## Quantum Mechanics

## Problem Sheet 1 - Quantum states

## Basics

1. This problem is meant to give you an idea of the typical energies involved in a quantum process. Compare to the typical energies of a macroscopic classical process.
2. Compute the integral that yields the norm of the state, choose the normalization constant in order to get a unit norm.
3. A useful relation.
4. Action of the position operator on the wave function in one dimension.
5. Useful relations involving Hermitian conjugates. If you can memorize some of these relations, you will find it much easier to solve problems in subsequent problem sheets.
6. Eigenfunctions of operators and results of measurements.
7. A first look at two-state systems. Use of the hermiticity condition, find the eigenstates.

## Further problems

1. Application of the two-state formalism to describe a qubit in quantum computation. Application of some of the concepts introduce above to this basic example.
2. The Jacobi identity for quantum operators.
3. This problem requires you to compute some integrals that characterize the system described by the given wave function. Try to perform the integrals, and then to understand their physical meaning. This second step is where you understand the physics!
4. Some mathematical relations about the eigenstates of compatible observables.

## Basics

1. The energy levels for the infinite 1-dimensional square well are given by

$$
\begin{equation*}
E_{n}=\frac{\hbar^{2} \pi^{2} n^{2}}{8 m a^{2}} \quad \text { for } n=1,2,3, \ldots \infty \tag{1}
\end{equation*}
$$

Calculate the energies of the first $(n=1)$ and second $(n=2)$ levels for the case of an electron of mass $9.1 \times 10^{-31} \mathrm{~kg}$, confined to a box of atomic dimensions ( $a=10^{-10}$ $\mathrm{m})$. Hence calculate the wavelength of a photon emitted in a transition between these levels.
2. The first and the third energy eigenstates of the harmonic oscillator are respectively:

$$
\begin{align*}
& \psi_{0}(x)=C_{0} \exp \left[-\alpha^{2} x^{2} / 2\right]  \tag{2}\\
& \psi_{2}(x)=C_{2}\left(4 \alpha^{2} x^{2}-2\right) \exp \left[-\alpha^{2} x^{2} / 2\right] \tag{3}
\end{align*}
$$

where $\alpha^{2}=m \omega / \hbar$.
Calculate explicitly the normalization constants for these two energy eigenstates, and verify that the eigenfunctions are orthogonal. Note that:

$$
\begin{equation*}
\int_{-\infty}^{\infty} \exp \left\{-\alpha^{2} x^{2}\right\} d x=\left(\pi / \alpha^{2}\right)^{\frac{1}{2}} \text { and } \int_{-\infty}^{\infty} x^{2} \exp \left\{-\alpha^{2} x^{2}\right\} d x=\frac{1}{2} \sqrt{\pi} / \alpha^{3} \tag{4}
\end{equation*}
$$

3. Show that:

$$
\begin{equation*}
\frac{1}{\hat{A}}-\frac{1}{\hat{B}}=\frac{1}{\hat{A}}(\hat{B}-\hat{A}) \frac{1}{\hat{B}} . \tag{5}
\end{equation*}
$$

Remember that $\hat{A}$ and $\hat{B}$ are operators.
4. When acting on the wave function, the position operator, $\hat{X}$, corresponds simply to multiplication by $x$ :

$$
\hat{X} \psi(x)=x \psi(x) .
$$

Use the definition of Hermitean conjugate given in lectures to show that $\hat{X}$ is Hermitean and hence that the potential energy operator $\hat{V} \equiv V(x)$ is also Hermitean.
5. Prove the following relations:

$$
\begin{align*}
\left(\hat{f}^{\dagger}\right)^{\dagger} & =\hat{f}  \tag{6}\\
(\hat{f} \hat{g})^{\dagger} & =\hat{g}^{\dagger} \hat{f}^{\dagger},  \tag{7}\\
{[\hat{f}, \hat{g} \hat{h}] } & =\hat{g}[\hat{f}, \hat{h}]+[\hat{f}, \hat{g}] \hat{h},  \tag{8}\\
{[\hat{f} \hat{g}, \hat{h}] } & =\hat{f}[\hat{g}, \hat{h}]+[\hat{f}, \hat{h}] \hat{g} . \tag{9}
\end{align*}
$$

