1. **Problem 1**

Free Particle

A particle moves along the x-axis in free space. At $t = 0$, we find it in the state

$$\Psi(x,0) = \langle x|\Psi(0)\rangle = \mathcal{N}e^{-\gamma|x|},\ \gamma = \text{real}$$

(a) Find:

- $\mathcal{N}$ so that $\Psi(x,0)$ is normalized.
- is $\gamma = -100\text{Å}^{-1}$ a valid choice?
- The probability density $P(x,0)$ to find the particle between x and $x + dx$ at $t = 0$.
- The probability-current density $J(x,0)$ at $t = 0$.
- The time derivative $\frac{\delta}{\delta t}P(x,t)$ of the probability density at $t = 0$.

(b) What are the possible outcomes of a measurement of the momentum at $t = 0$? What is the probability to measure each allowed value? Do you expect these probabilities to change with time? Explain.

(c) Find $\langle x\rangle$, $\langle p\rangle$, and Δx for $t = 0$ and for $t > 0$.

(d) Find the average value of the energy at a positive time $t > 0$.

Solution.
a.) For this, we simply directly solve the inner product of the wavefunction with itself, or the integral

$$\int_{-\infty}^{\infty}\Psi(x,0)^{\star}\Psi(x,0)dx = 1$$

$$\int_{-\infty}^{\infty}\mathcal{N}^2e^{-2\gamma|x|}dx = \mathcal{N}^2\int_{-\infty}^{\infty}e^{-2\gamma|x|}dx$$
$$= 2\mathcal{N}^2\int_{0}^{\infty}e^{-2\gamma|x|}dx$$

and then utilizing the exponential integral

$$\int_0^{\infty}e^{-ax} = \frac{1}{a}$$

we arrive at a normalization constant of

$$\mathcal{N} = \sqrt{\gamma}$$

Regarding the second bullet point, $\gamma = -100\text{Å}^{-1}$ is not a valid choice because if $\gamma < 0$ then our normalization integral would diverge, and we would end up with a non-normalizable wavefunction.

The probability density for a wavefunction is defined as

$$\rho(x,0) = |\Psi(x,0)|^2 = \gamma e^{-2\gamma|x|}$$

which we got to immediately because we utilize the probability density to normalize a function, which we have already done.

For the fourth bullet point, we say that for any real function the probability-current density is zero. You can see this if you write out the equation for probabiltiy-current density,

$$\mathbf{J}(\mathbf{r},t) = -\frac{i\hbar}{2m}\left[\psi^*\nabla\psi - \psi\nabla\psi^*\right]$$

For the last bullet point, we immediately see our probability density has no time dependence, so the derivative of it is zero.

b.) The possible outcomes for a measurement of momentum are all of them within the range of $-\infty \to \infty$, as this has been the only restriction placed, and the momentum operator has continuous eigenvalues, not discrete. The probability to measure the allowed values is given by the postulate

$$P = |\langle p|\Psi(x,0)\rangle|^2$$

Since the wavefunction is currently represented in the position basis, we need to apply the fourier transform to get it into the momentum basis(which is what this is saying), so we write

$$\langle p|\Psi\rangle = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}} \sqrt{\gamma} e^{-\gamma|x|} dx$$

Since this deals with the absolute value of x, we need to split this into two integrals in order to evaluate it correctly,

$$\begin{aligned}\langle p|\Psi\rangle &= \sqrt{\frac{\gamma}{2\pi\hbar}}\left[\int_0^{\infty} e^{-(\gamma+\frac{ip}{\hbar})x}dx + \int_{-\infty}^{0} e^{(\gamma-\frac{ip}{\hbar})x}dx\right] \\ &= \sqrt{\frac{\gamma}{2\pi\hbar}}\left[\frac{1}{\gamma+ip/\hbar} + \frac{1}{\gamma-ip/\hbar}\right] \\ &= \sqrt{\frac{\gamma}{2\pi\hbar}}\frac{2\gamma}{\gamma^2+(\frac{p}{\hbar})^2}\end{aligned}$$

Now we plug this back into our probability postulate, and arrive at

$$P = |\langle p|\Psi(x,0)\rangle|^2$$
$$P = \left|\sqrt{\frac{\gamma}{2\pi\hbar}}\frac{2\gamma}{\gamma^2 + (\frac{p}{\hbar})^2}\right|^2$$
$$P = \frac{2\gamma^3}{\pi\hbar}\frac{1}{[\gamma^2 + (\frac{p}{\hbar})^2]^2}$$

so the probability of a certain momentum measurement is dependent upon both the "tightening" factor γ and the momentum p.

No we do not expect the momentum to change with time. Momentum states are also eigenstates of the Hamiltonian, so the probability will not be time dependent, if we write

$$P = |\langle p|\Psi(t)\rangle|^2 = |\langle p|e^{-iHt/\hbar}|\Psi(0)\rangle|^2 = |e^{-i\epsilon_p t/\hbar}\langle p|\Psi(0)\rangle|^2$$

it can be seen the "wiggle factor" disappears.
c.) We find the expectation value for position and momentum at $t = 0$ through the application of

$$\langle x\rangle = \langle\Psi|x|\Psi\rangle\,,\ \langle p\rangle = \langle\Psi|p|\Psi\rangle$$

