Imperial College London

MATH96005

BSc, MSci and MSc EXAMINATIONS (MATHEMATICS)
May-June 2021

This paper is also taken for the relevant examination for the Associateship of the Royal College of Science

Quantum Mechanics 1

Date: Tuesday, 25 May 2021

Time: 09:00 to 11:00

Time Allowed: 2 hours

Upload Time Allowed: 30 minutes

This paper has 4 Questions.

Candidates should start their solutions to each question on a new sheet of paper.

Each sheet of paper should have your CID, Question Number and Page Number on the top.

Only use 1 side of the paper.

Allow margins for marking.

Any required additional material(s) will be provided.

Credit will be given for all questions attempted.

Each question carries equal weight.

SUBMIT YOUR ANSWERS ONE PDF TO THE RELEVANT DROPBOX ON BLACKBOARD INCLUDING A COMPLETED COVERSHEET WITH YOUR CID NUMBER, QUESTION NUMBERS ANSWERED AND PAGE NUMBERS PER QUESTION.

1. **Dirac notation and operator algebra**

(a) Consider a quantum system on a Hilbert space spanned by the complete set of orthonormal vectors $\{|\phi_1\rangle, |\phi_2\rangle\}$.

(i) Consider the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|\phi_1\rangle - \mathrm{i}|\phi_2\rangle)$. Construct a state $|\chi\rangle$ that is orthogonal to $|\psi\rangle$ and normalised. Verify that these two states form a resolution of the identity.

(5 marks)

(ii) Represent the operator $|\psi\rangle\langle\psi|$ as matrices in the bases $\{|\phi_n\rangle\}$ and $\{|\psi\rangle, |\chi\rangle\}$, respectively.

(5 marks)

(b) Show that

(i) $\hat{A}\hat{B}^n\hat{A}^{-1} = \left(\hat{A}\hat{B}\hat{A}^{-1}\right)^n$.

(ii) $\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}}\mathrm{e}^{-\hat{A}} = \mathrm{e}^{\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{-\hat{A}}}$.

(5 marks)

(c) (i) Use the Hadamard lemma to calculate

$$\langle\psi_0|\mathrm{e}^{\mathrm{i}\frac{\hat{p}^2}{2m}t/\hbar}\hat{q}\mathrm{e}^{-\mathrm{i}\frac{\hat{p}^2}{2m}t/\hbar}|\psi_0\rangle.$$

(3 marks)

(ii) How could you have deduced the result from Ehrenfest's theorem? (2 marks)

(Total: 20 marks)

2. **The principles of quantum mechanics - a two-level system**

Consider a system on a Hilbert space spanned by the orthonormal basis $\{|\phi_1\rangle, |\phi_2\rangle\}$. The Hamiltonian $\hat{H}$ and another operator $\hat{A}$ are represented by the matrices

$$\hat{H} = \begin{pmatrix} -E & 0 \\ 0 & E \end{pmatrix}, \qquad \text{and} \qquad \hat{A} = \begin{pmatrix} 1 & -\mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix}.$$

(a) Calculate the eigenvalues and a set of normalised eigenvectors of $\hat{A}$ in the basis $\{|\phi_1\rangle, |\phi_2\rangle\}$.

(4 marks)

(b) Assume that at some specific time the system is in the state

$$|\psi\rangle = |\phi_1\rangle.$$

(i) With what probability does a measurement of the energy H return which result and what is the expectation value of the energy?

(2 marks)

(ii) With what probability does a measurement of the observable A return which result and what is the expectation value of A?

(3 marks)

(iii) Check that the uncertainties of A and H are consistent with the uncertainty relation $\Delta A \Delta H \geq \frac{1}{2}|\langle[\hat{A}, \hat{H}]\rangle|$.

(5 marks)

(c) Assume that in an experiment the measurement of the observable A at time $t = 0$ yields the result 0. What is the probability that a subsequent measurement of A at time $t > 0$ yields the result 2?

(6 marks)

(Total: 20 marks)

3. **Quantum wave functions in a harmonic potential**

Consider a particle in a one-dimensional harmonic potential, described by the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{q}^2.$$

In what follows, we will use rescaled units with $m = 1 = \omega$, and $\hbar = 1$, to simplify calculations.

(a) Consider the wave functions

$$\phi_0(x) = \left(\frac{1}{\pi}\right)^{1/4} \mathrm{e}^{-\frac{1}{2}x^2}, \quad \text{and} \quad \phi_1(x) = \left(\frac{2}{\sqrt{\pi}}\right)^{1/2} x\mathrm{e}^{-\frac{1}{2}x^2}.$$

(i) Check that these wave functions are normalised to one.

