QP II

Final exam	Assignment date: July 5th, 2024, 15h15
2025	Due date: July 5th, 2024, 18h15

CORRECTION: PHYS-314 – Exam – room PO 01

- You must answer ALL questions in the short answer section.
- You must answer precisely 2 (out of 3) of the questions in the long answer section.

  Please mark clearly which two you have answered below and **start a new sheet for each of the long answer questions**.
- **Write your solutions in the indicated space.** Scrap paper will not be corrected.
- You are reminded that Examiners attach great importance to legibility, accuracy and clarity of expression.
- A simple calculator (without internet access) is allowed.
- Please write your name on the top right corner of each sheet you use.
- Good luck! Enjoy!

NAME STICKER GOES HERE

Short answers: Problem 1	/ 50
Problem A: YES or NO	/ 25
Problem B: YES or NO	/ 25
Problem C: YES or NO	/ 25
Total	/100

Short questions

1. **Bloch Sphere**

   Density matrices satisfy the following 3 conditions:

   - The density matrix is Hermitian: $\hat{\rho}^\dagger = \hat{\rho}$
   - It has trace 1: $\text{Tr}\hat{\rho} = 1$
   - It is positive or null : $\langle \Psi | \hat{\rho} | \Psi \rangle \geq 0, \quad \forall \Psi$

   a) Show that any density matrix $\hat{\rho}$ of a 2 level system can be written

   $$\hat{\rho} = \frac{1}{2}(\hat{I} + \hat{\boldsymbol{\sigma}}.\boldsymbol{r}), \tag{1}$$

   where $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$. Argue that $\boldsymbol{r}$ is a real vector of 3D space and $|\boldsymbol{r}| \leq 1$.

   Hint: The eigenvalues of $\hat{\rho}$ are $\frac{1}{2}(1 \pm |\boldsymbol{r}|)$.

   (3 marks)

   Any Hermitian operator acting on a two-level system can be written as a linear combination of the Pauli matrices together with the identity operator. Since density matrices are Hermitian, the density matrix ρ of an arbitrary two-level system can be written as

   $$\rho = a1 + b\sigma_x + c\sigma_y + d\sigma_z = a1 + \boldsymbol{\sigma} \cdot \boldsymbol{r}', \tag{2}$$

   where $a, b, c, d \in \mathbb{R}$, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ and $\boldsymbol{r}' = (b, c, d)$. Density matrices must additionally satisfy $\text{Tr}\rho = 1$, which gives the following constraint

   $$\text{Tr}\rho = \text{Tr}[a1] = 2a = 1 \implies a = 1/2, \tag{3}$$

   using that Pauli matrices are traceless and the trace operation is linear. So density matrices can be written as

   $$\rho = \frac{1}{2}(1 + \boldsymbol{\sigma} \cdot \boldsymbol{r}) \tag{4}$$

   where $\boldsymbol{r} = 2\boldsymbol{r}'$. We finally use the last condition that $\langle \Psi | \rho | \Psi \rangle \geq 0$ for all $|\Psi\rangle$, which implies that the eigenvalues should be non-negative. As provided by the hint, the eigenvalues of ρ are $\lambda_\pm \equiv (1 \pm |\boldsymbol{r}|)/2$ (in particular they sum up to 1 as required), and by imposing this last condition we get two constraints

   $$\frac{1}{2}(1 + |\boldsymbol{r}|) \geq 0 \qquad \text{and} \qquad \frac{1}{2}(1 - |\boldsymbol{r}|) \geq 0, \tag{5}$$

   where the first inequality is always satisfy, while the second inequality implies that $|\boldsymbol{r}| \leq 1$.

   b) A pure state is a density operator that can be written in the form $\rho = |\psi\rangle\langle\psi|$. Show that the Bloch vector $\boldsymbol{r}$ for a pure state has norm 1, $|\boldsymbol{r}| = 1$

(4 marks)

Method 1: We use the fact that pure states have a purity of 1, i.e. $\text{Tr}[\rho^2] = \text{Tr}[\rho] = 1$. In that case one has to expand ρ^2 and then take the trace. By expanding we get

$$\rho^2 = \frac{1}{4}(1 + 2(\boldsymbol{\sigma} \cdot \boldsymbol{r}) + (\boldsymbol{\sigma} \cdot \boldsymbol{r})^2). \tag{6}$$

