Quantum Mechanics

Problem Sheet 3

The Simple Harmonic Oscillator & Problems on Basic Quantum Mechanics

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January 21, 2024

The simple harmonic oscillator

3.1

Given that $\hat{H} = (\hat{p}^2 + \hat{x}^2)/2$ and $[\hat{x}, \hat{p}] = i$ and an energy eigenstate $|\psi\rangle$ with energy E, we have:

$$\begin{aligned}
\hat{H}(\hat{x} \mp i\hat{p})|\psi\rangle &= \frac{1}{2}(\hat{p}^2 + \hat{x}^2)(\hat{x} \mp i\hat{p})|\psi\rangle \\
&= \frac{1}{2}(\hat{p}^2\hat{x} \mp i\hat{p}^3 + \hat{x}^3 \mp i\hat{x}\hat{p}^2)|\psi\rangle \\
&= \frac{1}{2}[\hat{p}(\hat{x}\hat{p} - [\hat{x}, \hat{p}]) \mp i\hat{p}^3 + \hat{x}^3 \mp i(\hat{p}\hat{x} + [\hat{x}, \hat{p}])\hat{p}]|\psi\rangle \\
&= \frac{1}{2}[\hat{p}\hat{x}\hat{p} - i\hat{p} \mp i\hat{p}^3 + \hat{x}^3 \mp i\hat{p}\hat{x}\hat{p} \pm \hat{p}^2]|\psi\rangle
\end{aligned} \tag{1}$$

3.2

Consider the Hermitian conjugate of the annihilation operator $\hat{a}$:

$$\hat{a}^\dagger = \frac{m\omega\hat{x} - i\hat{p}}{\sqrt{2m\omega\hbar}} \tag{2}$$

We have:

$$\hat{a}^\dagger\hat{a} = \frac{m\omega\hat{x} - i\hat{p}}{\sqrt{2m\omega\hbar}}\frac{m\omega\hat{x} + i\hat{p}}{\sqrt{2m\omega\hbar}} = \frac{m^2\omega^2\hat{x}^2 + \hat{p}^2}{2m\omega\hbar} + \frac{i}{2\hbar}[\hat{x}, \hat{p}] = \hat{H}/\hbar\omega - 1/2 \tag{3}$$

This allows us to calculate:

$$|\hat{a}|n\rangle| = \langle n|\hat{a}^\dagger\hat{a}|n\rangle = \frac{E_n}{\hbar\omega} - \frac{1}{2} = n \tag{4}$$

On the other hand, this is just $|\alpha|n-1\rangle|^2 = \alpha^2$, which gives us $\alpha = \sqrt{n}$.

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3.3

The pendulum follows an approximately harmonic potential of the form:

$$V(x) = \frac{1}{2}m\omega^2x^2 \tag{5}$$

Given that $A = 3\,\mathrm{cm}$, we require:

$$\left(n+\frac{1}{2}\right)\hbar\omega=\frac{1}{2}m\omega^2A^2 \tag{6}$$

solving which gives the enormous energy level $n = 5.5 \times 10^{30}$.

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3.4

We minimise the function $E(p,x) = p^2/2m + m\omega^2x^2/2$ under the constraint $xp = \hbar/2$. Consider the function $f(p,x,\lambda) = E(p,x) + \lambda(xp - \hbar/2)$, we have need:

$$\begin{aligned}\frac{\partial f}{\partial p}&=\frac{p}{m}+\lambda x=0\\ \frac{\partial f}{\partial x}&=m\omega^2x+\lambda p=0\\ \frac{\partial f}{\partial \lambda}&=xp-\frac{\hbar}{2}=0\end{aligned} \tag{7}$$

Solving which gives us $E_{\min} = \hbar\omega/2$, which is indeed the ground state energy of the harmonic oscillator.

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3.5

The position representation of the n-th energy eigenstate of the harmonic oscillator is given by:

$$\psi_n(x)=A_nH_n(\xi)e^{-\xi^2/2} \tag{8}$$

where $\xi = \sqrt{m\omega/\hbar}x$ and A_n is a normalisation constant.

The nodes of the function are due to the Hermite polynomial $H_n(\xi)$, which is of degree n. By the fundamental theorem of algebra, it has n roots, which are the nodes of the wave function.

