Introduction to Quantum Mechanics – Solutions to Problem sheet 6

1. Harmonic oscillator eigenstates and Hermite polynomials

(a) Using the relation $H_n'(x) = 2nH_{n-1}(x)$ we find

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}x}H_n(x)\mathrm{e}^{-x^2/2} &= H_n'(x)\mathrm{e}^{-x^2/2} - xH_n(x)\mathrm{e}^{-x^2/2}\\ &= 2nH_{n-1}(x)\mathrm{e}^{-x^2/2} - xH_n(x)\mathrm{e}^{-x^2/2},\end{aligned}$$

and

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}H_n(x)\mathrm{e}^{-x^2/2} = \left(4n(n-1)H_{n-2}(x) - 4nxH_{n-1}(x) - (1-x^2)H_n(x)\right)\mathrm{e}^{-x^2/2}.$$

Thus, we find

$$-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}H_n(x)\mathrm{e}^{-x^2/2}+\frac{1}{2}x^2H_n(x)\mathrm{e}^{-x^2/2} = \left(-2n(n-1)H_{n-2}(x) + 2nxH_{n-1}(x) + \frac{1}{2}H_n(x)\right)\mathrm{e}^{-x^2/2}$$

On the other hand, we have the recursion relation $H_n(x) = 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x)$, and thus,

$$\hat{H}\left(H_n(x)\mathrm{e}^{-x^2/2}\right) = \left(n+\tfrac{1}{2}\right)H_n(x)\mathrm{e}^{-x^2/2}.$$

(b) Figure 1 shows the first five functions $H_n(x)\mathrm{e}^{-x^2/2}$.

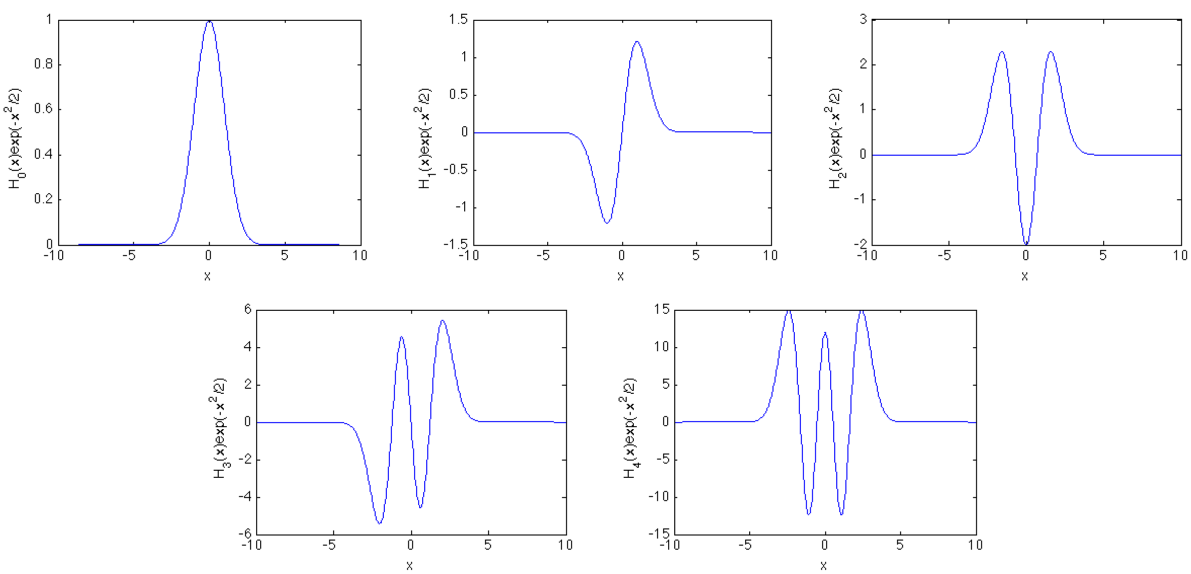

Figure 1: The first five of the unnormalised harmonic oscillator eigenfunctions.

2. Exercise: Momentum representation

(a) The eigenvalue equation for $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ reads

$$-i\hbar\frac{\partial}{\partial x}\phi_p(x) = p\phi_p(x),$$

from which it follows that $\phi_p(x) \propto \mathrm{e}^{i\frac{px}{\hbar}}$, for any $p \in \mathbb{C}$. That some of the eigenvalues are complex has to do with the fact that although $\hat{p}$ is Hermitian on $L^2(\mathbb{R})$, it is unbounded, and in fact does not have any eigenfunctions in $L^2(\mathbb{R})$ at all. None of the functions $\phi_p(x)$ is normalisable. For real values of p, however, $|\phi_p(x)|$ is bounded, while for complex p it diverges. Thus, $\hat{p}$ does not have eigenfunctions in L^2. Nevertheless the functions $\phi_p(x)$ with real p form a complete basis for the space L^2.

