Imperial College London

Department of Mathematics

M3A52 Quantum Mechanics II

Question	Examiner's Comments
Q 1	Most did very well in parts a-c. Part d was a bit more difficult, but some were able to also work this out.
Q 2	I was very happy to see a number of you with a clever and shorter approach to part b than was in the coursework solutions. Well done!
Q 3	The first two parts were directly from the notes. Part c was slightly tricky because the "unperturbed" Hamiltonian was not diagonal. Still, many did this correctly.
Q 4	I was overall impressed with how students did on this problem because we did not have any assessed coursework problems on time reversal.

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M45A52 Quantum Mechanics II

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Q 2	I was very happy to see a number of you with a clever and shorter approach to part b than was in the coursework solutions. Well done!
Q 3	The first two parts were directly from the notes. Part c was slightly tricky because the "unperturbed" Hamiltonian was not diagonal. Still, many did this correctly.
Q 4	This was similar to a coursework problem. In hindsight, I felt this problem was a bit too long. Since this was one of the more difficult coursework problems, I wanted to see how many of you went through the solutions carefully.
Q 5	I was overall impressed with how students did on this problem because we did not have any assessed coursework problems on time reversal.

Imperial College
London

M4/5A52

BSc, MSci and MSc EXAMINATIONS (MATHEMATICS)

May-June 2018

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

Quantum Mechanics II

Date: Friday, 25 May 2018

Time: 10:00 AM - 12:30 PM

Time Allowed: 2.5 hours

This paper has 5 questions.

Candidates should use ONE main answer book.

Supplementary books may only be used after the relevant main book(s) are full.

All required additional material will be provided.

- DO NOT OPEN THIS PAPER UNTIL THE INVIGILATOR TELLS YOU TO.
- Affix one of the labels provided to each answer book that you use, but DO NOT USE THE LABEL WITH YOUR NAME ON IT.
- Each question carries equal weight.
- Calculators may not be used.

1. The Heisenberg Picture.

In this problem we consider the quantum dynamics of a particle in one spatial dimension governed by the Hamiltonian

$$\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 + m\gamma\hat{x}$$

where γ is a real constant and m denotes the mass of the particle. As usual, $\hat{x}$ and $\hat{p}$ denote the canonically conjugate position and momentum operators: $[\hat{x}, \hat{p}] = i\hbar$.

(a) Show that the Heisenberg equations of motion for the position and momentum operators are

$$m\frac{d}{dt}\hat{x}_{\mathrm{H}} = \hat{p}_{\mathrm{H}}$$
$$\frac{d}{dt}\hat{p}_{\mathrm{H}} = -m\gamma$$

where $\hat{x}_{\mathrm{H}}$ and $\hat{p}_{\mathrm{H}}$ are the position and momentum operators in the Heisenberg picture.

(b) Solve the (operator) differential equations of part (a) with appropriate initial conditions to determine $\hat{x}_{\mathrm{H}}$ and $\hat{p}_{\mathrm{H}}$.

(c) Suppose that the initial wave function (at time $t = 0$) of the particle is

$$\psi_i(x) = \frac{1}{(2\pi\bar{\sigma}_x^2)^{1/4}} e^{-\frac{x^2}{4\bar{\sigma}_x^2}}$$

where $\bar{\sigma}_x > 0$. With this initial state, compute the expectation value of the position operator for later times. Comment on your result in the context of Ehrenfest's theorem.

(d) Determine the time-dependent variance of position:

$$\sigma_x^2(t) = \langle\psi(t)|\,\hat{x}^2\,|\psi(t)\rangle - \langle\psi(t)|\,\hat{x}\,|\psi(t)\rangle^2$$

where $|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}\,|\psi_i\rangle$.

2. Time-dependent unitary transformations.

(a) Suppose $|\psi(t)\rangle$ satisfies the time-dependent Schrödinger equation for some time-dependent Hamiltonian $\hat{\mathcal{H}}(t)$:

$$\hat{\mathcal{H}}(t)\,|\psi(t)\rangle = i\hbar\partial_t\,|\psi(t)\rangle\,.$$

Next introduce a new state related to $|\psi(t)\rangle$ via a time-dependent unitary transformation. In particular, let $|\psi'(t)\rangle = \hat{U}(t)\,|\psi(t)\rangle$ where $\hat{U}(t)$ is a time-dependent unitary operator. Show that $|\psi'(t)\rangle$ satisfies

$$\hat{\mathcal{H}}'(t)\,|\psi'(t)\rangle = i\hbar\partial_t\,|\psi'(t)\rangle$$

where $\hat{\mathcal{H}}'(t) = \hat{U}(t)\hat{\mathcal{H}}(t)\hat{U}^\dagger(t) - i\hbar\hat{U}(t)\partial_t\hat{U}^\dagger(t)$.