The $\hat{x}$ operator in position space is simply x, so for the expectation value of x we can write

$$\langle x\rangle = \int_{-\infty}^{\infty} x\rho(x,0) = \gamma\int_{-\infty}^{\infty} xe^{-2\gamma|x|}$$

and we see this is an odd function, so we can automatically see the result of this integral is 0, leaving us with

$$\langle x\rangle = 0$$

For the momentum, we could also see that it would be an odd function or from Ehrenfest theorem see that the expectation value of momentum would also be zero,

$$\langle p\rangle = 0$$

We find the standard deviation of an operator through

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$$

and we have already shown that the expectation value of x is zero, so all we need to find is the expectation value of x^2.

$$\langle x^2\rangle = \langle\Psi|x^2|\Psi\rangle$$
$$= \int_{-\infty}^{\infty} x^2\rho(x,0) = \gamma\int_{-\infty}^{\infty} x^2 e^{-2\gamma|x|}$$

utilizing another definite exponential integral, we have

$$\langle x^2 \rangle = \frac{1}{2\gamma^2},\ \Delta x = \frac{1}{\gamma\sqrt{2}}$$

For $t > 0$, from Ehrenfest we immediately see that $\langle x \rangle, \langle p \rangle$ are independent of time and do not change. The only thing that may change is the uncertainty in x, so we know from above that we need to find

$$\langle x^2 \rangle_t = ?$$

To solve for this, we utilize the *Heisenberg Equation of Motion*, which relates the time evolution of any operator to its ability to commute with the Hamiltonian of the system.

$$i\hbar \frac{\delta \langle A \rangle}{\delta t} = \langle [A, H] \rangle$$

so for our case we have

$$\frac{\delta \langle x^2 \rangle}{\delta t} = \frac{1}{i\hbar} \langle [x^2, H] \rangle$$

We can further simplify this by remembering that we are describing a free particle, so there is no potential to act on it, so we can rewrite our Hamiltonian as

$$\frac{\delta \langle x^2 \rangle}{\delta t} = \frac{1}{i\hbar} \langle \left[x^2, \frac{p^2}{2m} \right] \rangle$$

we factor out the constants, and our commutator simplifies to

$$\frac{\delta \langle x^2 \rangle}{\delta t} = \frac{1}{2m\hbar i} \langle [x^2, p^2] \rangle$$

so for our free particle we describe how the expectation value of x^2 changes in time in terms of the ability of this operator to commute with the p^2 operator of the system. Using commutation relations we factor out factors of x, p to attempt to get to the canonical commutation relation for position and momentum,

$$\begin{aligned} [x^2, p^2] &= x[x, p^2] + [x, p^2]x \\ x[x, p^2] &= xp[x, p] + x[x, p]p \\ [x, p^2]x &= p[x, p]x + [x, p]px \end{aligned}$$

$$\rightarrow [x^2, p^2] = xp[x, p] + x[x, p]p + p[x, p]x + [x, p]px$$

now we plug in $[x, p] = i\hbar$, and we have

$$\langle [x^2, p^2] \rangle = i\hbar \langle xp + xp + px + px \rangle = 2i\hbar \langle xp + px \rangle$$

So to turn back to how our expectation value of x^2 changes in time, we now have

$$\frac{\delta \langle x^2 \rangle}{\delta t} = \frac{1}{m} \langle xp + px \rangle$$

And now we must seek to describe how this expectation value changes in time. You may think we are kind of running in circles, but you will see that we will find a way to express this soon enough, just think of what we are doing as the same sort of process one takes when solving for a differential equation, where each expectation value can be thought of as the next function.

$$\frac{\delta \langle xp + px \rangle}{\delta t} = \frac{1}{2m\hbar i} \langle [xp + px, p^2] \rangle$$

I will omit the steps, but following the same process as the previous one, we arrive at

$$\frac{\delta \langle xp + px \rangle}{dt} = \frac{1}{2mi\hbar} 4i\hbar \langle p^2 \rangle = \frac{2 \langle p^2 \rangle_t}{m}$$

Our next step would be to check and see if the rabbit hole goes any deeper by seeing how this new operator changes in time, but we can see that this would now be zero due to $[p^2, H] = [p^2, p^2]$. We now see that when we plug these back into our time changing value of x^2, we arrive at

$$\frac{\delta \langle x^2 \rangle}{\delta t} = \frac{2 \langle p^2 \rangle_t}{m^2} t + \frac{1}{m} \langle xp + px \rangle_0$$

The integral of this results in(taking into account an offset by $\langle x^2 \rangle_0$),

$$\langle x^2 \rangle_t = \frac{\langle p^2 \rangle}{m^2} t^2 + \frac{\langle xp + px \rangle_0}{m} t + \langle x^2 \rangle_0$$

Now we just need to actually calculate these expectation values using integration. Without going through the process, we know what the last term is from our previous work, the second term ends up being zero due to an imaginary integral, and the first term gives a value of $\gamma^2 \hbar^2$. Plugging this all in, we now have our answer for this time dependent expectation value as

$$\langle x^2 \rangle_t = \frac{\hbar^2 \gamma^2}{m^2} t^2 + \frac{1}{2\gamma^2}$$

and our standard devation in time as

$$\Delta x = \sqrt{\frac{\hbar^2 \gamma^2}{m^2} t^2 + \frac{1}{2\gamma^2}}$$

d.) The Hamiltonian is invariant of time, so we write

$$\langle H \rangle = \langle \Psi | H | \Psi \rangle$$

or we can solve this quicker by realizing that we already solved for the expectation value of the only operator in the Hamiltonian, and instead write the following, finishing our solution.

$$H = \frac{\langle p^2 \rangle_0}{2m} = \frac{\gamma^2 \hbar^2}{2m}$$

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