(3 marks)

(ii) Verify that $\phi_0(x)$ and $\phi_1(x)$ are eigenfunctions of the Hamiltonian in position representation. What are the corresponding eigenvalues?

(7 marks)

(b) The eigenfunctions above are the position representations of the ground state, and first excited state of the system, respectively. Verify that the application of the creation operator $\hat{a}^\dagger = \frac{1}{\sqrt{2}}(\hat{q} - \mathrm{i}\hat{p})$ in position representation to $\phi_0(x)$ indeed yields $\phi_1(x)$.

(4 marks)

(c) Assume that in an experiment at time $t = 0$ the system is in a superposition of the ground state and the first excited state,

$$\psi(x, 0) = \frac{1}{\sqrt{2}}(\phi_0(x) + \phi_1(x)).$$

Use the fact that $\hat{q} = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger)$ to deduce the expectation value of the position at times $t > 0$.

(6 marks)

Hint: The following integrals might be useful:

$$\int_{-\infty}^{\infty} \mathrm{e}^{-ax^2} dx = \sqrt{\frac{\pi}{a}}, \qquad \int_{-\infty}^{\infty} x^2 \mathrm{e}^{-ax^2} dx = \frac{1}{2a}\sqrt{\frac{\pi}{a}},$$

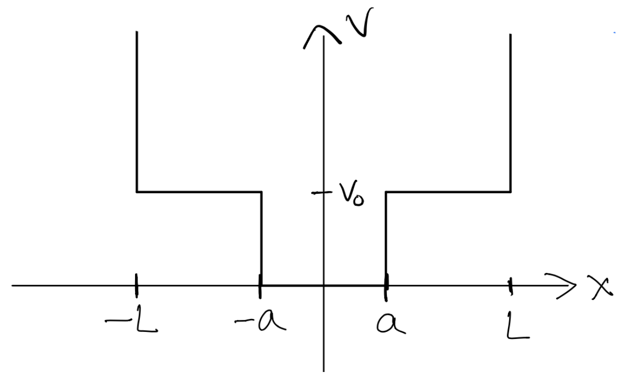
for $\mathrm{Re}(a) > 0$.

(Total: 20 marks)

4. Quantisation conditions for a piecewise constant potential well

Consider a potential of the form

$$V(x) = \begin{cases} \infty, & x \le -L \\ V_0, & -L < x \le -a \\ 0, & -a < x < a \\ V_0, & a \le x < L \\ \infty, & L \le x, \end{cases}$$



where V_0, L, and a are real and positive constants, and $a < L$.

(a) Write down an ansatz for possible bound states for the energy region $E > V_0$ using the known form of solutions of the time-independent Schrödinger equation in the different spatial regions.

(5 marks)

(b) Due to the symmetry of the potential the eigenstates are either even or odd. Refine your ansatz from (a) for even and odd states, respectively, reducing the number of free parameters.

(6 marks)

(c) Use the boundary conditions between the different regions to verify the following quantisation condition for the energies of the even bound states

$$k\tan(ka) = \tilde{k}\cot(\tilde{k}(L-a)),$$

where

$$k = \sqrt{2mE}/\hbar, \quad \text{and} \quad \tilde{k} = \sqrt{2m(E-V_0)}/\hbar.$$

(9 marks)

(Total: 20 marks)

5. **Mastery Question - Density matrices**

(a) Consider the density matrix $\hat{\rho}$ of a mixture of pure states $|\psi_j\rangle$, $\hat{\rho} = \sum_j w_j |\psi_j\rangle\langle\psi_j|$. Using the Schrödinger equation for the dynamics of the pure states $|\psi_j\rangle$ show that the dynamics of $\hat{\rho}$ is governed by the von Neuman equation

$$\mathrm{i}\hbar\dot{\hat{\rho}} = [\hat{H}, \hat{\rho}].$$

(3 marks)

(b) Show that the time evolution preserves

(i) The norm, i.e. $\mathrm{Tr}(\hat{\rho})$,

(ii) The purity (as measured by $\mathrm{Tr}(\hat{\rho}^2)$) of $\hat{\rho}$,

(iii) The positivity of $\hat{\rho}$.

