

PHASM426 / PHAS4426
Advanced Quantum Theory Problem Sheet 1

To be handed in by 5pm on Tuesday 31st October 2017.

Please hand in your completed work at the **end** of the lecture on that day. If you are unable to attend the lecture, you may scan your work, save it as a single PDF file and email it to me **prior** to this lecture. You may also bring the work to me in my office (B12) before the lecture. **Make sure your completed work is clearly labelled with your name and college.** Please note that UCL places severe penalties on late-submitted work.

1. Consider the vector space of real-valued polynomials of the power not larger than 3:

$$P_3(x) = a_0 + a_1x + a_2x^2 + a_3x^3.$$

- (a) Write down a set of functions that form a basis of this vector space. [1]
(b) What is the dimension of this vector space? [1]

Model answer: $P_3(x)$ is already written as a linear combination of the functions $f_0(x) = x^0$, $f_1(x) = x^1$, $f_2(x) = x^2$ and $f_3(x) = x^3$ which are linearly independent. The dimension of this basis is 4.

Marks: 1 mark for a correct answer for (a) or (b)

2. Consider the basis of vectors $|\phi_j\rangle$ where j spans from 1 to n . Show that if the basis of vectors $\{|\phi_j\rangle\}$ is linearly independent, then for any vector $|\Psi\rangle$ the coefficients c_j of the expansion

$$|\Psi\rangle = \sum_{j=1}^n c_j |\phi_j\rangle$$

are unique. *Hint:* To prove uniqueness you need to assume that there is another set of coefficients that will expand the state $|\Psi\rangle = \sum_{j=1}^n a_j |\phi_j\rangle$ and then prove that $a_j = c_j$. [2]

Model answer: Let's assume $|\Psi\rangle = \sum_{j=1}^n a_j |\phi_j\rangle$. Since $|\Psi\rangle$ belongs to a vector space, then its additive inverse exists, that is, there is a $|\neg\Psi\rangle$ such that $|\Psi\rangle + |\neg\Psi\rangle = 0$. Hence

$$\sum_{j=1}^n (c_j - a_j) |\phi_j\rangle = 0.$$

Since the basis $\{|\phi_j\rangle\}$ is linearly independent, then $c_j - a_j$ must equal zero for each j . Hence $c_j = a_j$.

Marks: 1 mark for correctly justifying the existence of the inverse additive, 1

marks for using correctly the argument of linear independence.

3. The Hamiltonian of a quantum system is written in its spectral decomposition as $H = \sum_{n=1}^d \lambda_n |\phi_n\rangle\langle\phi_n|$, with $\langle\phi_m|\phi_n\rangle = \delta_{m,n}$ where the closure relationship is satisfied i.e. $\mathbb{1} = \sum_{n=1}^d |\phi_n\rangle\langle\phi_n|$. Prove that the exponential of H takes the form $e^H = \sum_{n=1}^d e^{\lambda_n} |\phi_n\rangle\langle\phi_n|$. [3]

Model answer: In analogy of the series expansion of $e^x = \sum_{j=0}^{\infty} x^j/j!$ we expand e^H as

$$e^H = \mathbb{1} + H + \frac{H^2}{2} + \frac{H^3}{3!} + \cdots$$

Let us find out H^j for $j \geq 1$.

$$H^j = \left(\sum_{n=1}^d \lambda_n |\phi_n\rangle\langle\phi_n| \right)^j = \sum_{n=1}^d \lambda_n^j |\phi_n\rangle\langle\phi_n|$$

because $\langle\phi_n|\phi_m\rangle = \delta_{m,n}$. Hence

$$\begin{aligned} e^H &= \mathbb{1} + \sum_{n=1}^d \lambda_n |\phi_n\rangle\langle\phi_n| + \sum_{n=1}^d (\lambda_n^2/2) |\phi_n\rangle\langle\phi_n| + \cdots \\ &= \mathbb{1} + \sum_{n=1}^d (\lambda_n + \lambda_n^2/2 + \lambda_n^3/3! + \cdots) |\phi_n\rangle\langle\phi_n| \\ &= \mathbb{1} + \sum_{n=1}^d (e^{\lambda_n} - 1) |\phi_n\rangle\langle\phi_n| \\ &= \sum_{n=1}^d e^{\lambda_n} |\phi_n\rangle\langle\phi_n| + \mathbb{1} - \sum_{n=1}^d |\phi_n\rangle\langle\phi_n| \\ &= \sum_{n=1}^d e^{\lambda_n} |\phi_n\rangle\langle\phi_n|, \end{aligned}$$

where we have used the closure relationship $\mathbb{1} = \sum_{n=1}^d |\phi_n\rangle\langle\phi_n|$.