We previously encountered the term $(\boldsymbol{\sigma} \cdot \boldsymbol{r})^2$ in the exercies, and it gives $(\boldsymbol{\sigma} \cdot \boldsymbol{r})^2 = |\boldsymbol{r}|^2 1$. By using the fact that Pauli matrices are traceless, we directly recover the desired result

$$\text{Tr}[\rho^2] = \frac{1}{4}\text{Tr}[(1 + |\boldsymbol{r}|^2)1 + 2(\boldsymbol{\sigma} \cdot \boldsymbol{r})] = \frac{1}{4}(2(1 + |\boldsymbol{r}|^2)) = 1 \quad \Longrightarrow \quad |\boldsymbol{r}| = 1. \tag{7}$$

Method 2: Any quantum state $|\psi\rangle$ of a two-level system can be written as

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle, \quad \theta \in [0, \pi], \quad \phi \in [0, 2\pi[. \tag{8}$$

By expanding $|\psi\rangle\langle\psi|$ and equating the resulting expression to $(1 + \boldsymbol{\sigma} \cdot \boldsymbol{r})/2$, we can recover the Bloch vector

$$\boldsymbol{r} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta), \tag{9}$$

which represents a unit vector in spherical coordinates in $\mathbb{R}^3$.

c) A mixed state is a density operator that is a convex combination of pure states. That is,

$$\rho_{\text{mixed}} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

with $0 < p_i < 1$ and $\sum_i p_i = 1$.

Based on this definition of a mixed state give a geometric argument to show that the Bloch vector of a mixed state is always less than 1, $|\boldsymbol{r}_{\text{mixed}}| \leq 1$.

(3 marks)

A mixed state can be written as

$$\rho_{\text{mixed}} = \sum_{i=1}^{M} p_i |\psi_i\rangle\langle\psi_i| = \sum_{i=1}^{M} p_i \frac{1}{2}(1 + \boldsymbol{\sigma} \cdot \boldsymbol{r}_i) = \frac{1}{2}\left(1 + \boldsymbol{\sigma} \cdot \sum_i p_i \boldsymbol{r}_i\right), \tag{10}$$

using that $\sum_i p_i = 1$. We can then define

$$\boldsymbol{r}_{\text{mixed}} = \sum_i p_i \boldsymbol{r}_i, \tag{11}$$

which corresponds to the resulting Bloch vector of the mixed state ρ_{mixed}. This quantity indicates the degree of mixedness, and given that $0 < p_i < 1$, $\sum_i p_i = 1$, and $|\boldsymbol{r}_i| \leq 1$, it must satisfy $|\boldsymbol{r}_{\text{mixed}}| < 1$. (Geometrically, by summing the weighted arrows/vectors $p_i \boldsymbol{r}_i$, the resulting vector $\boldsymbol{r}_{\text{mixed}}$ will never escape from the unit sphere.)

2. **Entanglement**

Alice, Bob and Charlie share a three qubit state:

$$\hat{\rho}_{ABC} = \frac{1}{\sqrt{2}} (|000\rangle_{ABC} + |111\rangle_{ABC}) \tag{12}$$

where $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle$ are the ± 1 eigenstates of $\hat{\sigma}_x$ and $|0\rangle$ and $|1\rangle$ are the $+1$ and $\bar{1}$ eigenstates of $\hat{\sigma}_z$ respectively.

a) Suppose Bob measures his qubit in the $\hat{\sigma}_z$ basis. Find the output states for Alice and Charlie conditional on Bob's measuring 0 and conditional on Bob measuring 1.

(2 marks)

If Bob measures 0 (by applying $P_0 = I \otimes |0\rangle\langle 0| \otimes I$ to $|\psi\rangle_{ABC}$), the output state for Alice and Charlie collapses to

$$|\psi\rangle_{AC|B=0} = \frac{1}{\sqrt{2}} |00\rangle_{AC}, \tag{13}$$

while if he measures 1, the state collapses to

$$|\psi\rangle_{AC|B=1} = \frac{1}{\sqrt{2}} |11\rangle_{AC}. \tag{14}$$

b) What if Bob instead measures in the $\hat{\sigma}_x$ basis? State the output states for Alice and Charlie conditional on Bob's measurement outcomes in this case.