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3.6

The ground state wave function of the harmonic oscillator is given by:

$$\psi_0(x)=A_0e^{-\xi^2/2} \tag{9}$$

To obtain wave functions of higher energy states, we can apply the raising operator $\hat{a}^\dagger$ to the ground state wave function. Consider:

$$
\begin{aligned}
\langle x|\hat{a}^\dagger|0\rangle &= \frac{1}{\sqrt{2m\omega\hbar}}\,\langle x|m\omega\hat{x} - i\hat{p}|0\rangle \\
&= \left(\frac{x}{2l} - l\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_0(x)
\end{aligned} \tag{10}
$$

or, raising the state again:

$$
\psi_2 = \left(\frac{x}{2l} - l\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 \psi_0(x) \tag{11}
$$

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3.7

Consider the matrix element $\hat{x}_{jk} \equiv \langle j|\hat{x}|k\rangle$:

$$
\begin{aligned}
\hat{x}_{jk} &= \langle j|\hat{x}|k\rangle \\
&= l\,\langle j|\hat{a}^\dagger + \hat{a}|k\rangle \\
&= l(\sqrt{j}\,\langle j|k-1\rangle + \sqrt{j+1}\,\langle j|k+1\rangle) \\
&= l(\delta_{j,k-1}\sqrt{j} + \delta_{j,k+1}\sqrt{j+1})
\end{aligned} \tag{12}
$$

Thus, $\hat{x}_{jk}$ is non-zero only when $k = j \pm 1$, i,e., $\hat{x}$ is a tridiagonal matrix with the diagonal elements being zero.

For $\hat{p}$, we have the identity:

$$
\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}^\dagger - \hat{a}) \tag{13}
$$

which gives us:

$$
\begin{aligned}
\hat{p}_{jk} &= \langle j|\hat{p}|k\rangle \\
&= i\sqrt{\frac{m\omega\hbar}{2}}(\sqrt{j+1}\,\langle j|k+1\rangle - \sqrt{j}\,\langle j|k-1\rangle) \\
&= i\sqrt{\frac{m\omega\hbar}{2}}(\delta_{j,k+1}\sqrt{j+1} - \delta_{j,k-1}\sqrt{j})
\end{aligned} \tag{14}
$$

which is also a tridiagonal matrix with the upper 'diagonal' elements switching their signs.

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3.8

Since $\hat{x}$ and $\hat{H}$ commute and the Hamiltonian of a harmonic oscillator is time independent, we have by Ehrenfest's theorem that the expectation value of $\hat{x}$ is time independent. We can evaluate the ket $\hat{x}\left|\psi\right\rangle$:

$$\begin{aligned}\hat{x}\left|\psi\right\rangle &= l(\hat{a}+\hat{a}^\dagger)\left(\frac{1}{2}\left|N-1\right\rangle + \frac{1}{\sqrt{2}}\left|N\right\rangle + \frac{1}{2}\left|N+1\right\rangle\right) \\ &= l\left(\frac{1}{2}\sqrt{N}\left|N\right\rangle + \frac{1}{\sqrt{2}}\sqrt{N}\left|N-1\right\rangle + \frac{1}{\sqrt{2}}\sqrt{N+1}\left|N+1\right\rangle + \frac{1}{2}\sqrt{N+1}\left|N\right\rangle\right)\end{aligned} \tag{15}$$

where we have ignored $\left|N-2\right\rangle$ and $\left|N+2\right\rangle$ since they are orthogonal to $\left|\psi\right\rangle$.

We thus have the expectation value of $\hat{x}$:

$$\langle\psi|\hat{x}|\psi\rangle = \frac{l}{\sqrt{2}}(\sqrt{N}+\sqrt{N+1}) \tag{16}$$

where $l = \sqrt{\hbar/2m\omega}$.

This shows that while the position expectation of a single 'pure' state $\left|N\right\rangle$ is zero, that of a mixed state is not.

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Problems on basic quantum mechanics

3.9

$\hat{H}$ is obviously Hermitian since its complex conjugate is itself. $\hat{B}$ is not for the same reason.