Marks: 1 Mark for correctly expanding e^H , 1 mark for correctly finding H^j and 1 mark for using the closure relationship. Partial marks for partial answers.

4. Given two arbitrary vectors $|\phi_1\rangle$ and $|\phi_2\rangle$ belonging to the inner product space \mathcal{H} , the Cauchy-Schwartz inequality states that

$$|\langle\phi_1|\phi_2\rangle|^2 \leq \langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle. \quad (1)$$

The purpose of this problem is to use the properties of inner product to prove this inequality. To proceed with the proof consider the vector $|\Psi\rangle$ defined as:

$$|\Psi\rangle = |\phi_1\rangle + \lambda|\phi_2\rangle$$

where λ is a complex number that can be written as $\lambda = a + ib$.

- (a) Write an expression for the inequality $\langle\Psi|\Psi\rangle \geq 0$ as a function of λ i.e. $f(\lambda)$. Then, re-write this expression as a function of a and b i.e. $f(a, b)$. [2]

Model answer: As a function of a and b the the inner product $\langle\Psi|\Psi\rangle$ becomes

$$\begin{aligned}\langle\Psi|\Psi\rangle &= \langle\phi_1|\phi_1\rangle + \lambda\langle\phi_1|\phi_2\rangle + \lambda^*\langle\phi_2|\phi_1\rangle + |\lambda|^2\langle\phi_2|\phi_2\rangle \\ &= \langle\phi_1|\phi_1\rangle + a(\langle\phi_1|\phi_2\rangle + \langle\phi_2|\phi_1\rangle) + ib(\langle\phi_1|\phi_2\rangle - \langle\phi_2|\phi_1\rangle) \\ &\quad + (a^2 + b^2)\langle\phi_2|\phi_2\rangle \\ &= \langle\phi_1|\phi_1\rangle + 2a\text{Re}(\langle\phi_2|\phi_1\rangle) + 2b\text{Im}(\langle\phi_2|\phi_1\rangle) + (a^2 + b^2)\langle\phi_2|\phi_2\rangle \\ &=: f(a, b) \geq 0\end{aligned}$$

In writing the last line we have used the fact that $\langle\phi_2|\phi_1\rangle = \langle\phi_1|\phi_2\rangle^*$.

Marks: 1 mark for the correct expression as a function of λ , 1 for a correct expression as a function of a and b .

- (b) Show that the value of λ that minimises $\langle\Psi|\Psi\rangle$ is

$$\lambda_{min} = -\frac{\langle\phi_2|\phi_1\rangle}{\langle\phi_2|\phi_2\rangle} \quad (2)$$

Hint: Compute the derivatives of the function $f(a, b)$ obtained in (a) with respect to a and b . Solve these equations to obtain a_{min} and b_{min} and then compute λ_{min} . [2]

Model answer: To minimise $f(a, b)$ we need to calculate:

$$\begin{aligned}\frac{\partial f(a, b)}{\partial a} &= 2\text{Re}(\langle\phi_2|\phi_1\rangle) + 2a\langle\phi_2|\phi_2\rangle = 0 \\ \frac{\partial f(a, b)}{\partial b} &= 2\text{Im}(\langle\phi_2|\phi_1\rangle) + 2b\langle\phi_2|\phi_2\rangle = 0\end{aligned}$$

which leads to

$$a_{min} = -\frac{\text{Re}(\langle\phi_2|\phi_1\rangle)}{\langle\phi_2|\phi_2\rangle} \quad \text{and} \quad b_{min} = -\frac{\text{Im}(\langle\phi_2|\phi_1\rangle)}{\langle\phi_2|\phi_2\rangle}$$

such that

$$\lambda_{min} = a_{min} + ib_{min} = -\frac{\text{Re}(\langle\phi_2|\phi_1\rangle) + i\text{Im}(\langle\phi_2|\phi_1\rangle)}{\langle\phi_2|\phi_2\rangle} = -\frac{\langle\phi_2|\phi_1\rangle}{\langle\phi_2|\phi_2\rangle}.$$

Since $\langle \phi_2 | \phi_2 \rangle > 0$ the matrix of second derivatives is a positive definite and we therefore have found a minimum.