(3 marks)

We start by rewriting $|0\rangle_B$ and $|1\rangle_B$ in the wavefunction $|\psi\rangle_{ABC}$ in terms of $|\pm\rangle_B$

$$|\psi\rangle_{ABC} = \frac{1}{\sqrt{2}} \left[|0\rangle_A \left(\frac{1}{\sqrt{2}}(|+\rangle_B + |-\rangle_B) \right) |0\rangle_C + |1\rangle_A \left(\frac{1}{\sqrt{2}}(|+\rangle_B - |-\rangle_B) \right) |1\rangle_C \right] \tag{15}$$

$$= \frac{1}{2} \left[(|0\rangle_A |0\rangle_C + |1\rangle_A |1\rangle_C)|+\rangle_B + (|0\rangle_A |0\rangle_C - |1\rangle_A |1\rangle_C)|-\rangle_B \right]. \tag{16}$$

If Bob's measurement outcome is $|\pm\rangle$, the output state for Alice and Charlie will be

$$|\psi_\pm\rangle \equiv |\psi\rangle_{AC|B=\pm} = \frac{1}{2}(|00\rangle_{AC} \pm |11\rangle_{AC}), \tag{17}$$

c) Assuming Bob does not tell Alice or Charlie the output to his measurement, what is the mixed state that Alice and Charlie share after his measurement in the $\hat{\sigma}_z$ basis?

(2 marks)

If Bob does not reveal to Alice or Charlie his measurement outcome, the state that Alice and Charlie share is a mixture of the possible states after Bob's measurement. The mixed state is given by

$$\rho_{AC} = \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|). \tag{18}$$

d) Could Alice and Charlie use this state to violate a Bell inequality? Explain your answer.

(3 marks)

No, this state, being a mixture of product states, does not include non-classical correlations (through entanglement) that would allow Alice and Charlie to violate Bell inequality.

3. **Fermions and Bosons**

Which of the following states are valid Fermionic states and which are valid Bosonic states:

$$\text{(a)} \quad \left(\frac{1}{\sqrt{2}}|p\rangle_1|q\rangle_2 + \frac{1}{\sqrt{2}}|q\rangle_1|p\rangle_2\right)\left(\frac{1}{\sqrt{2}}|R\rangle_1|L\rangle_2 - \frac{1}{\sqrt{2}}|L\rangle_1|R\rangle_2\right) \tag{19}$$

$$\text{(b)} \quad \left(\frac{1}{\sqrt{2}}|p\rangle_1|q\rangle_2 - \frac{1}{\sqrt{2}}|q\rangle_1|p\rangle_2\right)|R\rangle_1|R\rangle_2 \tag{20}$$

$$\text{(c)} \quad \left(\frac{1}{\sqrt{2}}|p\rangle_1|q\rangle_2 + \frac{1}{\sqrt{2}}|q\rangle_1|p\rangle_2\right)\left(\frac{1}{\sqrt{2}}|R\rangle_1|L\rangle_2 + \frac{1}{\sqrt{2}}|L\rangle_1|R\rangle_2\right) \tag{21}$$

$$\text{(d)} \quad |p\rangle_1|q\rangle_2|R\rangle_1|L\rangle_2 \tag{22}$$

$$\text{(e)} \quad \left(\frac{1}{\sqrt{2}}|p\rangle_1|q\rangle_2 - \frac{1}{\sqrt{2}}|q\rangle_1|p\rangle_2\right)\left(\frac{1}{\sqrt{2}}|R\rangle_1|L\rangle_2 - \frac{1}{\sqrt{2}}|L\rangle_1|R\rangle_2\right) \tag{23}$$

(5 marks)

Valid fermionic states: (a), (b);
Valid bosonic states: (c), (e).

4. **Symmetry.** Consider a unitary irreducible representation $R(g) = U_g$ of group G.

a) Use the Grand Orthogonality Theorem to prove that

$$\frac{1}{N}\sum_g U_g X U_g^\dagger = \frac{1}{d}\,\mathrm{Tr}[X]\,I \tag{24}$$

where $d = \dim(X)$ and N is the order of the group.

(4 marks)

Given that the representation is unitary and irreducible, the Grand Orthogonality Theorem can be applied to prove the result of interest

$$\begin{aligned}
\frac{1}{N}\sum_g U_g X U_g^\dagger &= \frac{1}{N}\sum_{jklm}\sum_g [R(g)]_{lm} X_{mj} [R(g)^\dagger]_{jk} |l\rangle\langle k| \\
&= \frac{1}{d}\sum_{jklm} \delta_{lk}\delta_{jm} X_{mj} |l\rangle\langle k| \\
&= \frac{1}{d}\sum_{jk} X_{jj} |k\rangle\langle k| \\
&= \frac{1}{d}\mathrm{Tr}[X] I,
\end{aligned} \tag{25}$$

where d is the dimension of the vector space of the representation. In the lecture notes, this result is called the **Irrep Group Averaging Corollary**.