Apparently the eigenvalues of $\hat{H}$ are $\hbar\omega$ and $-\hbar\omega$, with the former having the eigenstate $|1\rangle$ and the latter (degenerate) corresponding to $|2\rangle$ and $|3\rangle$. It is trivial to show that the eigenvalues of $\hat{B}$ are 1 and -1. The former has the eigenstate $|1\rangle$ and $|2\rangle + |3\rangle$, while the latter has the eigenstate $|2\rangle - |3\rangle$.

Both $\hat{H}$ and $\hat{B}$ have degenerate eigenvalues so they cannot uniquely specify the eigenstates. Consider the commutator $[\hat{H}, \hat{B}]$:

$$
\begin{aligned}
[\hat{H}, \hat{B}] &= \hat{H}\hat{B} - \hat{B}\hat{H} \\
&= \hbar\omega b \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} - \hbar\omega b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\
&= \hbar\omega b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} - \hbar\omega b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \\
&= 0
\end{aligned} \tag{17}
$$

Since $[\hat{H}, \hat{B}] = 0$, the two operators share a common set of eigenstates. It is easy to see that the eigenstates of $\hat{B}$ are just linear combinations of those of $\hat{H}$, so we choose $|1\rangle$, $|2\rangle + |3\rangle$ and $|2\rangle - |3\rangle$ as the shared eigenstates.

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3.10

By Erfhenfest's theorem, we have the time derivative of the expectation value of an operator $\hat{A}$:

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle\psi|\hat{A}|\psi\rangle = \frac{i}{\hbar} \langle\psi|[\hat{H}, \hat{A}]|\psi\rangle + \langle\psi|\frac{\partial \hat{A}}{\partial t}|\psi\rangle \tag{18}$$

The second term is zero for a time-independent operator. The probability of measuring energy E_k is given by:

$$P_k = |\langle k|\psi\rangle|^2 \tag{19}$$

Consider the projection operator A_k onto the k-th energy eigenstate acting on the state $|\psi\rangle$:

$$A_k |\psi\rangle = |k\rangle \langle k|\psi\rangle \tag{20}$$

The expectation value of A_k is thus:

$$\langle\psi|A_k|\psi\rangle = \langle\psi|k\rangle \langle k|\psi\rangle = |\langle k|\psi\rangle|^2 \tag{21}$$

Since the projection operator commutes with the Hamiltonian, we have:

$$\frac{\mathrm{d}P_k}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \langle\psi|A_k|\psi\rangle = \frac{i}{\hbar} \langle\psi|[\hat{H}, A_k]|\psi\rangle = 0 \tag{22}$$

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3.11

The probability of measuring q_r is given by:

$$P(q_r|\psi) = |\langle q_r|\psi\rangle|^2 \tag{23}$$

The summation of all probabilities is:

$$\begin{aligned}\sum_r P(q_r|\psi) &= \sum_r |\langle q_r|\psi\rangle|^2 \\ &= \sum_r \langle\psi|q_r\rangle \langle q_r|\psi\rangle \\ &= \langle\psi|\psi\rangle \\ &= 1\end{aligned} \tag{24}$$

where we have used the completeness relation $\sum_r |q_r\rangle \langle q_r| = \mathbb{I}$.

Note that we can express a state in its position representation:

$$|\psi\rangle = \int \langle x|\psi\rangle |x\rangle \,\mathrm{d}x \tag{25}$$

where $\psi(x) \equiv \langle x|\psi\rangle$ is the wave function.

The expectation value of $\hat{Q}$ is given by:

$$\begin{aligned}\langle\psi|\hat{Q}|\psi\rangle &= \int\int \langle\psi|x'\rangle \langle x'|\,\hat{Q}\,|x\rangle \langle x|\psi\rangle \,\mathrm{d}x\,\mathrm{d}x' \\ &= \int \psi^*(x)\hat{Q}\psi(x)\,\mathrm{d}x\end{aligned} \tag{26}$$

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3.12

(a) Given the TISE in the position representation:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = E\psi(x) \tag{27}$$

we have the general solution:

$$\psi(x) = A\sin kx + B\cos kx \tag{28}$$

where $k \equiv \sqrt{2mE}/\hbar$.