(b) Suppose we managed to find a unitary transformation such that $\hat{\mathcal{H}}'$ is time-independent. For this case, show that the time-evolution operator (with initial time $t = 0$) for the original time-dependent Hamiltonian is

$$\hat{\mathcal{U}}(t) = \hat{U}^\dagger(t)e^{\frac{-i}{\hbar}\hat{\mathcal{H}}'t}\hat{U}(0).$$

(c) For the remainder of this problem restrict to the following Hamiltonian

$$\hat{\mathcal{H}} = \varepsilon\,|1\rangle\langle 1| + \frac{\Omega}{2}\left(|0\rangle\langle 1|\,e^{i\omega t} + |1\rangle\langle 0|\,e^{-i\omega t}\right).$$

Here $\{|0\rangle, |1\rangle\}$ form an orthonormal basis and ε, Ω and, ω are real constants. Consider the operator $\hat{U}(t) = |0\rangle\langle 0| + |1\rangle\langle 1|\,e^{i\omega t}$. Show that $\hat{U}(t)$ is unitary. Show that the transformed Hamiltonian $\hat{\mathcal{H}}'(t) = \hat{U}(t)\hat{\mathcal{H}}\hat{U}^\dagger(t) - i\hbar\hat{U}(t)\partial_t\hat{U}^\dagger(t)$ is

$$\hat{\mathcal{H}}' = (\varepsilon - \hbar\omega)\,|1\rangle\langle 1| + \frac{\Omega}{2}\left(|0\rangle\langle 1| + |1\rangle\langle 0|\right)$$

(d) For this part, restrict to the case of responance: $\hbar\omega = \varepsilon$. Suppose at time $t = 0$ the system is in state $|0\rangle$. Compute the probability for the system to be in state $|1\rangle$ at later time t.

3. Time-independent perturbation theory.

Consider the Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \lambda\hat{V}$ where λ is a small parameter. Here, $\hat{\mathcal{H}}_0$ and $\hat{V}$ are time-independent Hermitian operators. Denote the eigenstates and eigenenergies of $\hat{\mathcal{H}}_0$ as $|n\rangle$ and ε_n so that $\hat{\mathcal{H}}_0 |n\rangle = \varepsilon_n |n\rangle$. In this problem we restrict to the case where the ground state of $\hat{\mathcal{H}}_0$, $|n=0\rangle$, is non-degenerate.

(a) In one or two sentences carefully explain what it means for the state $|n=0\rangle$ to be non-degenerate.

(b) Show that the ground state energy including linear and second-order perturbative corrections in λ is

$$E_0 = \varepsilon_0 + \lambda \langle 0| \hat{V} |0\rangle + \lambda^2 \sum_{n\neq 0} \frac{|\langle n| \hat{V} |0\rangle|^2}{\varepsilon_0 - \varepsilon_n}$$

(c) For the remainder of the problem we focus on a two-dimensional Hilbert space spanned by the orthonormal basis $\{|R\rangle, |L\rangle\}$. We focus on the following Hamiltonian

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \lambda\hat{V} = -w(|R\rangle\langle L| + |L\rangle\langle R|) + \lambda\Delta(|L\rangle\langle L| - |R\rangle\langle R|)$$

where Δ and w are positive real constants and λ is our usual perturbative parameter. Such a Hamiltonian can provide an effective description of a particle in a double-well potential with a small tilt. Using perturbation theory, compute the ground state energy of this Hamiltonian to second order in λ.

(d) Compute the exact ground state of the Hamiltonian from (c). Show that this is consistent with the result from perturbation theory.

4. Time-dependent perturbation theory and the adiabatic limit.

In this problem we consider the time-dependent Hamiltonian given by

$$\hat{\mathcal{H}} = \varepsilon(|1\rangle\langle 1| - |0\rangle\langle 0|) + f(t)\lambda\Omega(|1\rangle\langle 0| + |0\rangle\langle 1|) = \hat{\mathcal{H}}_0 + \lambda\hat{V}(t).$$

where ε and Ω are positive constants and λ is our usual perturbative parameter. $\{|0\rangle, |1\rangle\}$ form an orthonormal basis. The time-dependent function appearing in the Hamiltonian is defined as $f(t) = e^{\eta t}$ for $t < 0$ and $f(t) = 1$ for $t \geq 0$ where η is a positive constant. Adjusting η allows us to control how quickly the second term in the Hamiltonian is 'turned on'.

Suppose that in the 'distant past', $t \to -\infty$, the system is in the ground state $|0\rangle$ of the Hamiltonian. In this problem we will focus on computing the probability $P_{0\to 1}$ for the system to be in the state $|1\rangle$ at time $t > 0$.

(a) Limit of small λ. Using time-dependent perturbation theory, show that to lowest non-trivial order in λ,

$$P_{0\to 1} = \frac{\lambda^2\Omega^2}{\hbar^2}\left|\frac{1}{2i\varepsilon/\hbar + \eta} + \frac{1}{2i\varepsilon/\hbar}(e^{2i\varepsilon t/\hbar} - 1)\right|^2.$$

Hint: recall the result from time-dependent perturbation theory

$$P_{0\to 1} = \frac{\lambda^2}{\hbar^2}\left|\int_{-\infty}^{t} dt' \langle 1|\hat{V}|0\rangle\, e^{-i(\varepsilon_0-\varepsilon_1)t'/\hbar}\right|^2.$$

(b) Limit of large η. In the limit when $\eta \to +\infty$, $f(t)$ becomes a step function. That is $f(t) = 0$ for $t < 0$ and $f(t) = 1$ for $t \geq 0$. Taking $f(t)$ to be a step function, compute the probability $P_{0\to 1}$ exactly. Show that it agrees with the result of (a) in the limit of small λ and large η.