The above relation for averaging over irreducible representations of finite groups generalizes to averaging over compact Lie groups. In this case the finite average $\frac{1}{N}\sum_g$ becomes a continuous integral over a uniform measure $\int d\mu(g)$ and we have:

$$\langle X\rangle_G := \int_G d\mu(g) U_g X U_g^\dagger = \frac{1}{d}\mathrm{Tr}[X]\, I \tag{26}$$

b) Use this result to explain why applying random single qubit rotations to any single qubit state on average results in the maximally mixed state.

(3 marks)

Given any single qubit state ρ, we do indeed find the maximally mixed state by averaging over all possible single-qubit rotations

$$\langle \rho\rangle_{SU(2)} = \int_{SU(2)} d\mu(g) U_g \rho U_g^\dagger = \frac{1}{2}\mathrm{Tr}[\rho] I = \frac{1}{2} I, \tag{27}$$

since density matrices have unit trace.

c) We now consider only random rotations about the x-axis. What is the relevant symmetry group and representation in this case? Why can Eq. (26) not be directly applied to compute this average?

(3 marks)

The relevant symmetry group is $U(1)$ and the associated representation is the set of rotation by an angle $\theta \in [0, 2\pi)$ about the x-axis: $\{U(\theta) := e^{-i\theta\sigma_x/2} | \theta \in [0, 2\pi)\}$. Eq. (26) cannot be directly applied because it only holds for irreps and $R_x = e^{-i\theta\sigma_x}$ is not an irrep.

d) Explain how a different version of Eq. (26) *can* be applied to compute the state that results on average from applying a random x rotation to a qubit.

(4 mark)

[Taken from the lecture notes] Here we are therefore looking for a generalization of Eq. (26) for reducible representations. Any reducible unitary representation can be written in the form

$$U(g) = \bigoplus_x U_x(g) = \sum_x U_x(g) \otimes I_{\bar{x}} \tag{28}$$

where $\bar{x}$ denotes the subspace that U_x does not act on. Again we'll do this calculation for a finite group but it generalises to continuous groups:

$$\begin{aligned}
\langle X \rangle_G &= \frac{1}{N} \sum_g U(g) X U(g)^\dagger \\
&= \frac{1}{N} \sum_g \sum_{xx'} (U_x(g) \otimes I_{\bar{x}}) X (U_{x'}(g)^\dagger \otimes I_{\bar{x}}) \\
&= \frac{1}{N} \sum_g \sum_x (U_x(g) \otimes I_{\bar{x}}) X (U_x(g)^\dagger \otimes I_{\bar{x}}) \\
&= \frac{1}{d_x} \sum_x \mathrm{Tr}[X \Pi_x] \Pi_x \otimes I_{\bar{x}} \\
&= \frac{1}{d_x} \bigoplus_x \mathrm{Tr}[X \Pi_x] \Pi_x
\end{aligned} \tag{29}$$

where Π_x denotes the identity projector onto the subspace spanned by the representation. That is, the input is projected down onto the irreps.

e) Hence compute the state that results on average from applying a random x rotation to a qubit.

(2 marks)

Now we can compute what happens when we average a state ρ by $R_x(\theta) = e^{-i\theta\sigma_x}$. The relevant symmetry group being $U(1)$, the irreps in this case are both 1D, namely $\{1\}$ and $\{e^{-i\theta}\}$, and we have:

$$U_g = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\theta} \end{pmatrix} = |+\rangle\langle+| + e^{-i\theta} |-\rangle\langle-| \tag{30}$$

such that $\Pi_+ = |+\rangle\langle+|$ and $\Pi_- = |-\rangle\langle-|$

$$\langle \rho \rangle_G = \frac{1}{1} \bigoplus_{x=+,-} \mathrm{Tr}[\rho \Pi_x] \Pi_x = \langle+|\rho|+\rangle |+\rangle\langle+| + \langle-|\rho|-\rangle |-\rangle\langle-| \,. \tag{31}$$

As expected, this averaging kills off all coherence and projects onto the x-axis.

5. **Variational Principle.** Consider the 1D Harmonic Oscillator with H:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

Use the variational principle with the trial wavefunction

$$\psi(x) = Ae^{-bx^2}$$

to upper bound the ground state energy of H.