For $\psi(0) = 0$, we have $B = 0$. For $\psi(a) = 0$, we have $k = n\pi/a$ where n is an integer. Thus, the energy levels are:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \tag{29}$$

To fix the normalisation constant A, we have:

$$|A|^2 \int_0^a \sin^2\frac{n\pi x}{a}\,\mathrm{d}x = 1 \tag{30}$$

which gives us $A = \sqrt{2/a}$.

(b) The expectation value of the position is given by:

$$\begin{aligned}\langle\psi|\hat{x}|\psi\rangle &= \int_0^a \psi^*(x)x\psi(x)\,\mathrm{d}x \\ &= \frac{2}{a}\int_0^a x\sin^2\frac{n\pi x}{a}\,\mathrm{d}x \\ &= \frac{a}{2}\end{aligned} \tag{31}$$

(c) The variance of the position is given by:

$$\left\langle (x - \langle x \rangle)^2 \right\rangle = \left\langle x^2 - 2x \langle x \rangle + \langle x \rangle^2 \right\rangle = \left\langle x^2 \right\rangle - \langle x \rangle^2 = \left\langle x^2 \right\rangle - \frac{a^2}{4} \tag{32}$$

where we treat $\langle x \rangle$ as a constant.

We evaluate $\langle x^2 \rangle$:

$$\begin{aligned} \left\langle x^2 \right\rangle &= \int_0^a \psi^*(x) x^2 \psi(x) \, \mathrm{d}x \\ &= \frac{2}{a} \int_0^a x^2 \sin^2 \frac{n\pi x}{a} \, \mathrm{d}x \\ &= a^2 \left(\frac{1}{3} - \frac{1}{2n^2\pi^2} \right) \end{aligned} \tag{33}$$

which gives us the variance:

$$\left\langle (x - \langle x \rangle)^2 \right\rangle = \frac{a^2}{12} \left(1 - \frac{6}{n^2\pi^2} \right) \tag{34}$$

(d) Consider a particle undergoing elastic collisions with the walls of the box. Suppose that the particle starts from $x = 0$ with a velocity v at $t = 0$. The position of the particle at time t is given by:

$$x(t) = \begin{cases} vt & 2na/v \leq t \leq (2n+1)a/v \\ a - vt & (2n+1)a/v \leq t \leq (2n+2)a/v \end{cases} \tag{35}$$

The average position of the particle is given by the integral:

$$\begin{aligned} \langle x \rangle &= \sum_{n=0}^{\infty} \frac{1}{a/v} \int_{2na/v}^{(2n+1)a/v} vt \, \mathrm{d}t + \sum_{n=0}^{\infty} \frac{1}{a/v} \int_{(2n+1)a/v}^{(2n+2)a/v} (a - vt) \, \mathrm{d}t \\ &= \frac{a}{2} \sum_{n=0}^{\infty} \left[(2n+1)^2 - (2n)^2 \right] + \frac{a}{2} \sum_{n=0}^{\infty} \left[2 - (2n+2)^2 + (2n+1)^2 \right] \\ &= 0 \end{aligned} \tag{36}$$

where as the variance is given by:

$$
\begin{aligned}
\left\langle (x-\langle x\rangle)^2\right\rangle &= \sum_{n=0}^{\infty}\frac{1}{a/v}\int_{2na/v}^{(2n+1)a/v}(vt)^2\,\mathrm{d}t + \sum_{n=0}^{\infty}\frac{1}{a/v}\int_{(2n+1)a/v}^{(2n+2)a/v}(a-vt)^2\,\mathrm{d}t \\
&= \frac{a^2}{3}\sum_{n=0}^{\infty}\left[(2n+1)^3-(2n)^3\right] + \frac{a^2}{3}\sum_{n=0}^{\infty}\left[(2n+1)^3-(2n)^3\right] \\
&= \frac{2a^2}{3}\sum_{n=0}^{\infty}\left[(2n+1)^3-(2n)^3\right]
\end{aligned} \tag{37}
$$

For the moment let n tend to a finite value N. We have:

$$
\begin{aligned}
\sum_{n=0}^{N}\left[(2n+1)^3-(2n)^3\right] &= \sum_{n=0}^{N}\left(12n^2+6n+1\right) \\
&= 12\frac{N(N+1)(2N+1)}{6} + 6\frac{N(N+1)}{2} + (N+1)
\end{aligned} \tag{38}
$$