Marks: 1 Marks for obtaining a_{min} , b_{min} and writing correctly λ_{min} and 1 mark for justifying why we have indeed a minimum. Partial marks for partial answers.

- (c) Substitute Eq. (2) in the expression of $f(\lambda)$ derived in (a) and show that it reduces to the expression for the Cauchy-Schwartz inequality (Eq. (1)). [2]

Model answer: Inserting Eq. (2) in the expression of $f(\lambda)$ we obtain

$$\begin{aligned} 0 &\leq \langle \phi_1 | \phi_1 \rangle - \frac{\langle \phi_2 | \phi_1 \rangle}{\langle \phi_2 | \phi_2 \rangle} \langle \phi_1 | \phi_2 \rangle - \frac{\langle \phi_1 | \phi_2 \rangle}{\langle \phi_2 | \phi_2 \rangle} \langle \phi_2 | \phi_1 \rangle + \left| \frac{\langle \phi_2 | \phi_1 \rangle}{\langle \phi_2 | \phi_2 \rangle} \right|^2 \langle \phi_2 | \phi_2 \rangle \\ &\leq \langle \phi_1 | \phi_1 \rangle - \frac{|\langle \phi_2 | \phi_1 \rangle|^2}{\langle \phi_2 | \phi_2 \rangle}, \end{aligned}$$

which is equivalent to Eq. (1).

Marks: 2 marks for deriving the correct expression.

- (d) Which relation do $|\phi_1\rangle$ and $|\phi_2\rangle$ satisfy such that the equality in Eq. (1) is realised? [1]

Model answer: Eq. (1) becomes an equality when $|\phi_1\rangle = c|\phi_2\rangle$ i.e. the vectors are linearly dependent. **Marks:** 1 mark for stating that $|\phi_1\rangle$ need to be linearly dependent.

- (e) Discuss in which cases the Cauchy-Schwartz inequality is important in quantum mechanics [1]

Model answer: The Cauchy-Schwartz inequality is important to demonstrate the generalised uncertainty principle for two arbitrary operators A and B .

5. Consider a Hermitian operator A with eigenvalues $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$ and eigenvectors $\{|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_n\rangle\}$. Show that A can be written in terms of a unitary transformation U as $A = UDU^\dagger$, where D is a diagonal matrix. [2]

Model answer: We write A in its spectral decomposition, that is: $A = \sum_i \lambda_i |\psi_i\rangle \langle \psi_i|$. Since the states $\{|\psi_i\rangle\}$ form an orthonormal basis there is a unitary transformation U such that $|\psi_i\rangle = U|\phi_i\rangle$ where $\{|\phi_i\rangle\}$ also form an orthonormal basis.

Hence we can re-write A as

$$A = \sum_i \lambda_i U |\phi_i\rangle \langle \phi_i| U^\dagger = U \left(\sum_i \lambda_i |\phi_i\rangle \langle \phi_i| \right) U^\dagger = U D U^\dagger.$$

Notice that $D = \sum_i \lambda_i |\phi_i\rangle \langle \phi_i|$ defines a diagonal matrix.

Marks: 1 for using the unitary transformation between basis and 1 for finding the diagonal matrix.

6. Consider a quantum system with Hamiltonian H and consider the measurement of an observable with a non-degenerate spectral decomposition $A = \sum_n a_n |\psi_n\rangle \langle \psi_n|$. The system is initially in the eigenstate $|\psi_n\rangle$ of A , with eigenvalue a_n . A series of ideal measurements on the observable A are carried out. The first measurement is carried out at time $t = \theta$. Then subsequent measurements are made at $t = 2\theta, t = 3\theta$ and so on. Here θ is very small.