(c) Now consider the opposite limit of η approaching zero (slow turn-on). Show that in this limit

$$P_{0\to 1} = \frac{1}{2}\left(1 - \frac{\varepsilon}{\sqrt{\varepsilon^2 + \lambda^2\Omega^2}}\right).$$

Argue that this result is consistent with that of (a).

(d) Finally, consider the case where there is different time-dependence: $f(t) = e^{-\eta t^2}$ where η is a positive real parameter and $t \in \mathbb{R}$. Suppose, again, that in the 'distant past', $t \to -\infty$, the particle is in the state $|0\rangle$. What is the probability for the particle to still be in the state $|0\rangle$ as $t \to \infty$ to leading non-trivial order in λ? In a few sentences explain why this result is consistent with the adiabatic limit of small η.

5 . (Mastery) Time reversal.

Consider an N-dimensional Hilbert space spanned by orthonormal basis $\{|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_N\rangle\}$. Let $\hat{K}$ be an anti-linear operator that acts on an arbitrary state $|\alpha\rangle = \sum_n \alpha_n |\phi_n\rangle$ (for scalar α_n's) as $\hat{K}|\alpha\rangle = \sum_n \alpha_n^* |\phi_n\rangle$. Denote the time-reversal operator as

$$\hat{T} = \hat{U}\hat{K}$$

where $\hat{U}$ is a unitary operator.

(a) Take two arbitrary states in this Hilbert space to be $|\alpha\rangle$ and $|\beta\rangle$. Let $|\alpha'\rangle = \hat{T}|\alpha\rangle$ and $|\beta'\rangle = \hat{T}|\beta\rangle$. Show that $\langle\alpha|\beta\rangle = \langle\beta'|\alpha'\rangle$ and hence $\hat{T}$ gives an anti-unitary transformation.

(b) Now consider a time-reversal invariant Hamiltonian acting in this Hilbert space: $\hat{\mathcal{H}} = \hat{T}\hat{\mathcal{H}}\hat{T}^{-1}$. Further suppose that $\hat{T}^2 = -\mathbb{1}$. Show that $\hat{\mathcal{H}}$ has no non-degenerate eigenstates.

(c) For the remainder of this problem, we consider the case of a spin-one system. Let $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ be the spin-one spin operators. Denote the eigenbasis of $\hat{S}_z$ as $\{|m\rangle\}$ so that $\hat{S}_z|m\rangle = \hbar m|m\rangle$ for $m = -1, 0, 1$. The time reversal operator for this system is $\hat{T} = \hat{U}\hat{K}$ where $\hat{U} = |1\rangle\langle -1| - |0\rangle\langle 0| + |-1\rangle\langle 1|$ and $\hat{K}$ is the anti-unitary operator that acts trivially on the $\hat{S}_z$ eigenkets: $\hat{K}|m\rangle = |m\rangle$.

Show that $\hat{U}$ is unitary. Also show that $\hat{T}^2 = \mathbb{1}$ (hint: consider how $\hat{T}$ acts on an arbitrary spin-one state).

(d) Consider the Hamiltonian

$$\hat{\mathcal{H}} = \gamma(\hat{S}_x^2 + \hat{S}_y^2)$$

where γ is a real constant. Find three simultaneous eigenstates of $\hat{\mathcal{H}}$ and $\hat{T}$.

Solutions for MA52 Exam, 2018

1. The Heisenberg Picture.

   In this problem we consider the quantum dynamics of a particle in one spatial dimension governed by the Hamiltonian

$$\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 + m\gamma\hat{x}$$

   where γ is a real constant and m denotes the mass of the particle. As usual, $\hat{x}$ and $\hat{p}$ denote the canonically conjugate position and momentum operators: $[\hat{x}, \hat{p}] = i\hbar$.

   (a) Show that the Heisenberg equations of motion for the position and momentum operators are

$$m\frac{d}{dt}\hat{x}_{\mathrm{H}} = \hat{p}_{\mathrm{H}}$$
$$\frac{d}{dt}\hat{p}_{\mathrm{H}} = -m\gamma$$

   where $\hat{x}_{\mathrm{H}}$ and $\hat{p}_{\mathrm{H}}$ are the position and momentum operators in the Heisenberg picture.

   Unseen/Seen: A similar problem was worked out for the free particle.

   5 Marks (Level 1)

   In the Heisenberg picture, operators evolve but states are time-independent. In particular $\hat{x}_{\mathrm{H}} = \hat{\mathcal{U}}^\dagger(t)\hat{x}\hat{\mathcal{U}}(t)$ where $\hat{\mathcal{U}}(t)$ is the time-evolution operator for $\hat{\mathcal{H}}$. Differentiating with respect to t gives $i\hbar\frac{d}{dt}\hat{x}_{\mathrm{H}} = \hat{\mathcal{U}}^\dagger(t)[\hat{x}, \hat{\mathcal{H}}]\hat{\mathcal{U}}(t)$. Evaluating the commutator gives $i\hbar\frac{d}{dt}\hat{x}_{\mathrm{H}} = \hat{\mathcal{U}}^\dagger(t)i\hbar\hat{p}/m\hat{\mathcal{U}}(t) = i\hbar\hat{p}_{\mathrm{H}}$. This gives our first equation of motion. A similar calculation gives the equation for $\hat{p}_{\mathrm{H}}$.