(9 marks)

You may find these integrals helpful:

$$\int_{-\infty}^{\infty} e^{-ax^2+bx}\, dx = e^{\frac{b^2}{4a}}\sqrt{\frac{\pi}{a}} \tag{32}$$

$$\int_0^{\infty} x^n e^{-ax^2}\, dx = \begin{cases} \frac{(n-1)(n-3)\dots 3\cdot 1}{2^{\frac{n}{2}} a^{\frac{n+1}{2}}}\sqrt{\frac{\pi}{a}}, & \text{for } n \text{ even} \\ \frac{1}{2}\frac{(n-1)!}{a^{\frac{n+1}{2}}}, & \text{for } n \text{ odd} \end{cases} \tag{33}$$

We start by normalizing the trial wavefunction by imposing the constraint

$$\int_{-\infty}^{\infty} dx|\psi(x)|^2 = A^2\int_{-\infty}^{\infty} dx e^{-2bx^2} = A^2\sqrt{\frac{\pi}{2b}} = 1, \tag{34}$$

which yields $A = (2b/\pi)^{1/4}$. The normalized trial wavefunction is therefore

$$\psi(x) = \left(\frac{2b}{\pi}\right)^{1/4} e^{-bx^2}. \tag{35}$$

To evaluate the expectation value of the Hamiltonian with respect to this trial wavefunction, we will need

$$\frac{d\psi}{dx} = \left(\frac{2b}{\pi}\right)^{1/4}(-2bx)e^{-bx^2}, \tag{36}$$

$$\frac{d^2\psi}{dx^2} = \left(\frac{2b}{\pi}\right)^{1/4}(4b^2x^2 - 2b)e^{-bx^2} = (4b^2x^2 - 2b)\psi(x). \tag{37}$$

We can now evaluate the expectation value

$$\langle\psi|H|\psi\rangle = \int_{-\infty}^{\infty} dx\psi(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\psi(x) \tag{38}$$

$$= \int_{-\infty}^{\infty} dx\psi(x)\left(-\frac{\hbar^2}{2m}(4b^2x^2-2b)+\frac{1}{2}m\omega^2x^2\right)\psi(x) \tag{39}$$

$$= \sqrt{\frac{2b}{\pi}}\left(-\frac{2\hbar^2b^2}{m}+\frac{1}{2}m\omega^2\right)\int_{-\infty}^{\infty} dx x^2 e^{-2bx^2}+\frac{\hbar^2 b}{m}\int_{-\infty}^{\infty} dx|\psi(x)|^2 \tag{40}$$

$$= \sqrt{\frac{2b}{\pi}}\left(-\frac{2\hbar^2b^2}{m}+\frac{1}{2}m\omega^2\right)\frac{\sqrt{\pi}}{2^{5/2}b^{3/2}}+\frac{\hbar^2 b}{m} \tag{41}$$

$$= -\frac{\hbar^2 b}{2m}+\frac{m\omega^2}{8b}+\frac{\hbar^2 b}{m} \tag{42}$$

$$= \frac{m\omega^2}{8b}+\frac{\hbar^2 b}{2m}. \tag{43}$$

To find the optimal value for b, we minimize $\langle H\rangle$ with respect to b

$$\frac{d}{db}\left(\frac{m\omega^2}{8b}+\frac{\hbar^2 b}{2m}\right)=0 \quad\Longrightarrow\quad -\frac{m\omega^2}{8b^2}+\frac{\hbar^2}{2m}=0 \quad\Longrightarrow\quad b=\frac{m\omega}{2\hbar}. \tag{44}$$

Substituting this optimal value for b back into $\langle H\rangle$, we get

$$\langle H\rangle = \frac{m\omega^2}{8}\left(\frac{2\hbar}{m\omega}\right)+\frac{\hbar^2}{2m}\left(\frac{m\omega}{2\hbar}\right)=\frac{\hbar\omega}{4}+\frac{\hbar\omega}{4}=\frac{\hbar\omega}{2}. \tag{45}$$

We thus conclude that the ground state energy is at most equal to $\hbar\omega/2$. Here in fact it is exactly $\hbar\omega/2$, because the Gaussian trial wavefunction is precisely the correct ground state.

Longer questions

Please **pick 2 questions** to attempt - mark your choices clearly on the cover sheet.

Start a new sheet for each question.

