Quantum Mechanics I - PSet 3

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Exercise 1

- (a) We compute the RHS

$$\begin{aligned} [A, B]C + B[A, C] &= (AB - BA)C + B(AC - CA) \\ &= ABC - BAC + BAC - BCA \\ &= [A, BC]. \end{aligned} \tag{1.1}$$

- (b) The idea is the same as above.

- (c) We have

$$\begin{aligned} [A, [B, C]] + [C, [A, B]] + [B, [C, A]] &= A(BC - CB) - (BC - CB)A \\ &+ C(AB - BA) - (AB - BA)C + B(CA - AC) - (CA - AC)B = 0. \end{aligned} \tag{1.2}$$

- (d) Consider the action on a test function ϕ

$$\begin{aligned} [\hat{x}^n, \hat{p}]\phi &= x^n \frac{\hbar}{i}\frac{\partial \phi}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}\left(x^n \phi\right) \\ &= x^n \frac{\hbar}{i}\frac{\partial \phi}{\partial x} - \frac{\hbar}{i}\left(n x^{n-1}\phi + x^n \frac{\partial \phi}{\partial x}\right) \\ &= \left(i\hbar n x^{n-1}\right)\phi. \end{aligned} \tag{1.3}$$

Let $\partial_n := \partial^n / \partial x^n$. We have

$$[\hat{x}, \hat{p}^n]\phi = x\frac{\hbar^n}{i^n}\frac{\partial^n \phi}{\partial x^n} - \frac{\hbar^n}{i^n}\frac{\partial^n}{\partial x^n}\left(x\phi\right). \tag{1.4}$$

Let us look at

$$\begin{aligned} \partial_n \left(x\phi\right) &= \partial_{n-1}\left(\phi + x\partial_1\phi\right) = \partial_{n-1}\phi + \partial_{n-2}\left(\partial_1\phi + x\partial_2\phi\right) \\ &= 2\partial_{n-1}\phi + \partial_{n-2}\left(x\partial_2\phi\right) \\ &= 3\partial_{n-1}\phi + \partial_{n-3}\left(x\partial_3\phi\right) \end{aligned} \tag{1.5}$$

We now prove by induction that

$$\partial_n \left(x\phi\right) = n\partial_{n-1}\phi + x\partial_n\phi. \tag{1.6}$$

For $n = 1$ this is clearly true, note that $\partial_0 = Id$, the identity. Using the induction hypothesis, we have

$$\begin{aligned}
\partial_{n+1}(x\phi) &= \partial_1 \left(n\partial_{n-1}\phi + x\partial_n\phi\right) \\
&= n\partial_n\phi + \partial_n\phi + x\partial_{n+1}\phi \\
&= (n+1)\partial_n\phi + x\partial_{n+1}\phi,
\end{aligned} \tag{1.7}$$

as we wanted to show. We conclude then that

$$[\hat{x}, \hat{p}^n] = -\frac{\hbar^n}{i^n} n\partial_{n-1}. \tag{1.8}$$

- (e)

$$\begin{aligned}
[\hat{x}\hat{p}, \hat{x}^2]\phi &= x\hat{p}\left(x^2\phi\right) - x^3\hat{p}\phi = x\frac{\hbar}{i}(2x\phi + x^2\partial_x\phi) - x^3\frac{\hbar}{i}\partial_x\phi \\
&= 2x^2\frac{\hbar}{i}\phi.
\end{aligned} \tag{1.9}$$

Therefore $[\hat{x}\hat{p}, \hat{x}^2] = -2i\hbar x^2$. Finally,

$$\begin{aligned}
[\hat{x}\hat{p}, \hat{p}^2]\phi &= ix\hbar^3\partial_3\phi - i\hbar^3\partial_2\left(x\partial_1\phi\right) \\
&= ix\hbar^3\partial_3\phi - i\hbar^3\left(2\partial_2\phi + x\partial_3\phi\right) \\
&= -2i\hbar^3\partial_2\phi.
\end{aligned} \tag{1.10}$$

where we used the previous result. Therefore $[\hat{x}\hat{p}, \hat{p}^2] = -2i\hbar^3\partial_2 = 2i\hbar\hat{p}^2$.