(6 marks)

(c) Consider a spin 1 system described by the density matrix

$$\hat{\rho} = \begin{pmatrix} \frac{1}{4} & \frac{1}{2\sqrt{2}} & \frac{1}{4} \\ \frac{1}{2\sqrt{2}} & \frac{1}{2} & \frac{1}{2\sqrt{2}} \\ \frac{1}{4} & \frac{1}{2\sqrt{2}} & \frac{1}{4} \end{pmatrix}.$$

Verify that the state is normalised, and check whether it is a pure state or a mixed state.

(3 marks)

(d) Consider a spin 1 system with the pure states $\psi = (1,0,0)^T$ and $\phi = \frac{1}{\sqrt{2}}(1,0,1)^T$, in the standard basis. Assume the system is described by a Hamiltonian $\hat{H} = \omega\hat{J}_3$, which, in the standard basis is represented by the matrix

$$\hat{H} = \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

where ω is a real valued frequency.

(i) Assuming that the system is in the pure states ψ. Write down the corresponding density matrix, and calculate the expectation value of the energy in that state. (3 marks)

(ii) Assuming that the system is in a mixture of the pure states ψ and ϕ with equal weighting $w_\psi = \frac{1}{2} = w_\phi$. Write down the corresponding density matrix, and calculate the expectation value of the energy in that state. (5 marks)

(Total: 20 marks)

Quantum Mechanics 2020/21 Exam Solutions

1. Dirac notation and operator algebra

(a) (i) **[seen similar in homework - category A]**
A normalised state orthogonal to $|\psi\rangle$ would be

$$|\chi\rangle = \frac{1}{\sqrt{2}}\left(-\mathrm{i}|\phi_1\rangle + |\phi_2\rangle\right)$$

Resolution of identity:

$$\begin{aligned}
|\chi\rangle\langle\chi| + |\psi\rangle\langle\psi| &= \frac{1}{2}\left(-\mathrm{i}|\phi_1\rangle + |\phi_2\rangle\right)\left(\mathrm{i}\langle\phi_1| + \langle\phi_2|\right) \\
&+ \frac{1}{2}\left(|\phi_1\rangle - \mathrm{i}|\phi_2\rangle\right)\left(\langle\phi_1| + \mathrm{i}\langle\phi_2|\right) \\
&= \frac{1}{2}\big(|\phi_1\rangle\langle\phi_1| - \mathrm{i}|\phi_1\rangle\langle\phi_2| + \mathrm{i}|\phi_2\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2| \\
&+ |\phi_1\rangle\langle\phi_1| + \mathrm{i}|\phi_1\rangle\langle\phi_2| - \mathrm{i}|\phi_2\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|\big) \\
&= |\phi_1\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2| = \hat{I},
\end{aligned}$$

since $\{|\phi_n\rangle\}$ is an orthonormal basis.

[5 marks]

(ii) **[Unseen but fairly straight-forward - category C]**
Matrix representation of $|\psi\rangle\langle\psi|$ in basis $\{|\psi\rangle, |\chi\rangle\}$:

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

In basis $\{|\phi_1\rangle, |\phi_2\rangle\}$: We have

$$\begin{aligned}
|\psi\rangle\langle\psi| &= \frac{1}{2}\left(|\phi_1\rangle - \mathrm{i}|\phi_2\rangle\right)\left(\langle\phi_1| + \mathrm{i}\langle\phi_2|\right) \\
&= \frac{1}{2}\left(|\phi_1\rangle\langle\phi_1| + \mathrm{i}|\phi_1\rangle\langle\phi_2| - \mathrm{i}|\phi_2\rangle\langle\phi_1| + |\phi_2\rangle\langle\phi_2|\right).
\end{aligned}$$

From this we find the matrix representation

$$\left(\langle\phi_j|\psi\rangle\langle\psi|\phi_k\rangle\right) = \begin{pmatrix} \frac{1}{2} & \frac{\mathrm{i}}{2} \\ -\frac{\mathrm{i}}{2} & \frac{1}{2} \end{pmatrix}.$$

[5 marks]

(b) (i) **[Seen briefly in class and straight forward - category A]**
Insert $\hat{A}^{-1}\hat{A} = \hat{I}$ n times:

$$\begin{aligned}
\hat{A}\hat{B}^n\hat{A}^{-1} &= (\hat{A}\hat{B}\hat{A}^{-1})\hat{A}\hat{B}^{n-1}\hat{A}^{-1} \\
&= \cdots \\
&= \left(\hat{A}\hat{B}\hat{A}^{-1}\right)^n
\end{aligned}$$

[2 marks]