Question A - Perturbation Theory

Consider a free particle in a box of width a, with sides at $x = 0$ and $x = a$. The unperturbed problem is well-known: the eigenvalues are

$$E_n^{(0)} = n^2\hbar^2\pi^2/2ma^2 = n^2 E_1^{(0)},$$

and the eigenfunctions are

$$\langle x|n_0\rangle = u_n(x) = \sqrt{2/a}\sin(n\pi x/a).$$

(a) We now add a perturbation

$$H_1 = W\cos(\pi x/a).$$

Sketch the perturbed potential well as a function of x. Show that all the first-order energy shifts are zero.

(4 marks)

The original potential for a particle in a box is $V(x) = 0$ for $0 < x < a$ and infinite otherwise. The perturbation potential is:

$$H_1 = V(x) = W\cos\left(\frac{\pi x}{a}\right)$$

This means the potential is modified by a cosine function with a period twice the width of the box (since $\cos\left(\frac{\pi x}{a}\right)$ completes half a period across the box width). The sketch should show a cosine wave oscillating between W and $-W$ within the interval 0 to a.

First-Order Energy Shifts

The first-order energy shift for a state $|n_0\rangle$ is given by:

$E_n^{(1)} = \langle n_0|H_1|n_0\rangle = \int_0^a u_n(x)H_1u_n(x)\,dx$

Substituting the given wavefunction and perturbation, we get:

$E_n^{(1)} = \int_0^a \left(\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\right) W\cos\left(\frac{\pi x}{a}\right)\left(\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\right)\,dx = \frac{2W}{a}\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)\cos\left(\frac{\pi x}{a}\right)\,dx$

...

$E_n^{(1)} = 0.$

Thus, all first-order energy shifts are zero.

(b) Find the first order correction to the ground state wavefunction. Sketch the ground state wavefunction and the correction.

(7 marks)

The first-order correction to the ground state wavefunction $|1\rangle$ is given by:

$$|1^{(1)}\rangle = \sum_{m\neq 1} \frac{\langle m|H_1|1\rangle}{E_1^{(0)} - E_m^{(0)}} |m\rangle.$$

Calculating the matrix elements:

$$\langle m|H_1|1\rangle = \int_0^a \psi_m(x) W \cos\left(\frac{\pi x}{a}\right) \psi_1(x)\, dx.$$

Substituting the wavefunctions:

$$\langle m|H_1|1\rangle = \frac{2W}{a} \int_0^a \sin\left(\frac{m\pi x}{a}\right) \cos\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi x}{a}\right) dx.$$

Using trigonometric identities and orthogonality:

$$\sin(A)\cos(B) = \frac{1}{2}[\sin(A+B) + \sin(A-B)],$$

we get:

$$\langle m|H_1|1\rangle = \frac{2W}{a} \int_0^a \frac{1}{2} \left[\sin\left(\frac{(m+1)\pi x}{a}\right) + \sin\left(\frac{(m-1)\pi x}{a}\right)\right] dx.$$

Only terms with $m = 2$ will be non-zero:

$$\langle 2|H_1|1\rangle = \frac{W}{a} \int_0^a \sin\left(\frac{2\pi x}{a}\right) \sin\left(\frac{\pi x}{a}\right) dx.$$

This evaluates to:

$$\langle 2|H_1|1\rangle = \frac{W}{2}.$$

So the first-order correction is:

$$|1^{(1)}\rangle = \frac{\frac{W}{2}}{E_1^{(0)} - E_2^{(0)}} |2\rangle.$$

With $E_1^{(0)} = \frac{\hbar^2\pi^2}{2ma^2}$ and $E_2^{(0)} = 4E_1^{(0)}$:

$$|1^{(1)}\rangle = \frac{\frac{W}{2}}{E_1^{(0)} - 4E_1^{(0)}} |2\rangle = -\frac{W}{6E_1^{(0)}} |2\rangle.$$

The corrected ground state wavefunction is:

$$\psi_1(x) + \psi_1^{(1)}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) - \frac{W}{6E_1^{(0)}} \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right).$$

(c) What constraints are required on W for perturbation theory to be a suitable approximation method?

