{5}}\left(\left|0\right\rangle + 2e^{i\pi/2}e^{-i\omega t}\left|1\right\rangle\right)$$

$$= \sqrt{\tfrac{\hbar}{2m\omega}}\,\tfrac{1}{5}\left[2e^{i\pi/2}e^{-i\omega t}\left\langle 0\middle| a \middle| 1\right\rangle + 2e^{-i\pi/2}e^{+i\omega t}\left\langle 1\middle| a^\dagger \middle| 0\right\rangle\right]$$

$$= \sqrt{\tfrac{\hbar}{2m\omega}}\,\tfrac{2}{5}\left[ie^{-i\omega t}\sqrt{1} - ie^{+i\omega t}\sqrt{1}\right] = \sqrt{\tfrac{\hbar}{2m\omega}}\,\tfrac{4}{5}\sin\omega t$$

Momentum expectation value:

$$\langle p\rangle = \left\langle \psi(t)\middle| p \middle| \psi(t)\right\rangle = i\sqrt{\tfrac{m\omega\hbar}{2}}\left\langle \psi(t)\middle| a^\dagger - a \middle|\psi(t)\right\rangle$$

$$= i\sqrt{\tfrac{m\omega\hbar}{2}}e^{+i\omega t/2}\,\tfrac{1}{\sqrt{5}}\left(\left\langle 0\right| + 2e^{-i\pi/2}e^{+i\omega t}\left\langle 1\right|\right)\left(a^\dagger - a\right)e^{-i\omega t/2}\,\tfrac{1}{\sqrt{5}}\left(\left|0\right\rangle + 2e^{i\pi/2}e^{-i\omega t}\left|1\right\rangle\right)$$

$$= i\sqrt{\tfrac{m\omega\hbar}{2}}\,\tfrac{1}{5}\left[-2e^{i\pi/2}e^{-i\omega t}\left\langle 0\middle| a \middle| 1\right\rangle + 2e^{-i\pi/2}e^{+i\omega t}\left\langle 1\middle| a^\dagger \middle| 0\right\rangle\right]$$

$$= i\sqrt{\tfrac{m\omega\hbar}{2}}\,\tfrac{2}{5}\left[-ie^{-i\omega t}\sqrt{1} - ie^{+i\omega t}\sqrt{1}\right] = \sqrt{\tfrac{m\omega\hbar}{2}}\,\tfrac{4}{5}\cos\omega t$$

b) Ehrenfest's theorem in this case is

$$\langle p\rangle = m\frac{d}{dt}\langle x\rangle = m\frac{d}{dt}\left[\sqrt{\tfrac{\hbar}{2m\omega}}\,\tfrac{4}{5}\sin\omega t\right] = m\sqrt{\tfrac{\hbar}{2m\omega}}\,\tfrac{4}{5}\left[\omega\cos\omega t\right] = \sqrt{\tfrac{m\omega\hbar}{2}}\,\tfrac{4}{5}\cos\omega t$$

So it is satisfied.

c) Energy expectation value

$$\langle E\rangle = \left\langle \psi\middle| H \middle|\psi\right\rangle = e^{+i\omega t/2}\,\tfrac{1}{\sqrt{5}}\left(\left\langle 0\right| + 2e^{-i\pi/2}e^{+i\omega t}\left\langle 1\right|\right)He^{-i\omega t/2}\,\tfrac{1}{\sqrt{5}}\left(\left|0\right\rangle + 2e^{i\pi/2}e^{-i\omega t}\left|1\right\rangle\right)$$

$$= \tfrac{1}{5}\left[\left\langle 0\middle| H \middle| 0\right\rangle + 4\left\langle 1\middle| H \middle| 1\right\rangle\right]$$

$$= \tfrac{1}{5}\left[\tfrac{1}{2}\hbar\omega + 4\,\tfrac{3}{2}\hbar\omega\right]$$

$$= \tfrac{13}{10}\hbar\omega$$

Now find the standard deviation of the energy.

$$\Delta E = \sqrt{\left\langle \left(E - \langle E\rangle\right)^2 \right\rangle} = \sqrt{\left\langle E^2 - 2E\langle E\rangle + \langle E\rangle^2 \right\rangle} = \sqrt{\left\langle E^2\right\rangle - \langle E\rangle^2}$$

$$\begin{aligned}
\left\langle E^2\right\rangle &= \langle\psi|H^2|\psi\rangle = e^{+i\omega t/2}\tfrac{1}{\sqrt{5}}\left(\langle 0| + 2e^{-i\pi/2}e^{+i\omega t}\langle 1|\right)H^2 e^{-i\omega t/2}\tfrac{1}{\sqrt{5}}\left(|0\rangle + 2e^{i\pi/2}e^{-i\omega t}|1\rangle\right)\\
&= \tfrac{1}{5}\left[\langle 0|H^2|0\rangle + 4\langle 1|H^2|1\rangle\right]\\
&= \tfrac{1}{5}\left[\left(\tfrac{1}{2}\hbar\omega\right)^2 + 4\left(\tfrac{3}{2}\hbar\omega\right)^2\right]\\
&= \tfrac{37}{20}\hbar^2\omega^2
\end{aligned}$$