   (b) Solve the (operator) differential equations of part (a) with appropriate initial conditions to determine $\hat{x}_{\mathrm{H}}$ and $\hat{p}_{\mathrm{H}}$.

   Unseen/Seen:

   5 Marks (Level 2)

   Noting that $\hat{x}(t=0) = \hat{x}$ and $\hat{p}(t=0) = \hat{p}$ we can solve these coupled differential equations. The solution is

$$\hat{x}_{\mathrm{H}} = \hat{x} + \frac{1}{m}\hat{p}t - \frac{1}{2}\gamma t^2$$
$$\hat{p}_{\mathrm{H}} = \hat{p} - m\gamma t.$$

   (c) Suppose that the initial wave function (at time $t = 0$) of the particle is

$$\psi_i(x) = \frac{1}{(2\pi\bar{\sigma}_x^2)^{1/4}}e^{-\frac{x^2}{4\bar{\sigma}_x^2}}$$

where $\bar{\sigma}_x > 0$. With this initial state, compute the expectation value of the position operator for later times. Comment on your result in the context of Ehrenfest's theorem.

Unseen/Seen:

5 Marks (Level 1)

Using the given expression for $\psi_i(x)$ we can determine that

$$\langle\psi_i|\,\hat{x}\,|\psi_i\rangle = \int dx|\psi_i(x)|^2 x = 0$$
$$\langle\psi_i|\,\hat{p}\,|\psi_i\rangle = \int dx\psi_i^*(x)(-i\hbar\partial_x)\psi_i(x) = 0.$$

Then, with the result of (b) we have

$$\langle\psi(t)|\,\hat{x}\,|\psi(t)\rangle = \langle\psi_i|\,\hat{x}_{\mathrm{H}}\,|\psi_i\rangle = -\frac{1}{2}\gamma t^2.$$

This is the trajectory a classical particle under the analogous potential would follow (with zero initial momentum and position). This agreement is due to Ehrenfest's theorem.

(d) Determine the time-dependent variance of position:

$$\sigma_x^2(t) = \langle\psi(t)|\,\hat{x}^2\,|\psi(t)\rangle - \langle\psi(t)|\,\hat{x}\,|\psi(t)\rangle^2$$

where $|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}\,|\psi_i\rangle$.

Unseen/Seen

5 Marks (Level 4)

It is intended that the Heisenberg picture is again used for this part. Several Gaussian integrals need to be computed to obtain the desired result. Many of these can be seen to vanish without actually doing the integrals. The result is

$$\sigma_x^2 = \bar{\sigma}_x^2 + \frac{\hbar^2 t^2}{4m\bar{\sigma}_x{}^2}.$$

2. Time-dependent unitary transformations.

(a) Suppose $|\psi(t)\rangle$ satisfies the time-dependent Schrodinger equation for some time-dependent Hamiltonian $\hat{\mathcal{H}}(t)$:

$$\hat{\mathcal{H}}(t)\,|\psi(t)\rangle = i\hbar\partial_t\,|\psi(t)\rangle\,.$$

Next introduce a new state related to $|\psi(t)\rangle$ via a time-dependent unitary transformation. In particular, let $|\psi'(t)\rangle = \hat{U}(t)\,|\psi(t)\rangle$ where $\hat{U}(t)$ is a time-dependent unitary operator. Show that $|\psi'(t)\rangle$ satisfies

$$\hat{\mathcal{H}}'(t)\,|\psi'(t)\rangle = i\hbar\partial_t\,|\psi'(t)\rangle$$

where $\hat{\mathcal{H}}'(t) = \hat{U}(t)\hat{\mathcal{H}}(t)\hat{U}^\dagger(t) - i\hbar\hat{U}(t)\partial_t\hat{U}^\dagger(t)$.

Seen

5 Marks (Level 1)

Substituting $|\psi\rangle = \hat{U}^\dagger\,|\psi'\rangle$ in the TDSE we have

$$i\hbar(\partial_t\hat{U}^\dagger)\,|\psi'\rangle + i\hbar\hat{U}^\dagger\partial_t\,|\psi'\rangle = \hat{\mathcal{H}}\hat{U}^\dagger\,|\psi'\rangle\,.$$

Next, we multiply both sides of this equation by $\hat{U}$. Remembering that $\hat{U}$ is unitary, and rearranging we have

$$i\hbar\partial_t\,|\psi'\rangle = \left(\hat{U}\hat{\mathcal{H}}\hat{U}^\dagger - i\hbar\hat{U}\partial_t\hat{U}^\dagger\right)|\psi'\rangle\,.$$

This is the desired result.

