Quantum Mechanics

Problem Sheet 3

The Simple Harmonic Oscillator & Problems on Basic Quantum Mechanics

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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:

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

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 implies $\alpha = \sqrt{n}$.

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3.3

The pendulum follows an approximately harmonic potential of the form:

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

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

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

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

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3.4

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

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

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:

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

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:

$$\psi_0(x) = A_0 e^{-m\omega x^2/2\hbar} = A_0 e^{-x^2/4l^2} \tag{9}$$

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:

$$\begin{aligned}\psi_2 &= \left(\frac{x}{2l} - l\frac{\mathrm{d}}{\mathrm{d}x}\right)^2\psi_0(x) \\ &= A_0\left(\frac{x^2}{l^2} - 1\right)e^{-x^2/2l^2}\end{aligned} \tag{11}$$

The normalisation constant is given by:

$$A_0 = \frac{1}{\int e^{-x^2/2l^2}\,\mathrm{d}x} = \left(\frac{l}{\sqrt{2\pi}}\right)^{1/2} \tag{12}$$

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3.7

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

$$\begin{aligned}\hat{x}_{jk} &= \langle j|\hat{x}|k\rangle \\ &= l\,\langle j|\hat{a}^\dagger + \hat{a}|k\rangle \\ &= l(\sqrt{j}\,\langle j|k-1\rangle + \sqrt{j+1}\,\langle j|k+1\rangle) \\ &= l(\delta_{j,k-1}\sqrt{j} + \delta_{j,k+1}\sqrt{j+1})\end{aligned} \tag{13}$$

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:

$$\hat{p} = i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a}^\dagger - \hat{a}) \tag{14}$$

which gives us:

$$\begin{aligned}\hat{p}_{jk} &= \langle j|\hat{p}|k\rangle \\ &= i\sqrt{\frac{m\omega\hbar}{2}}(\sqrt{j+1}\,\langle j|k+1\rangle - \sqrt{j}\,\langle j|k-1\rangle) \\ &= i\sqrt{\frac{m\omega\hbar}{2}}(\delta_{j,k+1}\sqrt{j+1} - \delta_{j,k-1}\sqrt{j})\end{aligned} \tag{15}$$

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 $\hat{x}\,|\psi\rangle$:

$$\begin{aligned}\hat{x}\,|\psi\rangle &= l(\hat{a}+\hat{a}^\dagger)\left(\frac{1}{2}\,|N-1\rangle + \frac{1}{\sqrt{2}}\,|N\rangle + \frac{1}{2}\,|N+1\rangle\right) \\ &= l\left(\frac{1}{2}\sqrt{N}\,|N\rangle + \frac{1}{\sqrt{2}}\sqrt{N}\,|N-1\rangle + \frac{1}{\sqrt{2}}\sqrt{N+1}\,|N+1\rangle + \frac{1}{2}\sqrt{N+1}\,|N\rangle\right)\end{aligned} \tag{16}$$

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

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

$$\langle\psi|\hat{x}|\psi\rangle = \frac{l}{\sqrt{2}}(\sqrt{N}+\sqrt{N+1}) \tag{17}$$

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

This shows that while the position expectation of a single 'pure' state $|N\rangle$ 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 $[\hat{H}, \hat{B}]$:

$$\begin{aligned}
[\hat{H}, \hat{B}] &= \hat{H}\hat{B} - \hat{B}\hat{H} \\
&= \hbar\omega b \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} - \hbar\omega b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\
&= \hbar\omega b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} - \hbar\omega b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \\
&= 0
\end{aligned} \tag{18}$$

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 $\hat{A}$:

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle\psi|\hat{A}|\psi\rangle = \frac{i}{\hbar} \langle\psi|[\hat{H}, \hat{A}]|\psi\rangle + \langle\psi|\frac{\partial \hat{A}}{\partial t}|\psi\rangle \tag{19}$$

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

$$P_k = |\langle k|\psi\rangle|^2 \tag{20}$$

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

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

The expectation value of A_k is thus:

$$\langle\psi|A_k|\psi\rangle = \langle\psi|k\rangle \langle k|\psi\rangle = |\langle k|\psi\rangle|^2 \tag{22}$$

Consider the commutator $[\hat{H}, A_k]$ acting on $|\psi\rangle$:

$$\begin{aligned}
\hat{H}A_k |\psi\rangle - A_k\hat{H} |\psi\rangle &= \hat{H} |k\rangle \langle k|\psi\rangle - |k\rangle \langle k|\hat{H}|\psi\rangle \\
&= E_k |k\rangle \langle k|\psi\rangle - |k\rangle \sum_r \langle k|\hat{H}|r\rangle \langle r|\psi\rangle \\
&= E_k |k\rangle \langle k|\psi\rangle - |k\rangle \sum_r E_r \langle k|r\rangle \langle r|\psi\rangle \\
&= E_k |k\rangle \langle k|\psi\rangle - E_k |k\rangle \langle k|\psi\rangle \\
&= 0
\end{aligned} \tag{23}$$

where at the second step we expand $|\psi\rangle$ in terms of energy eigenstates and at the fourth step we have used the orthogonality relation $\langle k|r\rangle = \delta_{k,r}$.