$$\Delta E = \sqrt{\tfrac{37}{20}\hbar^2\omega^2 - \left(\tfrac{13}{10}\right)^2\hbar^2\omega^2} = \hbar\omega\sqrt{\tfrac{16}{100}}$$

$$\boxed{\Delta E = \tfrac{4}{10}\hbar\omega}$$

2. a) When the energy of the incident particles is less than the height of the potential energy step, the wave function on the right side is a decaying exponential:

$$\varphi_E(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0 \\ Ce^{-qx}, & x > 0 \end{cases}$$

where

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

$$q = \sqrt{\frac{2m\left(V_0 - E\right)}{\hbar^2}}$$

The boundary conditions at the step are

$$\varphi(0): A + B = C$$

$$\left.\frac{d\varphi(x)}{dx}\right|_{x=0} : ikA - ikB = -qC$$

Substitute the first equation into the second equation and solve for the ratio of the reflected amplitude to the incident amplitude

$$ikA - ikB = -q\left(A + B\right)$$

$$ikA + qA = ikB - qB$$

$$\frac{B}{A} = \frac{ik + q}{ik - q}$$

The absolute square of this gives the reflection coefficient

$$R = \frac{|B|^2}{|A|^2} = \frac{ik + q}{ik - q} = \frac{k^2 + q^2}{k^2 + q^2} = 1$$

To conserve particles, we require that $R+T=1$, so the transmission is

$$T = 1 - R = 0$$

So 100% of the particles are reflected and there is no probability of transmission. There is some penetration of the wave function into the step, but the wave function decays to zero and never reaches infinity (where your detector is).

b) When the energy of the incident particles is greater than the height of the potential energy step, the wave function on the right side is a complex exponential:

$$\varphi_E(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x}, & x<0 \\ Ce^{ik_2x}, & x>0 \end{cases}$$

where

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$
$$k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

The boundary conditions at the step are

$$\varphi(0): A+B=C$$
$$\left.\frac{d\varphi(x)}{dx}\right|_{x=0} : ik_1A - ik_1B = ik_2C$$

Substitute the first equation into the second equation and solve for the ratio of the reflected amplitude to the incident amplitude

$$ik_1A - ik_1B = ik_2(A+B)$$
$$ik_1A - ik_2A = ik_1B + ik_2B$$
$$\frac{B}{A} = \frac{k_1-k_2}{k_1+k_2}$$

The absolute square of this gives the reflection coefficient

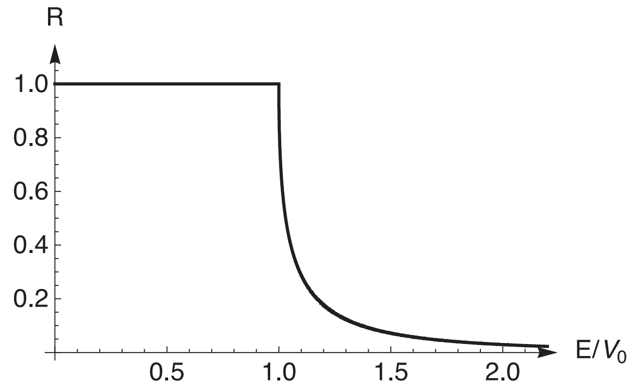
$$R = \frac{|B|^2}{|A|^2} = \frac{(k_1-k_2)^2}{(k_1+k_2)^2} = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2$$

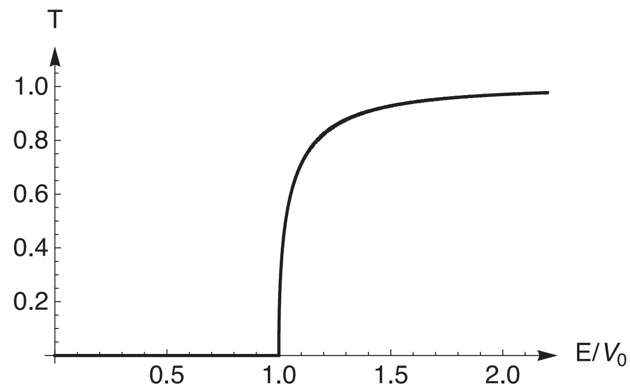
So less than 100% of the particles are reflected and there is some probability of transmission. To conserve particles, we require that $R+T=1$, so the transmission is

$$T = 1-R = 1-\frac{(k_1-k_2)^2}{(k_1+k_2)^2} = \frac{(k_1+k_2)^2-(k_1-k_2)^2}{(k_1+k_2)^2} = \frac{4k_1k_2}{(k_1+k_2)^2} = \frac{4\sqrt{E}\sqrt{E-V_0}}{\left(\sqrt{E}+\sqrt{E-V_0}\right)^2}$$

Note that $T \neq |C|^2 / |A|^2$ in this problem because the wave speeds on the two sides are different.

c) Plots:





The reflection is unity until the energy exceeds the step height, after which the reflection decreases monotonically. In the limit of large energy, $T \to 1$, as you might expect because the step becomes insignificant.