(b) Suppose we managed to find a unitary transformation such that $\mathcal{H}'$ is time-independent. For this case, show that the time-evolution operator (with initial time $t = 0$) for the original time-dependent Hamiltonian is

$$\hat{\mathcal{U}}(t) = \hat{U}^\dagger(t)e^{\frac{-i}{\hbar}\hat{\mathcal{H}}'t}\hat{U}(0).$$

Unseen/Seen (A student might have seen a similar expression in an optional problem). Would be a Level 4 problem if completely unseen.

4 Marks (Level 3) + 1 Mark (Level 4)

The time evolution operator for $\hat{\mathcal{H}}(t)$ is the operator $\hat{\mathcal{U}}(t)$ that satisfies satisfies $i\hbar\partial_t\hat{\mathcal{U}}(t) = \hat{\mathcal{H}}(t)\hat{\mathcal{U}}(t)$ with initial condition $\hat{\mathcal{U}}(t=0) = \mathbb{1}$. We can readily verify that $\hat{\mathcal{U}}(t=0) = \mathbb{1}$. Differentiating $\hat{\mathcal{U}}(t)$, and letting $\hat{\mathcal{U}}'(t) = e^{\frac{-i}{\hbar}\hat{\mathcal{H}}'t}$, we find

$$i\hbar\partial_t\hat{\mathcal{U}}(t) = i\hbar\partial_t\hat{U}^\dagger(t)\hat{\mathcal{U}}'(t)\hat{U}(0) + \hat{U}^\dagger(t)\hat{\mathcal{H}}'\hat{\mathcal{U}}'(t)\hat{U}(0).$$

Next, inserting $\hat{U}(t)\hat{U}^\dagger(t) = \mathbb{1}$ in two places in the above we find

$$i\hbar\partial_t\hat{\mathcal{U}}(t) = (i\hbar\partial_t\hat{U}^\dagger(t)\hat{U}(t) + \hat{\mathcal{H}}')\hat{\mathcal{U}}(t)$$

By inverting the result of (a), the term in parenthesis above is found to be just $\hat{\mathcal{H}}$.

(c) For the remainder of this problem restrict to the following Hamiltonian

$$\hat{\mathcal{H}} = \varepsilon \left|1\right\rangle \left\langle 1\right| + \frac{\Omega}{2}\left(\left|0\right\rangle \left\langle 1\right| e^{i\omega t} + \left|1\right\rangle \left\langle 0\right| e^{-i\omega t}\right).$$

Here $\{\left|0\right\rangle, \left|1\right\rangle\}$ form an orthonormal basis and ε, Ω and, ω are real constants. Consider the operator $\hat{U}(t) = \left|0\right\rangle \left\langle 0\right| + \left|1\right\rangle \left\langle 1\right| e^{i\omega t}$. Show that $\hat{U}(t)$ is unitary. Show that the transformed Hamiltonian $\hat{\mathcal{H}}'(t) = \hat{U}(t)\hat{\mathcal{H}}\hat{U}^\dagger(t) - i\hbar\hat{U}(t)\partial_t\hat{U}^\dagger(t)$ is

$$\hat{\mathcal{H}}' = (\varepsilon - \hbar\omega)\left|1\right\rangle \left\langle 1\right| + \frac{\Omega}{2}\left(\left|0\right\rangle \left\langle 1\right| + \left|1\right\rangle \left\langle 0\right|\right)$$

Unseen

5 Marks (Level 1)

By taking the adjoint, we find $\hat{U}^\dagger(t) = \left|0\right\rangle \left\langle 0\right| + \left|1\right\rangle \left\langle 1\right| e^{-i\omega t}$. A direct calculation shows that $\hat{U}^\dagger(t)\hat{U}(t) = \left|0\right\rangle \left\langle 0\right| + \left|1\right\rangle \left\langle 1\right| = \mathbb{1}$. Therefore, $\hat{U}(t)$ is unitary.

Through a calculation involving a few steps, we can work out that the transformed Hamiltonian is

$$\hat{\mathcal{H}}' = (\varepsilon - \hbar\omega)\left|1\right\rangle \left\langle 1\right| + \frac{\Omega}{2}\left(\left|0\right\rangle \left\langle 1\right| + \left|1\right\rangle \left\langle 0\right|\right)$$

which is indeed time-independent.

(d) For this part, restrict to the case of responance: $\hbar\omega = \varepsilon$. Suppose at time $t = 0$ the system is in state $\left|0\right\rangle$. Compute the probability for the system to be in state $\left|1\right\rangle$ at later time t.

Unseen

5 Marks (Level 4)

One must first recognise that this probability is given by

$$P = |\left\langle 1\right| \hat{\mathcal{U}}(t) \left|0\right\rangle|^2.$$

This calculation uses the results of (b) and (c). One also needs to diagonalise $\hat{\mathcal{H}}'$ so that its evolution operator can be found. The result is

$$P = \sin^2\left(\frac{\Omega t}{2\hbar}\right).$$

3. Time-independent perturbation theory. Consider Hamiltonian $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \lambda\hat{V}$ where λ is a small parameter. Here, $\hat{\mathcal{H}}_0$ and $\hat{V}$ are time-independent Hermitian operators. Denote the eigenstates and eigenenergies of $\hat{\mathcal{H}}_0$ as $|n\rangle$ and ε_n so that $\hat{\mathcal{H}}_0 |n\rangle = \varepsilon_n |n\rangle$. In this problem we restrict to the case where the ground state of $\hat{\mathcal{H}}_0$, $|n = 0\rangle$, is non-degenerate.