(ii) **[Unseen but straight forward - category B]**

Taylor expand $\mathrm{e}^{\hat{B}}$:

$$\begin{aligned}
\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}}\mathrm{e}^{-\hat{A}} &= \mathrm{e}^{\hat{A}}\sum_n \frac{\hat{B}^n}{n!}\left(\mathrm{e}^{\hat{A}}\right)^{-1} \\
&= \sum_n \frac{1}{n!}\mathrm{e}^{\hat{A}}\hat{B}^n(\mathrm{e}^{\hat{A}})^{-1} \\
&= \sum_n \frac{1}{n!}(\mathrm{e}^{\hat{A}}\hat{B}(\mathrm{e}^{\hat{A}})^{-1})^n \\
&= \mathrm{e}^{\mathrm{e}^{\hat{A}}\hat{B}\mathrm{e}^{-\hat{A}}}.
\end{aligned}$$

[3 marks]

(c) (i) **[Unseen but should be very straight forward - category A]**

$$\mathrm{e}^{\mathrm{i}\frac{\hat{p}^2}{2m}t/\hbar}\hat{q}\mathrm{e}^{-\mathrm{i}\frac{\hat{p}^2}{2m}t/\hbar} = \hat{q} + \frac{\mathrm{i}t}{2m\hbar}\left[\hat{p}^2,\hat{q}\right] + \frac{1}{2!}(\frac{\mathrm{i}t}{2m\hbar})^2\left[\hat{p}^2,\left[\hat{p}^2,\hat{q}\right]\right] + \cdots$$

We have

$$\left[\hat{p}^2,\hat{q}\right] = \hat{p}\left[\hat{p},\hat{q}\right] + \left[\hat{p},\hat{q}\right]\hat{p} = -2\mathrm{i}\hbar\hat{p},$$

and thus

$$\left[\hat{p}^2,\left[\hat{p}^2,\hat{q}\right]\right] = 0,$$

and all higher order nested commutators vanish too. Thus we find

$$\mathrm{e}^{\mathrm{i}\frac{\hat{p}^2}{2m}t/\hbar}\hat{q}\mathrm{e}^{-\mathrm{i}\frac{\hat{p}^2}{2m}t/\hbar} = \hat{q} + \frac{\hat{p}}{m}t,$$

that is,

$$\langle\psi_0|\mathrm{e}^{\mathrm{i}\frac{\hat{p}^2}{2m}t/\hbar}\hat{q}\mathrm{e}^{-\mathrm{i}\frac{\hat{p}^2}{2m}t/\hbar}|\psi_0\rangle = \langle\psi_0|\hat{q}|\psi_0\rangle + \frac{1}{m}\langle\psi_0|\hat{p}|\psi_0\rangle t.$$

[3 marks]

(ii) **[Easy but does require understanding - category B]**
This is the time-dependent expectation value of $\hat{q}$ under the time-evolution generated by the free-particle Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m}$, for which the Ehrenfest theorem holds exactly, i.e. we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{q}\rangle = \frac{\partial\langle\hat{H}\rangle}{\partial\langle\hat{p}\rangle} = \frac{\langle\hat{p}\rangle}{m},$$

that is

$$\langle\hat{q}\rangle(t) = \langle\hat{q}\rangle(0) + \frac{\langle\hat{p}\rangle}{m}t.$$

[2 marks]

2. The principles of quantum mechanics - a two-level system

(a) **[straight forward - category A]**

We find from the characteristic polynomial of $\hat{A}$

$$(1-\lambda)^2 - 1 = 0,$$

that is the two eigenvalues of $\hat{A}$ are

$$\lambda = 0,\, 2.$$

For the corresponding eigenvectors $\chi_{0,2} = \begin{pmatrix} x_{0,2} \\ y_{0,2} \end{pmatrix}$ we find from

$$\begin{pmatrix} 1 & -\mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix} \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = 0$$

that

$$x_0 = \mathrm{i} y_0,$$

and from

$$\begin{pmatrix} 1 & -\mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix} \begin{pmatrix} x_2 \\ y_2 \end{pmatrix} = 2 \begin{pmatrix} x_2 \\ y_2 \end{pmatrix}$$

that

$$y_2 = \mathrm{i} x_2.$$

Thus, a set of normalised eigenvectors (up to phase factors) is given by

$$\chi_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathrm{i} \\ 1 \end{pmatrix}, \quad \text{and} \quad \chi_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} -\mathrm{i} \\ 1 \end{pmatrix}.$$

[4 marks]

(b) (i) **[Seen similar - category A]**

The measurement of H yields the outcome $-E$ with probability 1. The expectation value is also $\langle \hat{H} \rangle = -E$

[2 marks]