Exercise 2

- (a) The phase is time-independent and given by $\varphi(k) = ikx$. It is stationary when $(d\varphi/dk)(k_0) = 0 = ix$. Thus, we expect the maximum of $|\Psi(x)|$ to occur at $x = 0$. Computing the integral explicitly we have

$$\int_{\mathbb{R}} e^{-L^2(k-k_0)^2+ikx}dk = e^{-L^2k_0^2}\int_{\mathbb{R}} e^{-L^2k^2+k\left(2L^2k_0+ix\right)}dk. \tag{1.11}$$

Using the given integral with $a = L^2 > 0$ and $b = (2L^2k_0 + ix)$ we have that

$$\Psi(x) = e^{-L^2k_0^2}\frac{\sqrt{\pi}}{L}e^{\frac{(2L^2k_0+ix)^2}{4L^2}} = \frac{\sqrt{\pi}}{L}e^{-\left(\frac{x}{2L}\right)^2}e^{ik_0x}. \tag{1.12}$$

Thus

$$|\Psi(x)| = \frac{\sqrt{\pi}}{L}e^{-\left(\frac{x}{2L}\right)^2}, \tag{1.13}$$

which is a Gaussian with a maximum at $x = 0$.

- (b) We now have $\varphi(k) = ik(x-x_0)$ and, as before, it is stationary when $(d\varphi/dk)(k_0) = 0 = i(x-x_0)$, i.e. when $x = x_0$. By explicit computation we have

$$\int_{\mathbb{R}} e^{-L^2(k-k_0)^2+ikx}dk = e^{-L^2k_0^2}\int_{\mathbb{R}} e^{-L^2k^2+k\left(2L^2k_0+i(x-x_0)\right)}dk. \tag{1.14}$$

We conclude, comparing with the above result, that

$$\Psi(x) = \frac{\sqrt{\pi}}{L}e^{-\left(\frac{x-x_0}{2L}\right)^2}e^{ik_0(x-x_0)}, \tag{1.15}$$

and therefore $|\Psi(x)|$ will have a maximum at $x = x_0$, being given by a Gaussian centered at x_0.

Exercise 3

- (a) We consider the Schrödinger's equation for the free particle in 1D

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}, \tag{1.16}$$

and we want to show that it is Galilean invariant. Let $x' = x - vt$, $t' = t$ and suppose

$$\Psi'(x', t') = f(x,t)\Psi(x,t), \tag{1.17}$$

also satisfies

$$i\hbar\frac{\partial\Psi'}{\partial t'} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi'}{\partial x'^2}. \tag{1.18}$$

We want to determine $f(x,t)$. We have

$$\frac{\partial\Psi'}{\partial t'} = \partial_t(f\Psi)\frac{dt}{dt'} + \partial_x(f\Psi)\frac{\partial x}{\partial t'} = f_t\Psi + f\Psi_t + vf_x\Psi + fv\Psi_x, \tag{1.19}$$

and

$$\frac{\partial\Psi'}{\partial x'} = \partial_x(f\Psi)\frac{\partial x}{\partial x'} = f_x\Psi + f\Psi_x, \tag{1.20}$$

and finally

$$\frac{\partial^2\Psi'}{\partial x'^2} = f_{xx}\Psi + 2f_x\Psi_x + f\Psi_{xx}. \tag{1.21}$$

Replacing on the Schrödinger's equation in the prime coordinates we get

$$i\hbar\left(f_t\Psi + f\Psi_t + vf_x\Psi + vf\Psi_x\right) = -\frac{\hbar^2}{2m}\left(f_{xx}\Psi + 2f_x\Psi_x + f\Psi_{xx}\right). \tag{1.22}$$

Using Schrödinger's equation on the (x,t) frame we get

$$i\hbar\left(f_t\Psi + vf_x\Psi + vf\Psi_x\right) = -\frac{\hbar^2}{2m}\left(f_{xx}\Psi + 2f_x\Psi_x\right), \tag{1.23}$$

and thus

$$\left(i\hbar f_t + i\hbar v f_x + (\hbar^2/(2m))f_{xx}\right)\Psi = \left(-i\hbar v f - (\hbar^2/m)f_x\right)\Psi_x. \tag{1.24}$$

If this is to hold for any Ψ we must have

$$\begin{cases} i\hbar f_t + i\hbar v f_x + (\hbar^2/(2m))f_{xx} = 0 \\ -i\hbar v f - (\hbar^2/m)f_x = 0. \end{cases} \tag{1.25}$$