(3 marks)

For perturbation theory to be valid, the perturbation must be small compared to the unperturbed Hamiltonian. This means that the energy shifts and wavefunction corrections due to the perturbation should be much smaller than the unperturbed quantities.

$$\left|\frac{\langle\phi_m|\hat{H}_1|\phi_1\rangle}{E_1^{(0)} - E_m^{(0)}}\right| \ll 1 \implies \left|\frac{\alpha}{-3E_1^{(0)}}\right| \ll 1 \implies |W| \ll 6E_1^{(0)},$$

where $E_1^{(0)} = \frac{\hbar^2\pi^2}{2ma^2}$ is the ground state energy of the unperturbed system.

(d) What is the second-order shift $E_n^{(2)}$ for $n = 1$ and $n = 2$?

(11 marks)

Hint: You will find the evaluation of the integrals much simplified if you start by proving for the perturbation a relationship of the form

$$H_1 u_n = \alpha(u_{n\bar{1}} + u_{n+1}).$$

This relationship turns the integrals into orthogonality integrals. You will need to think about the meaning of this equation for $n = 1$ since $n - 1$ is then zero, while u_n is only defined for $n > 0$.

The second-order energy shift is given by:

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle m|H_1|n\rangle|^2}{E_n^{(0)} - E_m^{(0)}}.$$

Using the hint:

$$H_1\psi_n = \alpha(\psi_{n-1} + \psi_{n+1}),$$

we get:

$$\langle m|H_1|n\rangle = \alpha(\delta_{m,n-1} + \delta_{m,n+1}).$$

For $n = 1$:

$$H_1\psi_1 = \alpha\psi_2.$$

Thus:

$$\langle 2|H_1|1\rangle = \alpha.$$

The second-order shift for $n = 1$ is:

$$E_1^{(2)} = \sum_{m \neq 1} \frac{|\langle m|H_1|1\rangle|^2}{E_1^{(0)} - E_m^{(0)}} = \frac{|\alpha|^2}{E_1^{(0)} - E_2^{(0)}} = \frac{|\alpha|^2}{-3E_1^{(0)}} = -\frac{|\alpha|^2}{3E_1^{(0)}}.$$

For $n = 2$:

$$H_1\psi_2 = \alpha(\psi_1 + \psi_3).$$

Thus:

$$\langle 1|H_1|2\rangle = \alpha, \quad \langle 3|H_1|2\rangle = \alpha.$$

The second-order shift for $n = 2$ is:

$$E_2^{(2)} = \frac{|\alpha|^2}{E_2^{(0)} - E_1^{(0)}} + \frac{|\alpha|^2}{E_2^{(0)} - E_3^{(0)}}.$$

Since $E_2^{(0)} = 4E_1^{(0)}$:

$$E_2^{(2)} = \frac{|\alpha|^2}{3E_1^{(0)}} + \frac{|\alpha|^2}{E_2^{(0)} - 9E_1^{(0)}}.$$

Evaluating the second term:

$$E_2^{(2)} = \frac{|\alpha|^2}{3E_1^{(0)}} + \frac{|\alpha|^2}{4E_1^{(0)} - 9E_1^{(0)}} = \frac{|\alpha|^2}{3E_1^{(0)}} - \frac{|\alpha|^2}{5E_1^{(0)}}.$$

Simplifying:

$$E_2^{(2)} = |\alpha|^2\left(\frac{1}{3E_1^{(0)}} - \frac{1}{5E_1^{(0)}}\right) = |\alpha|^2\left(\frac{5-3}{15E_1^{(0)}}\right) = \frac{2|\alpha|^2}{15E_1^{(0)}}.$$

Thus, the second-order shifts are:

$$E_1^{(2)} = -\frac{|\alpha|^2}{3E_1^{(0)}},$$

$$E_2^{(2)} = \frac{2|\alpha|^2}{15E_1^{(0)}}.$$

Question B - Symmetry

The quaternion group Q_8 is an order 8 non-abelian group which is isomorphic to the quaternions under multiplication. Do not worry if you do not know anything about quaternions, all you need to know to address this question is that Q_8 has the following Cayley table:

	e	$\bar{e}$	i	$\bar{i}$	j	$\bar{j}$	k	$\bar{k}$
e	e	$\bar{e}$	i	$\bar{i}$	j	$\bar{j}$	k	$\bar{k}$
$\bar{e}$	$\bar{e}$	e	$\bar{i}$	i	$\bar{j}$	j	$\bar{k}$	k
i	i	$\bar{i}$	$\bar{e}$	e	k	$\bar{k}$	$\bar{j}$	j
$\bar{i}$	$\bar{i}$	i	e	$\bar{e}$	$\bar{k}$	k	j	$\bar{j}$
j	j	$\bar{j}$	$\bar{k}$	k	$\bar{e}$	e	i	$\bar{i}$
$\bar{j}$	$\bar{j}$	j	k	$\bar{k}$	e	$\bar{e}$	$\bar{i}$	i
k	k	$\bar{k}$	j	$\bar{j}$	$\bar{i}$	i	$\bar{e}$	e
$\bar{k}$	$\bar{k}$	k	$\bar{j}$	j	i	$\bar{i}$	e	$\bar{e}$