(ii) **[Seen similar - category A]**

We calculate

$$P(0) = |\langle \chi_0 | \phi_1 \rangle|^2 = \frac{1}{2},$$

and

$$P(2) = |\langle \chi_2 | \phi_1 \rangle|^2 = \frac{1}{2}.$$

For the expectation value we find

$$\langle \hat{A} \rangle = 0 \times P(0) + 2 \times P(2) = 1.$$

[3 marks]

(iii) **[Unseen - category C/D]**

The uncertainty of the energy is zero, that is $\Delta H \Delta A = 0$.
Now check that

$$|\langle \phi_1 | [\hat{H}, \hat{A}] | \phi_1 \rangle| = 0:$$

We have

$$[\hat{H}, \hat{A}] = \begin{pmatrix} -E & 0 \\ 0 & E \end{pmatrix} \begin{pmatrix} 1 & -\mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix} - \begin{pmatrix} 1 & -\mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix} \begin{pmatrix} -E & 0 \\ 0 & E \end{pmatrix} = \begin{pmatrix} 0 & 2\mathrm{i}E \\ 2\mathrm{i}E & 0 \end{pmatrix} \tag{1}$$

And indeed

$$\langle \phi_1 | [\hat{H}, \hat{A}] | \phi_1 \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}^T \begin{pmatrix} 0 & 2\mathrm{i}E \\ 2\mathrm{i}E & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0,$$

which is consistent with the uncertainty relation.

[5 marks]

(c) **[Seen similar, but conceptually demanding - category D]**

A measurement of the value 0 at time $t = 0$ projects the system onto the corresponding eigenstate of $\hat{A}$, the vector

$$|\psi(t=0)\rangle = |\chi_0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathrm{i} \\ 1 \end{pmatrix},$$

which is not an eigenstate of $\hat{H}$.

We can use the method of stationary states to find $|\psi(t)\rangle$ as

$$|\psi(t)\rangle = \frac{\mathrm{i}}{\sqrt{2}} \mathrm{e}^{\mathrm{i}Et/\hbar} |\phi_1\rangle + \frac{1}{\sqrt{2}} \mathrm{e}^{-\mathrm{i}Et/\hbar} |\phi_2\rangle,$$

The probability to measure the result 2 in an A measurement at a later time is thus given by

$$P(2) = |\langle \phi_2 | \psi \rangle|^2 = \frac{1}{4} | - \mathrm{e}^{\mathrm{i}Et/\hbar} + \mathrm{e}^{-\mathrm{i}Et/\hbar}|^2 = \sin^2(Et/\hbar).$$

[6 marks]

3. **Quantum wave functions in a harmonic potential**

(a) (i) **[Seen similar and straight forward - category A]**
Normalisation:
$$\int_{-\infty}^{+\infty} |\phi_0(x)|^2 \mathrm{d}x = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-x^2} \mathrm{d}x = 1.$$
and
$$\int_{-\infty}^{+\infty} |\phi_1(x)|^2 \mathrm{d}x = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{+\infty} x^2 \mathrm{e}^{-x^2} \mathrm{d}x = 1.$$

[3 marks]

(ii) **[Seen similar and mostly straight forward - category A/B]**
Applying $\hat{H}$ in position representation to $\phi(x)$ yields
$$\langle x|\hat{H}|\phi\rangle = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\phi(x) + \frac{1}{2}x^2\phi(x).$$
We have
$$\frac{\partial}{\partial x}\phi_0(x) = -x\phi_0(x),$$
and
$$\frac{\partial^2}{\partial x^2}\phi_0(x) = (x^2-1)\phi_0(x),$$
and thus
$$\langle x|\hat{H}|\phi_0\rangle = \frac{1}{2}\phi_0(x),$$
that is, $\phi_0(x)$ is an eigenfunction of $\hat{H}$ with eigenvalue $\frac{1}{2}$.
For $\phi_1(x)$ we find
$$\frac{\partial^2}{\partial x^2}\phi_1(x) = (-3+x^2)\phi_1(x),$$
that is
$$\langle x|\hat{H}|\phi_1\rangle = \frac{3}{2}\phi_0(x),$$
which means that $\phi_1(x)$ is an eigenfunction of $\hat{H}$ with eigenvalue $\frac{3}{2}$.