From the second equation we have

$$i\hbar v f = -(\hbar^2/m)f_x, \tag{1.26}$$

or equivalently

$$\frac{f_x}{f} = -\frac{imv}{\hbar}. \tag{1.27}$$

Integrating both sides on x we get

$$f(x,t) = g(t)e^{-\frac{imvx}{\hbar}}, \tag{1.28}$$

for some $g(t)$ which we still have to find. Using our first equation we have

$$i\hbar g'(t)e^{-\frac{imvx}{\hbar}} + mv^2 g(t)e^{-\frac{imvx}{\hbar}} - \frac{mv^2}{2}g(t)e^{-\frac{imvx}{\hbar}} = 0, \tag{1.29}$$

$$g'(t)i\hbar = -g(t)\left(\frac{mv^2}{2}\right), \tag{1.30}$$

Integrating in t we obtain

$$g(t) = Ce^{\frac{imv^2}{2\hbar}t}, \tag{1.31}$$

for some constant $C \in \mathbb{R}$. Thus, taking $C = 1$, we finally obtain

$$f(x,t) = e^{-i\left(\frac{mv}{\hbar}x - \frac{mv^2}{2\hbar}t\right)}. \tag{1.32}$$

- (b) Let

$$\Psi(x,t) = Ae^{i(kx-\omega t)}, \tag{1.33}$$

and thus

$$\Psi'(x',t') = Ae^{-i\left(\frac{mv}{\hbar}(x'+vt') - \frac{mv^2}{2\hbar}t'\right)}e^{i(k(x'+vt')-\omega t')}. \tag{1.34}$$

We just need to check that this indeed solves the Schrödinger equation. We first simplify to obtain

$$\Psi'(x',t') = Ae^{i\left(k-\frac{mv}{\hbar}\right)x' + i\left(kv-\omega-\frac{mv^2}{2\hbar}\right)t'}. \tag{1.35}$$

We compute

$$\frac{\partial\Psi'}{\partial t'} = i\left(kv-\omega-\frac{mv^2}{2\hbar}\right)Ae^{i\left(k-\frac{mv}{\hbar}\right)x' + i\left(kv-\omega-\frac{mv^2}{2\hbar}\right)t'}, \tag{1.36}$$

and

$$\frac{\partial^2\Psi'}{\partial x'^2} = -\left(k-\frac{mv}{\hbar}\right)^2 Ae^{i\left(k-\frac{mv}{\hbar}\right)x' + i\left(kv-\omega-\frac{mv^2}{2\hbar}\right)t'}. \tag{1.37}$$

We use now the fact that $E = \hbar\omega$, $p = \hbar k$ and $E = p^2/2m$ to get $\omega = \frac{\hbar k^2}{2m}$. Thus, the LHS is given by

$$\begin{aligned} & -\hbar\left(kv - \frac{\hbar k^2}{2m} - \frac{mv^2}{2\hbar}\right) \\ = \quad & -\hbar kv + \frac{\hbar^2 k^2}{2m} + \frac{mv^2}{2}, \end{aligned} \tag{1.38}$$

while the RHS is

$$\begin{aligned} & \frac{h^2}{2m}\left(k^2 - \frac{2kmv}{\hbar} + \frac{m^2v^2}{\hbar^2}\right) \\ = \quad & \frac{\hbar^2k^2}{2m} - kv\hbar + \frac{mv^2}{2}, \end{aligned} \tag{1.39}$$

confirming that indeed $\Psi'(x',t')$ is a solution to Schrödinger's equation in the primed frame. We also have, from (1.35)

$$k' = k - \frac{mv}{\hbar}, \tag{1.40}$$

and

$$\omega' = kv - \omega - \frac{mv^2}{2\hbar} = kv - \frac{\hbar k^2}{2m} - \frac{mv^2}{2\hbar}. \tag{1.41}$$

Thus

$$\hbar\omega' = kv\hbar - \frac{\hbar^2k^2}{2m} - \frac{mv^2}{2} = -\frac{\hbar^2}{2m}\left(k-\frac{mv}{\hbar}\right)^2 = -\frac{\hbar^2k'^2}{2m}. \tag{1.42}$$

Remark 1.1. *The minus sign disappears if we take*

$$\Psi'(x',t') = Ae^{i\left(k-\frac{mv}{\hbar}\right)x' - i\left(-kv+\omega+\frac{mv^2}{2\hbar}\right)t'}. \tag{1.43}$$

Exercise 4

The Schrödinger's equation in 3D is given by

$$i\hbar\frac{\partial\Psi}{\partial t}(\vec{x},t) = -\frac{\hbar^2}{2m}\left(\Delta\Psi(\vec{x},t) + V(\vec{x},t)\right). \tag{1.44}$$