If $\hat{f}, \hat{g}$ are Hermitean, show that $\hat{f} \hat{g}+\hat{g} \hat{f}$, and $i[\hat{f}, \hat{g}]$ are also Hermitean. Show that for any operator $\hat{A}$,

$$
\begin{equation*}
\left\langle A^{\dagger} A\right\rangle \geq 0 \tag{10}
\end{equation*}
$$

for any state.
6. The observables $\mathcal{A}$ and $\mathcal{B}$ are represented by operators $\hat{A}$ and $\hat{B}$ with eigenfunctions $\left\{u_{i}(x)\right\}$ and $\left\{v_{i}(x)\right\}$ respectively, such that

$$
\begin{aligned}
v_{1}(x) & =\left\{\sqrt{3} u_{1}(x)+u_{2}(x)\right\} / 2 \\
v_{2}(x) & =\left\{u_{1}(x)-\sqrt{3} u_{2}(x)\right\} / 2 \\
v_{n}(x) & =u_{n}(x), \quad n \geq 3
\end{aligned}
$$

Verify that these relations are consistent with orthonormality of both bases. A certain system is subjected to three successive measurements:
(i) a measurement of $\mathcal{A}$
(ii) a measurement of $\mathcal{B}$
(iii) another measurement of $\mathcal{A}$

Show that if measurement (i) yields any of the values $A_{3}, A_{4}, \ldots$ then (iii) gives the same result but that if (i) yields the value $A_{1}$ there is a probability of $\frac{5}{8}$ that (iii) will yield $A_{1}$ and a probability of $\frac{3}{8}$ that it will yield $A_{2}$. What may be said about the compatibility of $\mathcal{A}$ and $\mathcal{B}$ ?
7. Consider a two-state system. We denote the two orthonormal states by $|1\rangle$, and $|2\rangle$. In the general case, the Hamiltonian of the system can be written as a $2 \times 2$ matrix, where the elements of the matrix are given by:

$$
H_{i j}=\langle i| \hat{H}|j\rangle
$$

Let us consider the Hamiltonian:

$$
\hat{H}=\left(\begin{array}{cc}
E_{0} & -\eta  \tag{11}\\
-\eta & E_{0}
\end{array}\right), \quad E_{0} \quad \text { real }
$$

(a) Write the action of $\hat{H}$ on the states $|1\rangle$ and $|2\rangle$.
(b) Show that $\eta$ has to be real.
(c) Compute the eigenvalues of $\hat{H}$, and the normalized eigenvectors.

## Further problems

1. A two-state quantum system describes a qubit in quantum computing. Consider a qubit described by the Hamiltonian:

$$
\hat{H}=E_{0}\left(\begin{array}{cc}
1 & 0  \tag{12}\\
0 & -1
\end{array}\right),
$$

and two observables described by the operators:

$$
\hat{A}=\left(\begin{array}{cc}
0 & -i  \tag{13}\\
i & 0
\end{array}\right), \quad \hat{B}=\left(\begin{array}{cc}
2 & -\sqrt{2} i \\
\sqrt{2} i & 1
\end{array}\right) .
$$

(a) Find the eigenvalues and eigenvectors for $\hat{A}$, and $\hat{B}$.
(b) Are $\hat{A}$ and $\hat{B}$ compatible? Do they commute with the Hamiltonian?
(c) Suppose that an observation of $\hat{A}$ has resulted in $A=1$, what would be the results for $\hat{B}$, and what would be the respective probabilities?
(d) What would be the probability of finding $A=1$ if a second measurement is made immediately after the first one?
(e) What is the probability of finding $A=1$ if a measurement of $A$ is made immediately after a measurement of $B$ that yielded the larger eigenvalue of $B$ ?
2. Let us consider three operators $\hat{f}, \hat{g}$, and $\hat{h}$. Show that:

$$
\begin{equation*}
[\hat{f},[\hat{g}, \hat{h}]]+[\hat{g},[\hat{h}, \hat{f}]]+[\hat{h},[\hat{f}, \hat{g}]]=0 \tag{14}
\end{equation*}
$$