[7 marks]

(b) **[Unseen but fairly straight forward - category B]**
We have
$$\langle x|\hat{a}^\dagger|\phi\rangle = \frac{1}{\sqrt{2}}(x\phi(x) - \frac{\partial}{\partial x}\phi(x)).$$
And for $\phi_0(x)$ we have as in (a)
$$\frac{\partial}{\partial x}\phi_0(x) = -x\phi_0(x),$$
that is
$$\langle x|\hat{a}^\dagger|\phi_0\rangle = \sqrt{2}x\phi_0(x),$$
and indeed
$$\phi_1(x) = \sqrt{2}x\phi_0(x).$$

[4 marks]

(c) **[Unseen and combines various ideas - category D]**

We have

$$\langle\psi(t)|\hat{q}|\psi(t)\rangle = \frac{1}{\sqrt{2}}\langle\psi(t)|\hat{a}+\hat{a}^\dagger|\psi(t)\rangle.$$

The time-dependent state is given by

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{-iE_0 t}|0\rangle + \mathrm{e}^{-iE_1 t}|1\rangle\right).$$

That is

$$\langle\psi(t)|\hat{q}|\psi(t)\rangle = \frac{1}{\sqrt{8}}\Big(\langle 0|\hat{a}|0\rangle + \langle 0|\hat{a}^\dagger|0\rangle + \mathrm{e}^{\mathrm{i}(E_0-E_1)t}\langle 0|\hat{a}|1\rangle + \mathrm{e}^{\mathrm{i}(E_0-E_1)t}\langle 0|\hat{a}^\dagger|1\rangle$$
$$\mathrm{e}^{\mathrm{i}(E_1-E_0)t}\langle 1|\hat{a}|0\rangle + \mathrm{e}^{\mathrm{i}(E_1-E_0)t}\langle 1|\hat{a}^\dagger|0\rangle + \langle 1|\hat{a}|1\rangle + \langle 1|\hat{a}^\dagger|1\rangle\Big).$$

With

$$\hat{a}^\dagger|n\rangle - \sqrt{n+1}|n+1\rangle, \quad \text{and} \quad \hat{a}|n\rangle = \sqrt{n}|n-1\rangle,$$

and $\langle n|m\rangle = \delta_{nm}$ we find

$$\langle\psi(t)|\hat{q}|\psi(t)\rangle = \frac{1}{\sqrt{2}}\cos\left((E_0-E_1)t\right) = \frac{1}{\sqrt{2}}\cos\left(t\right).$$

[6 marks]

4. Quantisation conditions for a piecewise constant potential well

[Conceptually very similar to an exam question from 2019, where the central part was raised rather than lowered]

(a) **[Seen similar and straight forward - Category A]**

The solutions of the time-independent Schrödinger equation in the separate regions are of the form $a\mathrm{e}^{\mathrm{i}kx} + b\mathrm{e}^{-\mathrm{i}kx}$ with $k = \sqrt{2m(E - V_j)}/\hbar$, where V_j is the value of the constant potential in region j. For $E > V_j$ we can rewrite this as $A\cos(kx) + B\sin(kx)$.

Here we are looking for *bound states*, that is $\phi(x \to \pm\infty) \to 0$. The solutions are of the form

$$\phi_E(x) = \begin{cases} A_1 \cos(\tilde{k}x) + A_2 \sin(\tilde{k}x), & -L \leq x \leq -a \\ B_1 \cos(kx) + B_2 \sin(kx), & -a < x < a \\ C_1 \cos(\tilde{k}x) + C_2 \sin(\tilde{k}x), & a \leq x \leq L, \end{cases} \tag{2}$$

with $k = \frac{\sqrt{2mE}}{\hbar}$ and $\tilde{k} = \frac{\sqrt{2m(E-V_0)}}{\hbar}$.

[5 marks]

(b) **[Unseen, but seen similar - Category B/C]**

Let us now consider even and odd solutions separately. For the functions (2) to be even, i.e. $\phi_E(-x) = \phi_E(x)$ it needs to hold $B_2 = 0$ and from

$$A_1 \cos(\tilde{k}x) - A_2 \sin(\tilde{k}x) = C_1 \cos(\tilde{k}x) + C_2 \sin(\tilde{k}x)$$

we find $A_1 = C_1$, and $A_2 = -C_2$. That is, the ansatz for even function simplifies to

$$\phi_E(x) = \begin{cases} A_1 \cos(\tilde{k}x) + A_2 \sin(\tilde{k}x), & -L \leq x \leq -a \\ B \cos(kx), \quad -a < x < a \\ A_1 \cos(\tilde{k}x) - A_2 \sin(\tilde{k}x), & a \leq x \leq L, \end{cases} \tag{3}$$