(a) In one or two sentences carefully explain what it means for the state $|n = 0\rangle$ to be non-degenerate.

Seen

3 Marks (Level 1)

It means that all eigenstates of $\hat{\mathcal{H}}_0$ with eigenenergy ε_0 are proportional to $|n = 0\rangle$.

(b) Show that the ground state energy including linear and second-order perturbative corrections in λ is

$$E_0 = \varepsilon_0 + \lambda \langle 0|\hat{V}|0\rangle + \lambda^2 \sum_{n\neq 0} \frac{|\langle n|\hat{V}|0\rangle|^2}{\varepsilon_0 - \varepsilon_n}$$

Seen

4 Marks (Level 1) + 2 Marks (Level 2)

This is a standard calculation (appearing in most QM textbooks). Still, there are several steps involved with the derivation.

(c) For the remainder of the problem we focus on a two-dimensional Hilbert space spanned by the orthonormal basis $\{|R\rangle, |L\rangle\}$. We focus on the following Hamiltonian

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \lambda\hat{V} = -w(|R\rangle\langle L| + |L\rangle\langle R|) + \lambda\Delta(|L\rangle\langle L| - |R\rangle\langle R|)$$

where Δ and w are positive real constants and λ is our usual perturbative parameter. Such a Hamiltonian can provide an effective description of a particle in a double-well potential with a small tilt. Using perturbation theory, compute the ground state energy of this Hamiltonian to second order in λ.

Unseen

6 Marks (Level 3)

Examples done in lecture focused on cases where $\hat{\mathcal{H}}_0$ is diagonal. For this problem, one needs to diagonalise $\hat{\mathcal{H}}_0$ before employing the expressions from (b). The result is

$$E_0 = -w + \frac{\lambda^2\Delta^2}{2w}.$$

(d) Compute the exact ground state of the Hamiltonian from (c). Show that this is consistent with the result from perturbation theory.

Similar Seen

5 Marks (Level 1)

The result is

$$E_0 = -\sqrt{w^2 + \lambda^2\Delta^2}.$$

Expanding this in λ to second order gives a result in agreement with (c).

4. Time-dependent perturbation theory and the adiabatic limit.

In this problem we consider the time-dependent Hamiltonian given by

$$\hat{\mathcal{H}} = 2\varepsilon |1\rangle\langle 1| + f(t)\lambda\Omega\left[|1\rangle\langle 0| + |0\rangle\langle 1|\right] = \hat{\mathcal{H}}_0 + \lambda\hat{V}(t).$$

where ε and Ω are positive constants and λ is our usual perturbative parameter. $\{|0\rangle, |1\rangle\}$ form an orthonormal basis. The time-dependent function appearing in the Hamiltonian is defined as $f(t) = e^{\eta t}$ for $t < 0$ and $f(t) = 1$ for $t \geq 0$ where η is a positive constant. Adjusting η allows us to control how quickly the second term in the Hamiltonian is 'turned on'.

Suppose that in the 'distant past', $t \to -\infty$, the system is in the ground state $|0\rangle$ of the Hamiltonian. In this problem we will focus on computing the probability $P_{0\to1}$ for the system to be in the state $|1\rangle$ at time $t > 0$.

(a) Limit of small λ. Using time-dependent perturbation theory, show that to lowest non-trivial order in λ,

$$P_{0\to1} = \frac{\lambda^2\Omega^2}{\hbar^2}\left|\frac{1}{2i\varepsilon/\hbar + \eta} + \frac{1}{2i\varepsilon/\hbar}(e^{2i\varepsilon t/\hbar} - 1)\right|^2.$$

Hint: recall the result from time-dependent perturbation theory

$$P_{0\to1} = \frac{\lambda^2}{\hbar^2}\left|\int_{-\infty}^{t} \langle 1|\hat{V}|0\rangle\, e^{-i(\varepsilon_0-\varepsilon_1)t/\hbar)}\right|^2$$

Similar Seen

5 Marks (Level 2)

Adapting for the problem at hand, we have

$$P_{0\to1} = \frac{\lambda^2}{\hbar^2}\left|\int_{-\infty}^{t} dt' e^{2i\varepsilon t/\hbar} f(t)\Omega\right|^2.$$

Performing the integral gives the desired result.

(b) Limit of large η. In the limit when $\eta \to +\infty$, $f(t)$ becomes a step function. That is $f(t) = 0$ for $t < 0$ and $f(t) = 1$ for $t \geq 0$. Taking $f(t)$ to be a step function, compute the probability $P_{0\to1}$ exactly. Show that it agrees with the result of (a) in the limit of small λ and large η.