3. First we need to find the energy eigenvalue and eigenstates. Diagonalizing H yields the eigenvalues

$$\begin{vmatrix} E_0 - \lambda & 0 & A \\ 0 & E_1 - \lambda & 0 \\ A & 0 & E_0 - \lambda \end{vmatrix} = 0 \quad \Rightarrow \quad (E_0 - \lambda)^2 (E_1 - \lambda) - A^2 (E_1 - \lambda) = 0$$

$$\Rightarrow \quad (E_1 - \lambda)\left\{(E_0 - \lambda)^2 - A^2\right\} = 0 \quad \Rightarrow \quad \lambda = E_1, E_0 + A, E_0 - A$$

and the eigenvectors

$$\begin{pmatrix} E_0 & 0 & A \\ 0 & E_1 & 0 \\ A & 0 & E_0 \end{pmatrix}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = E_1\begin{pmatrix} u \\ v \\ w \end{pmatrix} \quad \Rightarrow \quad \begin{matrix} E_0 u + Aw = E_1 u \\ E_1 v = E_1 v \\ Au + E_0 w = E_1 w \end{matrix} \quad \Rightarrow \quad u = w = 0$$

$$|u|^2 + |v|^2 + |w|^2 = 1 \quad \Rightarrow \quad |v|^2 = 1 \quad \Rightarrow \quad u = 0, v = 1, w = 0 \quad \Rightarrow \quad |E_1\rangle = |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} E_0 & 0 & A \\ 0 & E_1 & 0 \\ A & 0 & E_0 \end{pmatrix}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = (E_0 \pm A)\begin{pmatrix} u \\ v \\ w \end{pmatrix} \quad \Rightarrow \quad \begin{matrix} E_0 u + Aw = (E_0 \pm A) u \\ E_1 v = (E_0 \pm A) v \\ Au + E_0 w = (E_0 \pm A) w \end{matrix} \quad \Rightarrow \quad v = 0, u = \pm w$$

$$|u|^2 + |v|^2 + |w|^2 = 1 \quad \Rightarrow \quad 2|u|^2 = 1 \quad \Rightarrow \quad u = \tfrac{1}{\sqrt{2}}, v = 0, w = \pm\tfrac{1}{\sqrt{2}}$$

$$\Rightarrow \quad |E_0 \pm A\rangle = \tfrac{1}{\sqrt{2}}|1\rangle \pm \tfrac{1}{\sqrt{2}}|3\rangle \doteq \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ \pm 1 \end{pmatrix}$$

(a) The initial state is

$$|\psi(0)\rangle = |2\rangle = |E_1\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

The time-evolved state is

$$|\psi(t)\rangle = e^{-iE_1 t/\hbar}|E_1\rangle \doteq \begin{pmatrix} 0 \\ e^{-iE_1 t/\hbar} \\ 0 \end{pmatrix}$$

The probability of measuring the system to be in state $|2\rangle$ is

$$\mathcal{P}_2 = \left|\langle 2|\psi(t)\rangle\right|^2 = \left|\langle 2|e^{-iE_1 t/2\hbar}|2\rangle\right|^2 = \left|e^{-iE_1 t/2\hbar}\right|^2 = 1$$

(b) The initial state is

$$|\psi(0)\rangle = |3\rangle = \tfrac{1}{\sqrt{2}}\left(|E_0 + A\rangle - |E_0 - A\rangle\right) \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

The time-evolved state is

$$
\begin{aligned}
\left|\psi(t)\right\rangle &= \tfrac{1}{\sqrt{2}}\left(e^{-i(E_0+A)t/\hbar}\left|E_0+A\right\rangle - e^{-i(E_0-A)t/\hbar}\left|E_0-A\right\rangle\right)\\
&\doteq \tfrac{1}{\sqrt{2}}e^{-i(E_0+A)t/\hbar}\tfrac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix} - \tfrac{1}{\sqrt{2}}e^{-i(E_0-A)t/\hbar}\tfrac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix}\\
&\doteq \tfrac{1}{2}e^{-iE_0t/\hbar}\begin{pmatrix}-2i\sin(At/\hbar)\\0\\2\cos(At/\hbar)\end{pmatrix}
\end{aligned}
$$

The probability of measuring the system to be in state $\left|3\right\rangle$ is

$$
\mathcal{P}_3 = \left|\left\langle 3\middle|\psi(t)\right\rangle\right|^2 = \left|\tfrac{1}{2}e^{-iE_0t/\hbar}2\cos(At/\hbar)\right|^2 = \cos^2(At/\hbar) = \tfrac{1}{2}\left(1+\cos(2At/\hbar)\right)
$$