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

$$\frac{\mathrm{d}P_k}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \langle\psi|A_k|\psi\rangle = \frac{i}{\hbar} \langle\psi|[\hat{H}, A_k]|\psi\rangle = 0 \tag{24}$$

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3.11

The probability of measuring q_r is given by:

$$P(q_r|\psi) = |\langle q_r|\psi\rangle|^2 \tag{25}$$

The summation of all probabilities is:

$$
\begin{aligned}
\sum_r P(q_r|\psi) &= \sum_r |\langle q_r|\psi\rangle|^2 \\
&= \sum_r \langle\psi|q_r\rangle \langle q_r|\psi\rangle \\
&= \langle\psi|\psi\rangle \\
&= 1
\end{aligned}
\tag{26}
$$

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:

$$
|\psi\rangle = \int \langle x|\psi\rangle \, |x\rangle \, \mathrm{d}x \tag{27}
$$

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

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

$$
\begin{aligned}
\langle\psi|\hat{Q}|\psi\rangle &= \int\int \langle\psi|x'\rangle \langle x'| \hat{Q} |x\rangle \langle x|\psi\rangle \, \mathrm{d}x \, \mathrm{d}x' \\
&= \int \psi^*(x)\hat{Q}\psi(x) \, \mathrm{d}x
\end{aligned}
\tag{28}
$$

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3.12

(a) Given the TISE in the position representation:

$$
-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} = E\psi(x) \tag{29}
$$

we have the general solution:

$$
\psi(x) = A\sin kx + B\cos kx \tag{30}
$$

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:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \tag{31}$$

To fix the normalisation constant A, we have:

$$|A|^2 \int_0^a \sin^2 \frac{n\pi x}{a} \, \mathrm{d}x = 1 \tag{32}$$

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

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

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

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

$$\left\langle (x - \langle x \rangle)^2 \right\rangle = \left\langle x^2 - 2x \langle x \rangle + \langle x \rangle^2 \right\rangle = \left\langle x^2 \right\rangle - \langle x \rangle^2 = \left\langle x^2 \right\rangle - \frac{a^2}{4} \tag{34}$$

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

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

$$\begin{aligned} \left\langle x^2 \right\rangle &= \int_0^a \psi^*(x) x^2 \psi(x) \, \mathrm{d}x \\ &= \frac{2}{a} \int_0^a x^2 \sin^2 \frac{n\pi x}{a} \, \mathrm{d}x \\ &= a^2 \left(\frac{1}{3} - \frac{1}{2n^2\pi^2} \right) \end{aligned} \tag{35}$$

which gives us the variance:

$$\left\langle (x - \langle x \rangle)^2 \right\rangle = \frac{a^2}{12} \left(1 - \frac{6}{n^2\pi^2} \right) \tag{36}$$

(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:

$$x(t) = \begin{cases} vt & 2na/v \le t \le (2n+1)a/v \\ a - vt & (2n+1)a/v \le t \le (2n+2)a/v \end{cases} \tag{37}$$

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

$$\begin{aligned} \langle x \rangle &= \sum_{n=0}^{\infty} \frac{1}{a/v} \int_{2na/v}^{(2n+1)a/v} vt \, \mathrm{d}t + \sum_{n=0}^{\infty} \frac{1}{a/v} \int_{(2n+1)a/v}^{(2n+2)a/v} (a - vt) \, \mathrm{d}t \\ &= \frac{a}{2} \sum_{n=0}^{\infty} \left[(2n+1)^2 - (2n)^2\right] + \frac{a}{2} \sum_{n=0}^{\infty} \left[2 - (2n+2)^2 + (2n+1)^2\right] \\ &= 0 \end{aligned} \tag{38}$$

where as the variance is given by:

$$\begin{aligned} \left\langle (x - \langle x \rangle)^2 \right\rangle &= \lim_{N\to\infty} \frac{v}{Na} \int_0^{Na/v} x^2 \, \mathrm{d}t \\ &= \lim_{N\to\infty} \frac{v}{2Na} \left(\sum_{n=0}^{N-1} \int_{2na/v}^{(2n+1)a/v} (vt)^2 \, \mathrm{d}t + \sum_{n=0}^{N-1} \int_{(2n+1)a/v}^{(2n+2)a/v} (a - vt)^2 \, \mathrm{d}t \right) \\ &= \lim_{N\to\infty} \frac{a^2}{2Nv} \left(\sum_{n=0}^{N-1} \frac{1 + 6n + 12n^2}{3} + \sum_{n=0}^{N-1} \frac{(a-vt)^2}{a^2} \right) \\ &= \lim_{N\to\infty} \frac{a^2(4N^2 - 3N + 3) - 6avt + 3vt^2}{6} \\ &\approx \left(\frac{2}{3} N^2 - \frac{1}{2} N \right) a^2 \end{aligned} \tag{39}$$