We have

$$\begin{aligned}
\frac{\partial\rho(\vec{x},t)}{\partial t} &= \frac{\partial}{\partial t}|\Psi(\vec{x},t)|^2 = \frac{\partial}{\partial t}\left(\Psi^*(\vec{x},t)\Psi(\vec{x},t)\right) = \Psi_t^*\Psi + \Psi^*\Psi_t \\
&= -\frac{i\hbar}{2m}\left(\Delta\Psi^* + V\Psi^*\right)\Psi + \frac{i\hbar}{2m}\Psi^*\left(\Delta\Psi + V\Psi\right) \\
&= \frac{i\hbar}{2m}\left(\Psi^*(\Delta\Psi) - (\Delta\Psi^*)\Psi\right) \\
&= \nabla\cdot\left[\frac{i\hbar}{2m}\left(\Psi^*(\nabla\Psi) - (\nabla\Psi^*)\Psi\right)\right] \\
&= -\nabla\cdot\left[\frac{\hbar}{m}\left(\mathrm{Im}(\Psi^*\nabla\Psi)\right)\right].
\end{aligned} \tag{1.45}$$

Thus, defining

$$\vec{J} = \frac{\hbar}{m}\left(\mathrm{Im}(\Psi^*\nabla\Psi)\right), \tag{1.46}$$

we obtain

$$\frac{\partial\rho(\vec{x},t)}{\partial t} = -\nabla\cdot\vec{J}(\vec{x},t), \tag{1.47}$$

or

$$\frac{\partial\rho(\vec{x},t)}{\partial t} + \nabla\cdot\vec{J}(\vec{x},t) = 0. \tag{1.48}$$

Exercise 5

We have

$$\Psi(x,0) = \Psi_1(x,0) + \Psi_2(x,0). \tag{1.49}$$

The overlap is given by

$$\gamma(t) = \int_{\mathbb{R}}\Psi_1^*(x,t)\Psi_2(x,t)dx. \tag{1.50}$$

We are interest in how $\gamma(t)$ evolves in time so we look at

$$\frac{\partial\gamma}{\partial t} = \int_{\mathbb{R}}\partial_t\Psi_1^*(x,t)\Psi_2(x,t) + \Psi_1^*(x,t)\partial_t\Psi_2(x,t)dx. \tag{1.51}$$

Assuming both particles are under the action of the same Hermitian Hamiltonian operator $\hat{H}$, we have by the Schrödinger's equation

$$\frac{\partial\gamma}{\partial t} = \int_{\mathbb{R}}\frac{i}{\hbar}\left((\hat{H}\Psi_1)^*\Psi_2 - \Psi_1^*(\hat{H}\Psi_2)\right)dx = 0, \tag{1.52}$$

by using Hermiticity of $\hat{H}$, i.e. $(\hat{H}\Psi_1)^*\Psi_2 = \Psi_1^*\hat{H}\Psi_2$. Thus, we conclude that

$$|\gamma(t)| = |\gamma(0)|. \tag{1.53}$$

Exercise 6

Recalling the definition

$$J = \frac{\hbar}{m} \left(\text{Im}(\Psi^* \partial_x \Psi) \right). \tag{1.54}$$

- (a) We have

  $$J = \frac{\hbar}{m} \text{Im} \left(A^* e^{\gamma x} A \gamma e^{\gamma x} \right) = \frac{\hbar}{m} \text{Im} \left(\gamma |A|^2 e^{\gamma x} \right) = 0, \tag{1.55}$$

  since $\gamma \in \mathbb{R}$.

- (b) We have

  $$J = \frac{\hbar}{m} \text{Im} \left(N(x) e^{-iS(x)/\hbar} iS'(x) N(x)/\hbar e^{iS(x)/\hbar} \right) = \frac{N^2(x) S'(x)}{m}. \tag{1.56}$$

  since $N(x), S(x) \in \mathbb{R}$.

- (c) We have

  $$\begin{aligned} J &= \frac{\hbar}{m} \text{Im} \left[\left(A^* e^{-ikx} + B^* e^{ikx} \right) \left(ikAe^{ikx} - ikBe^{-ikx} \right) \right] \\ &= \frac{\hbar}{m} \text{Im} \left[ik|A|^2 - ikA^* Be^{-2ikx} + ikB^* Ae^{2ikx} - ik|B|^2 \right] \\ &= \frac{\hbar}{m} \text{Im} \left[ik|A|^2 + ik \left(2i \text{Im}((Be^{-2ikx})^* A) \right) - ik|B|^2 \right] \\ &= \frac{\hbar}{m} \text{Im} \left[ik|A|^2 - k \left(2 \text{Im}((Be^{-2ikx})^* A) \right) - ik|B|^2 \right] \\ &= \frac{\hbar k}{m} \left(|A|^2 - |B|^2 \right), \end{aligned} \tag{1.57}$$

  where $A, B \in \mathbb{C}$.