- (a) Expand the state of the system to second order in time t and show that the probability of obtaining the eigenvalue a_n at $t = \theta$ is given by

$$w_{nn}(\theta) \simeq 1 - (\Delta E)_n^2 \theta^2,$$

where $(\Delta E)_n^2 = \langle \psi_n | H^2 | \psi_n \rangle - \langle \psi_n | H | \psi_n \rangle^2$. Notice that $w_{nn}(\theta)$ is the probability that the system is still in the initial state. [3]

Model answer: We consider $\hbar = 1$ and the time-evolution of the initial state $|\psi_n\rangle$ given by $|\Psi(t)\rangle = e^{iHt} |\psi_n\rangle$. Expanding the state to second order means to expand the exponential as $e^{iHt} = 1 - iHt - H^2 t^2 / 2$, hence $|\Psi(t)\rangle = (1 - iHt - H^2 t^2 / 2) |\psi_n\rangle$. For $t = \theta$ we have

$$|\Psi(\theta)\rangle = (1 - iH\theta - H^2 \theta^2 / 2) |\psi_n\rangle.$$

Then the probability of obtaining the eigenvalue a_n is $w_{nn}(\theta) = |\langle \psi_n | \Psi(\theta) \rangle|^2$. We have $\langle \psi_n | \Psi(\theta) \rangle = 1 - i\theta \langle \psi_n | H | \psi_n \rangle - (1/2)\theta^2 \langle \psi_n | H^2 | \psi_n \rangle$ and therefore

$$\begin{aligned} w_{nn}(\theta) &= (1 - i\theta \langle \psi_n | H | \psi_n \rangle - (1/2)\theta^2 \langle \psi_n | H^2 | \psi_n \rangle) \times \\ &\quad (1 + i\theta \langle \psi_n | H | \psi_n \rangle - (1/2)\theta^2 \langle \psi_n | H^2 | \psi_n \rangle) \\ &= 1 - \theta^2 \langle \psi_n | H | \psi_n \rangle^2 - \theta^2 \langle \psi_n | H^2 | \psi_n \rangle + \text{terms of higher order} \\ &\simeq 1 - (\Delta E)_n^2 \theta^2 \end{aligned}$$

Above we discarded the higher order terms as they depend on powers of θ greater than 2. Since θ is small, such terms can be neglected.

Marks: 1 mark for expanding the state correctly, 1 mark for writing the correct definition of the probability and 1 mark for justifying discarding the higher order terms

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- (b) Show that after k measurements i.e. at $\tau = k\theta$, the probability $w_{nn}(\tau)$ becomes

$$w_{nn}(\tau) \simeq [1 - (\Delta E)_n^2 \theta^2]^k.$$

[3]

Model answer: To compute the probability after k measurements we need to know the state after k measurements.

$$\tau = \theta \rightarrow |\Psi'(\theta)\rangle = \frac{|\psi_n\rangle \langle \psi_n | \Psi(\theta) \rangle}{\sqrt{w_{nn}(\theta)}} = |\psi_n\rangle$$

$\tau = 2\theta \rightarrow |\Psi(2\theta)\rangle = U(\theta)|\psi_n\rangle$ and probability of finding a_n is approximately $w_{nn}(\theta)$.

Hence after two measurements the probability of finding the system in state $|\psi_n\rangle$ is $w_{nn}(2\theta) \simeq w_{nn}(\theta) \times w_{nn}(\theta)$. We can then generalize this to k measurements or $\tau = k\theta$ such that

$$w_{nn}(k\theta) \simeq \underbrace{w_{nn}(\theta) \times w_{nn}(\theta) \cdots \times w_{nn}(\theta)}_{k \text{ times}} = w_{nn}(\theta)^k.$$

Marks: 1 for showing the state after measurement is $|\psi_n\rangle$ and 2 marks for correct argument of multiplying probabilities after k measurements. Partial marks for partial answers.

- (c) Assume k is large and τ is fixed such that $\theta/k \rightarrow 0$. Show that in this limit

$$w_{nn}(\tau) \simeq \exp[-(\Delta E)_n^2 \tau \theta] \rightarrow 1.$$

You may use without proof the fact that

[2]

$$e^x = \lim_{n \rightarrow \infty} \left(1 + \frac{x}{n}\right)^n.$$

Model answer: Write $\theta = \tau/k$. Hence $w_{nn}(\tau) \simeq [1 - (\Delta E)_n^2 \theta(\theta/k)]^k$. Set $x = -(\Delta E)_n^2 \theta$ so that $w_{nn}(\tau) \simeq [1 + x/k]^k$. Consider the limit of $k \rightarrow \infty$ and use the limit given so $w_{nn}(\tau) \simeq e^x = e^{-(\Delta E)_n^2 \theta}$. When $k \rightarrow \infty$ then $\theta \rightarrow 0$ and $w_{nn}(\tau) \rightarrow e^0 = 1$

Marks: 1 mark for replacing $\theta = \tau/k$ and 1 mark for using correctly the limit given. Partial marks for partial answers.