Similar Seen

5 Marks (Level 2)

In this limit, $\hat{\mathcal{H}} = \varepsilon|1\rangle\langle 1|$ for $t < 0$. So the state will simply be fixed at $|0\rangle$ for all negative times. For positive times, we can evolve the state with the time-independent Hamiltonian $\hat{\mathcal{H}} = \varepsilon|1\rangle\langle 1| + \lambda\Omega\left[|1\rangle\langle 0| + |0\rangle\langle 1|\right]$ with initial condition $|\psi(t = 0)\rangle = |0\rangle$. A calculation then gives

$$P_{0\to1} = \sin^2(Et/\hbar)\frac{\lambda^2\Omega^2}{E^2}$$

where $E = \sqrt{\varepsilon^2 + \lambda^2\Omega^2}$. To compare with the result of (b), we note that the present $P_{0\to 1}$ to second order in λ is

$$P_{0\to 1} = \sin^2(\varepsilon t/\hbar)\,\frac{\lambda^2\Omega^2}{\varepsilon^2}.$$

Taking the large η limit of the result from part (b) gives the same expression.

(c) Now consider the opposite limit of η approaching zero (slow turn-on). Show that in this limit

$$P_{0\to 1} = \frac{1}{2}\left(1 - \frac{\varepsilon}{\sqrt{\varepsilon^2 + \lambda^2\Omega^2}}\right).$$

Argue that this result is consistent with that of (a).

Similar Seen

3 Marks (Level 2) + 2 Marks (Level 3)

This is the adiabatic limit. Here, to a good approximation the time-dependent state will be an instantaneous eigenstate of the Hamiltonian:

$$|\psi(t)\rangle = e^{i\beta(t)}\,|\phi(t)\rangle$$

where $\hat{\mathcal{H}}\,|\phi\rangle = \mathcal{E}\,|\phi\rangle$. The phase factor $e^{i\beta(t)}$ is unimportant for this problem. Solving for the instantaneous eigenstate, one can evaluate

$$P_{0\to 1} = |\langle 1|\,\phi(t)\rangle|^2$$

to find the result. Expanding the result to lowest non-trivial order in λ gives $P = \frac{\lambda^2\Omega^2}{4\varepsilon^2}$. This expression can also be obtained by putting $\eta = 0$ into the result of (a).

(d) Finally, consider the case where there is different time-dependence: $f(t) = e^{-\eta t^2}$ where η is a positive real parameter. Suppose, again, that in the 'distant past', $t \to -\infty$, the particle is in the state $|0\rangle$. What is the probability for the particle to still be in the state $|0\rangle$ as $t \to \infty$ to leading non-trivial order in λ? In a few sentences explain why this result is consistent with the adiabatic limit of small η.

Unseen

5 Marks (Level 4)

In lecture, we focused only on transition probabilities $P_{n\to n'}$ where $n \neq n'$. The possibly tricky aspect of this problem is figuring out how to compute $P_{0\to 0}$. It is cumbersome to compute this directly by using TDPT. Instead, one can compute it as $P_{0\to 0} = 1 - P_{0\to 1}$. One finds

$$P_{0\to 1} = \frac{\lambda^2\Omega^2\pi}{\hbar^2\eta}e^{-2\varepsilon^2/\eta}.$$

Therefore,

$$P_{0\to0} = 1 - \frac{\lambda^2\Omega^2\pi}{\hbar^2\eta}e^{-2\varepsilon^2/\eta}.$$

In the limit of small η we have $P_{0\to0} = 1$. This is what one would expect in the adiabatic limit. For this case the state is typically close to an eigenstate of $\hat{\mathcal{H}}$. For the very early and very late times we thus have $|\psi\rangle \propto |0\rangle$.

5. (Mastery) Time reversal.

Consider an N-dimensional Hilbert space spanned by orthonormal basis $\{|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_N\rangle\}$. Let $\hat{K}$ be an anti-linear operator that acts on an arbitrary state $|\alpha\rangle = \sum_n \alpha_n |\phi_n\rangle$ (for scalar α_n's) as $\hat{K}|\alpha\rangle = \sum_n \alpha_n^* |\phi_n\rangle$. Denote the time-reversal operator as

$$\hat{T} = \hat{U}\hat{K}$$

where $\hat{U}$ is a unitary operator.

(a) Take two arbitrary states in this Hilbert space to be $|\alpha\rangle$ and $|\beta\rangle$. Let $|\alpha'\rangle = \hat{T}|\alpha\rangle$ and $|\beta'\rangle = \hat{T}|\beta\rangle$. Show that $\langle\alpha|\beta\rangle = \langle\beta'|\alpha'\rangle$ and hence $\hat{T}$ is an anti-unitary transformation.

Seen

5 Marks (Level 3)

Applying the time-reversal operator to arbitrary states we find:

$$\begin{aligned}\hat{T}|\alpha\rangle &= \sum_n \alpha_n^*\hat{U}|\phi_n\rangle \\ \hat{T}|\beta\rangle &= \sum_n \beta_n^*\hat{U}|\phi_n\rangle.\end{aligned}$$

Next, compute the overlap:

$$\begin{aligned}\langle\beta'|\alpha'\rangle &= \sum_{nm}\beta_n\alpha_m^*\langle\phi_n|\hat{U}^\dagger\hat{U}|\phi_m\rangle \\ &= \sum_{nm}\beta_n\alpha_m^*\langle\phi_n|\phi_m\rangle = \sum_{nm}\beta_n\alpha_m^*\delta_{nm} = \sum_n \beta_n\alpha_n^*.\end{aligned}$$

Working out $\langle\alpha|\beta\rangle$ gives the same result.