For odd functions $\phi_E(-x) = -\phi_E(x)$ we need $B_1 = 0$, and $A_1 = -C_1$, and $A_2 = C_2$, i.e.,

$$\phi_E(x) = \begin{cases} A_1 \cos(\tilde{k}x) + A_2 \sin(\tilde{k}x), & -L \leq x \leq -a \\ B \sin(kx), \quad -a < x < a \\ -A_1 \cos(\tilde{k}x) + A_2 \sin(\tilde{k}x), & a \leq x \leq L, \end{cases} \tag{4}$$

[6 marks]

(c) **[Unseen, but seen similar - category A/B]**

We have the boundary conditions:

$$\phi(\pm L) = 0,$$

and the wave function and its first derivative need to be continuous at $x = a$ and $x = -a$. This yields six boundary conditions. Due to the symmetry two of them each are equivalent, and we thus have only three independent conditions.

For even states the boundary conditions at $x = \pm L$ yield the following relation between A_1 and A_2:

$$A_2 \cos(\tilde{k}L) - A_2 \sin(\tilde{k}L) = 0,$$

that is

$$A_2 = A_1 \frac{\cos(\tilde{k}L)}{\sin(\tilde{k}L)}$$

The continuity of the wave function and its first derivative at $x = \pm a$ yield the two conditions

$$\begin{aligned} A_1 \cos(\tilde{k}a) - A_2 \sin(\tilde{k}a) &= B\cos(ka) && (5) \\ -A_1 \tilde{k} \sin(\tilde{k}a) - A_2 \tilde{k} \cos(\tilde{k}a) &= -kB\sin(ka) && (6) \end{aligned}$$

Inserting $A_2 = A_1 \frac{\cos(\tilde{k}L)}{\sin(\tilde{k}L)}$ into (5) and (6) yields

$$A_1 \frac{\sin(\tilde{k}(L-a))}{\sin(\tilde{k}L)} = B\cos(ka) \tag{7}$$

$$\tilde{k}A_1 \frac{\cos(\tilde{k}(L-a))}{\sin(\tilde{k}L)} = kB\sin(ka) \tag{8}$$

Dividing (8) by (7) yields the quantisation condition

$$k\tan(ka) = \tilde{k}\cot(\tilde{k}(L-a))$$

for even bound states.

[9 marks]

5. Mastery question - Density Matrices

Based on extra mastery Reading material: Sections 2.1, 2.2., and 2.3 from Ballentine's "Quantum Mechanics" and section 6.1 from Chris Isham's "Lectures on Quantum Theory"

(a) According to the definition we have

$$\mathrm{i}\hbar\dot{\rho} = \hbar \sum_j w_j(\mathrm{i}|\dot{\psi}_j\rangle\langle\psi_j| + \mathrm{i}|\psi_j\rangle\langle\dot{\psi}_j|).$$

Using the Schrödinger equation $\mathrm{i}\hbar|\dot{\psi}\rangle = \hat{H}|\psi\rangle$ and its conjugate equation $-\mathrm{i}\hbar\langle\dot{\psi}| = \langle\psi|\hat{H}$ yields

$$\mathrm{i}\hbar\dot{\rho} = \sum_j w_j\hat{H}|\psi_j\rangle\langle\psi_j| - w_j|\psi_j\rangle\langle\psi_j|\hat{H} = \hat{H}\hat{\rho} - \hat{\rho}\hat{H}.$$

[3 marks]

(b) (i)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathsf{Tr}(\hat{\rho}) = \mathsf{Tr}(\dot{\hat{\rho}}) = -\frac{\mathrm{i}}{\hbar}\mathsf{Tr}\left(\hat{H}\hat{\rho} - \hat{\rho}\hat{H}\right),$$

which vanishes since the trace is cyclic. Thus, the norm is indeed preserved.

(ii) Time derivative of the purity:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathsf{Tr}(\hat{\rho}^2) &= \mathsf{Tr}(\hat{\rho}\dot{\hat{\rho}} + \dot{\hat{\rho}}\hat{\rho}) \\ &= -\frac{\mathrm{i}}{\hbar}\mathsf{Tr}(\hat{\rho}(\hat{H}\hat{\rho} - \hat{\rho}\hat{H}) + (\hat{H}\hat{\rho} - \hat{\rho}\hat{H})\hat{\rho}) \\ &= 0.\end{aligned}$$

(iii) The eigenvalues of $\hat{\rho}$ are conserved during the time evolution. this can for example be seen by the fact that the traces of all the powers of $\hat{\rho}$ are constant in time.