(b) For real p the functions fulfil the generalised orthonormality condition

$$\int_{-\infty}^{\infty} \phi_p^*(x)\phi_{p'}(x)dx \propto \int_{-\infty}^{\infty} \mathrm{e}^{-i(p'-p)x/\hbar}dx = 2\pi\hbar\delta(p'-p),$$

where $\delta(x)$ denotes the Dirac delta function. Thus, we find the position representation of the "normalised" eigenfunctions

$$\langle x|\phi_p\rangle = \phi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{i\frac{px}{\hbar}}.$$

(c) Consider an arbitrary wave function $|\psi\rangle$, in the position representation this is described by

$$|\psi\rangle = \int_{-\infty}^{\infty} \psi(x)|x\rangle dx,$$

with the coefficients $\psi(x) = \langle x|\psi\rangle$.
We now want to deduce the coefficients $\tilde{\psi}(p)$ in the momentum basis with

$$|\psi\rangle = \int_{-\infty}^{\infty} \tilde{\psi}(p)|\phi_p\rangle dp,$$

in dependence on the $\psi(x)$. By definition these coefficients are given by

$$\tilde{\psi}(p) = \langle\phi_p|\psi\rangle.$$

That is

$$\begin{aligned}
\tilde{\psi}(p) &= \langle\phi_p|\left(\int_{-\infty}^{\infty} \psi(x)|x\rangle dx\right) \\
&= \int_{-\infty}^{\infty} \psi(x)\langle\phi_p|x\rangle dx \\
&= \int_{-\infty}^{\infty} \psi(x)\phi_p^*(x)dx \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \psi(x)\mathrm{e}^{-ipx/\hbar}dx
\end{aligned}$$

Thus the wave function in momentum representation is the Fourier transform of the wave function in position representation (up to a scaling factor of $\hbar$).
Remark: This is one way of thinking about Heisenberg's uncertainty principle: If $\psi(x)$ is a very sharp distribution (localised), $\tilde{\psi}(p)$ is very broad (delocalised).

3. Gaussian states and the lower limit of Heisenberg's uncertainty principle

For the state $|\psi\rangle$ to saturate the lower bound of the uncertainty relation it needs to hold

$$(\hat{A} - \langle\hat{A}\rangle - \mathrm{i}\lambda(\hat{B} - \langle\hat{B}\rangle))|\psi\rangle = 0,$$

for some $\lambda \in \mathbb{R}$. That is

$$\hat{A}|\psi\rangle = (\langle\hat{A}\rangle + \mathrm{i}\lambda(\hat{B} - \langle\hat{B}\rangle))|\psi\rangle.$$

In particular, for $\hat{p}$ and $\hat{q}$ in position representation that means

$$-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) = (\langle\hat{p}\rangle - \mathrm{i}\lambda\langle\hat{q}\rangle)\psi(x) + \mathrm{i}\lambda x\psi(x).$$

Separating variables and integrating that is

$$\begin{aligned} -\mathrm{i}\hbar\int\frac{\mathrm{d}\psi(x)}{\psi(x)} &= \int(\langle\hat{p}\rangle - \mathrm{i}\lambda\langle\hat{q}\rangle + \mathrm{i}\lambda x)\mathrm{d}x \\ -\mathrm{i}\hbar\ln(\psi(x)) &= (\langle\hat{p}\rangle - \mathrm{i}\lambda\langle\hat{q}\rangle)x + \mathrm{i}\frac{\lambda}{2}x^2. \end{aligned}$$

That is

$$\psi(x) = \exp\left(-\frac{\lambda}{2\hbar}x^2 + \frac{\mathrm{i}}{\hbar}\langle\hat{p}\rangle x + \frac{\lambda}{\hbar}\langle\hat{q}\rangle x\right)$$

Rewriting this slightly leads to

$$\psi(x) = \exp\left(-\frac{\lambda}{2\hbar}(x - \langle\hat{q}\rangle)^2 + \frac{\mathrm{i}}{\hbar}\langle\hat{p}\rangle(x - \langle\hat{q}\rangle) + \frac{\lambda}{2\hbar}\langle\hat{q}\rangle^2 + \frac{\mathrm{i}}{\hbar}\langle\hat{p}\rangle\langle\hat{q}\rangle\right),$$

up to a phase, for some $\lambda \in \mathbb{R}$, with the additional condition of $\lambda > 0$ to guarantee that $|\psi\rangle$ is normalisable. Comparing this to the Gaussian wave packet in the question we introduce $q = \langle\hat{q}\rangle$, $p = \langle\hat{p}\rangle$, $\alpha = \frac{\lambda}{2\hbar}$, and $\gamma = pq$, which are all real, with $\alpha > 0$ to write

$$\psi(x) = \exp\left(\frac{\lambda}{2\hbar}q^2\right)\exp\left(-\alpha(x - q)^2 + \frac{\mathrm{i}}{\hbar}p(x - q) + \frac{\mathrm{i}\gamma}{\hbar}\right),$$

that is

$$\psi(x) \propto \exp\left(-\alpha(x - q)^2 + \frac{\mathrm{i}}{\hbar}p(x - q) + \frac{\mathrm{i}\gamma}{\hbar}\right),$$

as claimed.