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3.13

Consider $\hat{H}^2$:

$$\begin{aligned} \hat{H}^2 &= \hat{f}^\dagger \hat{f} \hat{f}^\dagger \hat{f} \\ &= \hat{f}^\dagger (\mathbb{I} - \hat{f}^\dagger \hat{f}) \hat{f} \\ &= \hat{f}^\dagger \hat{f} \\ &= \hat{H} \end{aligned} \tag{40}$$

where the second term of the second equality is zero since $\hat{f}^2 = 0$.

Suppose that $\hat{H}\left|\psi\right\rangle = \lambda\left|\psi\right\rangle$, applying $\hat{H}$ to both sides of the equation gives us:

$$\hat{H}^2\left|\psi\right\rangle = \lambda^2\left|\psi\right\rangle = \hat{H}\left|\psi\right\rangle = \lambda\left|\psi\right\rangle \tag{41}$$

which implies that λ is either zero or unity.

Suppose that $\hat{H}\left|0\right\rangle = 0$ and $\langle 0|0\rangle = 1$. We have two cases. Either $\hat{f}^\dagger(\hat{f}\left|0\right\rangle) = 0$, which means that $\hat{f}\left|0\right\rangle$ is in the null space of $\hat{f}^\dagger$; or $\hat{f}\left|0\right\rangle = 0$, which means that $\left|0\right\rangle$ is in the null space of $\hat{f}$. Consider the condition $\hat{f}\hat{f}^\dagger + \hat{f}^\dagger\hat{f} = \mathbb{I}$ acting on $\left|0\right\rangle$:

$$\begin{aligned}(\hat{f}\hat{f}^\dagger + \hat{H})\left|0\right\rangle &= \left|0\right\rangle \\ \hat{f}\hat{f}^\dagger\left|0\right\rangle &= \left|0\right\rangle \\ \hat{f}\hat{f}\hat{f}^\dagger\left|0\right\rangle &= \hat{f}\left|0\right\rangle \\ 0 &= \hat{f}\left|0\right\rangle\end{aligned} \tag{42}$$

where at the third step we apply $\hat{f}$ to both sides of the equation and at the last step we use the fact that $\hat{f}^2 = 0$.

This implies that the second case is true. Thus $\left|a\right\rangle = \hat{f}\left|0\right\rangle$ is just zero. Now let us consider the other eigenstate $\left|1\right\rangle$ that satisfies $\hat{H}\left|1\right\rangle = \left|1\right\rangle$. We consider:

$$\begin{aligned}\hat{f}^\dagger\hat{f}\left|1\right\rangle &= (\hat{f}^\dagger\hat{f} + \hat{f}\hat{f}^\dagger)\left|1\right\rangle \\ \left|1\right\rangle &= \left|1\right\rangle + \hat{f}\hat{f}^\dagger\left|1\right\rangle\end{aligned} \tag{43}$$

which implies that $\hat{f}\hat{f}^\dagger\left|1\right\rangle = 0$.

There are still two possibilities. Either $\hat{f}(\hat{f}^\dagger\left|1\right\rangle) = 0$ or $\hat{f}^\dagger\left|1\right\rangle = 0$. We take the second case and view $\hat{f}^\dagger$ as the 'raising' operator and $\hat{f}$ as the 'lowering' operator. Suppose that $\hat{f}^\dagger\left|0\right\rangle = A\left|1\right\rangle$ and $\hat{f}\left|1\right\rangle = B\left|0\right\rangle$ for some constants A and B. We have:

$$\begin{aligned}\hat{H}\left|1\right\rangle &= \left|1\right\rangle \\ \hat{f}^\dagger\hat{f}\left|1\right\rangle &= \left|1\right\rangle \\ AB\left|1\right\rangle &= \left|1\right\rangle\end{aligned} \tag{44}$$

This implies that $AB = 1$. Therefore, $\hat{f}^\dagger\left|0\right\rangle = A\left|1\right\rangle$ is just some constant multiple of $\left|1\right\rangle$.

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