This result is known as the Jacobi identity.
3. Given the wavefunction

$$
\begin{equation*}
\psi(x)=\left(\frac{\pi}{\alpha^{2}}\right)^{-1 / 4} \exp \left(\frac{-\alpha^{2} x^{2}}{2}\right) \tag{15}
\end{equation*}
$$

calculate $\left\langle x^{n}\right\rangle$ and $\Delta x \equiv \sqrt{\left\langle x^{2}\right\rangle-\langle x\rangle^{2}}$.
Now calculate the momentum space wave function associated with $\psi(x)$ :

$$
\begin{equation*}
\tilde{\psi}(p)=\int \frac{d x}{\sqrt{2 \pi \hbar}} e^{i p x / \hbar} \psi(x) \tag{16}
\end{equation*}
$$

Using $\tilde{\psi}(p)$, calculate $\left\langle p^{n}\right\rangle$ and $\Delta p \equiv \sqrt{\left\langle p^{2}\right\rangle-\langle p\rangle^{2}}$.
With the above results, what do you find for $\Delta x \Delta p$ ?
4. Let us consider two Hermitean operators $\hat{f}, \hat{g}$, such that:

$$
\begin{equation*}
[\hat{f}, \hat{g}]=0 \tag{17}
\end{equation*}
$$

and let us denote $\psi_{n}$ the eigenfunctions of $\hat{g}$ :

$$
\begin{equation*}
\hat{g} \psi_{n}=g_{n} \psi_{n} . \tag{18}
\end{equation*}
$$

(a) Show that $\hat{f} \psi_{n}$ is an eigenstate of $\hat{g}$ with eigenvalue $g_{n}$.

In general there will be a finite number of eigenstates corresponding to the same eigenvalue $g_{n}$. We denote these orthonormal eigenstates by $\left\{\psi_{n}^{i}, i=1,2, \ldots, s\right\}$.
(b) Using the result in (a), deduce that:

$$
\begin{equation*}
\hat{f} \psi_{n}^{i}=\sum_{j=1}^{s} F_{i j} \psi_{n}^{j} \tag{19}
\end{equation*}
$$

where $F_{i j}$ are complex numbers.
(c) Show that $F_{i j}=F_{j i}^{*}$, i.e. that $F$ is an $s \times s$ Hermitean matrix.

Any finite-dimensional Hermitean matrix can be diagonalized by a unitary transformation $U$ :

$$
U^{\dagger} F U=\left(\begin{array}{cccc}
f_{1} & 0 & \ldots & 0  \tag{20}\\
0 & f_{2} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & f_{n}
\end{array}\right)
$$

We can choose the following set of orthonormal linear combinations of $\psi_{n}^{i}$, for a given $n: \phi_{n}^{i}=\sum_{j} U_{i j}^{\dagger} \psi_{n}^{j}$.
(d) Show that $\hat{f} \phi_{n}^{i}=f_{i} \phi_{n}^{i}$.

We have therefore found a basis of simultaneous eigenstates of $\hat{f}$ and $\hat{g}$ :

$$
\begin{align*}
\hat{f} \phi_{n}^{i} & =f_{i} \phi_{n}^{i}  \tag{21}\\
\hat{g} \phi_{n}^{i} & =g_{n} \phi_{n}^{i} \tag{22}
\end{align*}
$$

By repeating the same argument for all eigenvalues $g_{n}$, we can explicitly construct a basis of simultaneous eigenvalues of $\hat{f}$ and $\hat{g}$. The two observables are called compatible.