(b) Now consider a time-reversal invariant Hamiltonian acting in this Hilbert space: $\hat{\mathcal{H}} = \hat{T}\hat{\mathcal{H}}\hat{T}^{-1}$. Further suppose that $\hat{T}^2 = -\mathbb{1}$. Show that $\hat{\mathcal{H}}$ has no non-degenerate eigenstates.

Seen

5 Marks (Level 3)

This is Kramer's theorem. Suppose that $|\xi\rangle$ is a non-degenerate eigenstate of $\hat{\mathcal{H}}$: $\hat{\mathcal{H}}\,|\xi\rangle = \varepsilon\,|\xi\rangle$. Multiplying this equation on the left by $\hat{T}$ we have

$$\hat{T}\hat{\mathcal{H}}\,|\xi\rangle = \hat{T}\hat{\mathcal{H}}\hat{T}^{-1}\hat{T}\,|\xi\rangle = \hat{\mathcal{H}}\hat{T}\,|\xi\rangle = \varepsilon\hat{T}\,|\xi\rangle\,.$$

So $\hat{T}\,|\xi\rangle$ is also an eigenstate of $\hat{\mathcal{H}}$. Since ε is assumed to be non-degenerate it must be that

$$\hat{T}\,|\xi\rangle = \lambda\,|\xi\rangle\,.$$

Multiplying by $\hat{T}$ we have

$$-\,|\xi\rangle = \hat{T}^2\,|\xi\rangle = \lambda^*\hat{T}\,|\xi\rangle = |\lambda|^2\,|\xi\rangle\,.$$

This tells us that $|\lambda|^2 = -1$ and so we have reached a contradiction.

(c) For the remainder of this problem, we consider the case of a spin-one system. Let $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$ be the spin-one spin operators. Denote the eigenbasis of $\hat{S}_z$ as $\{|m\rangle\}$ so that $\hat{S}_z\,|m\rangle = \hbar m\,|m\rangle$ for $m = -1, 0, 1$. The time reversal operator for this system is $\hat{T} = \hat{U}\hat{K}$ where $\hat{U} = |1\rangle\langle -1| - |0\rangle\langle 0| + |-1\rangle\langle 1|$ and $\hat{K}$ is the anti-unitary operator that acts trivially on the $\hat{S}_z$ eigenkets: $\hat{K}\,|m\rangle = |m\rangle$.

Show that $\hat{U}$ is unitary. Also show that $\hat{T}^2 = \mathbb{1}$ (hint: consider how $\hat{T}$ acts on an arbitrary spin-one state).

Unseen

5 Marks (Level 3)

$\hat{U}^\dagger\hat{U} = \mathbb{1}$ is established by a direct calculation. Following the hint, take an arbitrary spin-one state $|\alpha\rangle = \alpha_1\,|1\rangle + \alpha_0\,|0\rangle + \alpha_{-1}\,|-1\rangle$. Applying $\hat{T}$, we can work out that

$$\hat{T}\,|\alpha\rangle = \alpha_1^*\,|1\rangle - \alpha_0^*\,|0\rangle + \alpha_{-1}^*\,|-1\rangle\,.$$

Applying $\hat{T}$ again gives $\hat{T}^2\,|\alpha\rangle = |\alpha\rangle$.

(d) Consider the Hamiltonian

$$\hat{\mathcal{H}} = \gamma(\hat{S}_x^2 + \hat{S}_y^2)$$

where γ is a real constant. Find three simultaneous eigenstates of $\hat{\mathcal{H}}$ and $\hat{T}$.

Unseen

5 Marks (Level 4)

It is very helpful to recognise that we can write this Hamiltonian as

$$\hat{\mathcal{H}} = \gamma(\hat{S}_x^2 + \hat{S}_y^2) = \gamma(\hat{S}^2 - \hat{S}_z^2) = \gamma(2\hbar^2 - \hat{S}_z^2).$$

Therefore its eigenstates are just the eigenstates of $\hat{S}_z$. The eigenstates of $\hat{S}_z$, however, are not all eigenstates of $\hat{T}$. The state $|0\rangle$ is a non-degenerate eigenstate of $\hat{\mathcal{H}}$ and so it will be an eigenstate of $\hat{T}$. Since the states $|1\rangle$ and $|-1\rangle$ are degenerate eigenstates of $\hat{\mathcal{H}}$ we can take linear combinations of these to make eigenstates of $\hat{T}$. The resulting three simultaneous eigenstates are:

$$
\begin{aligned}
|\nu_1\rangle &= |0\rangle \\
|\nu_1\rangle &= (|1\rangle + |-1\rangle)/\sqrt{2} \\
|\nu_3\rangle &= (|1\rangle - |-1\rangle)/\sqrt{2}.
\end{aligned}
$$