[6 marks]

(c) Normalisation:

$$\mathsf{Tr}(\hat{\rho}) = \frac{1}{4} + \frac{1}{2} + \frac{1}{4} = 1.$$

Purity:

$$\mathsf{Tr}\begin{pmatrix}\frac{1}{4} & * & * \\ * & \frac{1}{4} & * \\ * & * & \frac{1}{2}\end{pmatrix} = 1$$

[3 marks]

(d) (i) The density matrix is given by

$$\hat{\rho} = \begin{pmatrix}1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0\end{pmatrix}$$

and we find

$$\mathsf{Tr}(\hat{H}\rho) = \hbar\omega\mathsf{Tr}\begin{pmatrix}1 & * & * \\ * & 0 & * \\ * & * & 0\end{pmatrix} = \hbar\omega$$

[3 marks]

(ii) We have

$$\hat{\rho} = \frac{1}{2}\begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}1 & 0 & 0\end{pmatrix} + \frac{1}{4}\begin{pmatrix}1\\0\\1\end{pmatrix}\begin{pmatrix}1 & 0 & 1\end{pmatrix} = \frac{1}{4}\begin{pmatrix}3 & 0 & 1\\0 & 0 & 0\\1 & 0 & 1\end{pmatrix}$$

and

$$\mathsf{Tr}(\hat{H}\rho) = \frac{\hbar\omega}{4}\mathsf{Tr}\begin{pmatrix}3 & * & *\\ * & 0 & *\\ * & * & -1\end{pmatrix} = \frac{\hbar\omega}{2}.$$

[5 marks]

If your module is taught across multiple year levels, you might have received this form for each level of the module. You are only required to fill this out once for each question.

Please record below, some brief but non-trivial comments for students about how well (or otherwise) the questions were answered. For example, you may wish to comment on common errors and misconceptions, or areas where students have done well. These comments should note any errors in and corrections to the paper. These comments will be made available to students via the MathsCentral Blackboard site and should not contain any information which identifies individual candidates. Any comments which should be kept confidential should be included as confidential comments for the Exam Board and Externals. If you would like to add formulas, please include a sperate pdf file with your email.

<table>
<tr><th>ExamModuleCode</th><th>QuestionNumber</th><th>Comments for Students</th></tr>
<tr><td>MATH96005 and
MATH97014
MATH97093</td><td>1</td><td>As anticipated most parts of this question were answered without further problems by most students. A common mistake in part a was to think that |psi><psi| was the identity. That is impossible for any vector in a two-dimensional Hilbert space! Part c)ii concerning the Ehrenfest theorem was answered correctly by a good number of students, but a surprisingly large number of students did not realise that V(q)=0 here and that the dynamical equation dq/dt=p/m is not solved by q(t)=p_0/m t if p is not constant!</td></tr>
<tr><td>MATH96005 and
MATH97014
MATH97093</td><td>2</td><td>Question 2 was solved well by most. In part b (iii) many wasted time by calculating the uncertainties of A and H explicilty, while it should have been clear from b (ii) that the uncertainty of H was zero. Part c was intended to test the understanding of the measurement concept, and not surprisingly there were more issues here than with the rest of the question. There was still a large number of student solving the whole problem excellently.</td></tr>
<tr><td>MATH96005 and
MATH97014
MATH97093</td><td>3</td><td>As intended,everyone who knew what a normalised wavefunction is solved part a (i) correectly. Part a(ii) went smoothly for many, but a fairly common mistake was to regard an x-dependent expression as an eigenvlue. H phi(x)=f(x)phi(x) does not mean that phi(x) is an eigenfunction of H with eigenvalue f(x)!!! Part b was fine, and part c, which combined different ideas from the course did reveal a lack of understanding for some, but was fully solved by many. I hope the fact that a considerable number of students solved this part and part c in Q2 so well reflects that many have learned some important aspects of quantum foundations succesfully this year due to the hard work they have invested into the course.</td></tr>
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MATH96005 and MATH97014 MATH97093	4	Question 4 was very very similar to an exam question from last year, but with crucial differences. While many solved the whole question very well, sadly there were quite a few students who tried to follow last year's solution and ran into inconsistencies. Since this was an open book exam and since the final expression to be dervied was provided in the question, I demanded a certain level of detail in the last steps of the derivation in part c to obtain full marks.
MATH96005 and MATH97014 MATH97093	5	A small number of students did not attempt the mastery question at all or wrote very very little. This may have been due to time constraints. Most part of the quesiton were rather straight forward, and solved well by most. The most challenging part seems to have been part b.