1. What order are the proper (i.e., non-trivial) subgroups of Q_8?

   (2 marks)

   1 point Stating langranges theorem

   1 point Finding that the order of the subgroups are 4,2. 2

   Equivalently

   2 point for any equivalent way of finding the orders (i.e. finding all the subgroups...)

   Note, without justification:

   - 2 point Write 2 and 4
   - 1 point write 2 or 4
   - 0 point write some wrong (random guess)

   The order of the subgroups is 4 and 2 (for the subgroup only involving $\{e, \bar{e}\}$). We can check by using Lagrange theorem that this are the only options. Indeed, because $|G|/|H| = n \in \mathbb{N}$, we can only have $|H| \in \{2, 4\}$.

2. Find two of the proper subgroups of Q_8

   (3 marks)

   1 point per $\{e, \bar{e}\}$.

   2 point for any other (up to 3 points).

   As mentioned, one of the subgroups is $\{e, \bar{e}\}$. We can also find $\{e, \bar{e}, i, \bar{i}\}$.

3. The conjugacy classes of Q_8 are

$$\{e\}, \{\bar{e}\}, \{i, \bar{i}\}, \{j, \bar{j}\}, \{k, \bar{k}\}$$

Verify that $\{e\}$ and $\{k, \bar{k}\}$ are indeed conjugacy classes.

(3 marks)

1 point Define conjugacy class (or use the definition implicitely).

1 point for verifying identity $\{e\}$.

1 point for verifying the $\{k, \overline{k}\}$.

Note:

- 2 point If they make a mistake identifying the k conjugacy class.
  - Wrongly identify $\bar{e}$ as the inverse of e.
  - Say that $u = k$
- They put all the products that they can think of without identifying which one is the correct.

For x, y to be a conjugacy class there has to exist some u such that $uxu^{-1} = y$. Trivially, if we choose $u = e$, then $eee = e$. Also if we choose $u = i$ $u^{-1} = \bar{i}$, then $ik\bar{i} = \overline{k}$.

4. What is an irreducible representation (or, 'irrep' for short)? How many (non-equivalent) irreducible representations does Q_8 have?

(3 marks)

1 point Definition of irrep. General definition (not very accurate, just enough to make sense)

1 point State the useful lemma.

1 point Saying how many irreps.

The number of conjugacy classes is equal to the number of non-equivalent irreps. Thus we have 5 non-equivalent irreps.

5. Consider this representation of Q_8:

$$e \mapsto \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \bar{e} \mapsto \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$
$$i \mapsto \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \quad \bar{i} \mapsto \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$$
$$j \mapsto \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \bar{j} \mapsto \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$
$$k \mapsto \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \quad \bar{k} \mapsto \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}$$

State a theorem that allows you to determine whether a representation is irreducible. Hence determine whether this representation is irreducible.

(3 marks)

1 point For saying that Schur's second lemma can help with this (and stating it).

1 point For stating that it is impossible for a matrix that is not proportional to identity to commute with all of them.

1 point For proving it. The ideal way of determining this is by saying that there is no matrix A different than identity that can be diagonalised in the basis of all of them at the same time.

---

1 point Th 7.11.4

2 point Using it to find that it is an irrep.

The second Schurs lemma can help with this. Indeed there is no matrix A except for $\lambda\mathbb{1}$ such that $[A, X] = 0\, X \in \{e, i, j, k, \bar{e}, \bar{i}, \bar{j}, \bar{k}\}$

6. State a theorem that allows you to determine the dimensions of a groups irreps. Hence, what are the dimensions of each of the quarternion's groups irreps?

   (3 marks)

   1 point Identifying Burnside lemma and stating it (directly or indirectly)

   1 point Identifying that the trivial representation exists. (even if it is not explicitely, i.e. they find the correct dim).

   1 point Computing all the other dimensions.

   Burnside lemma. Because the previous irrep has dimension 2, we need

$$\sum_i l_i^2 = h \tag{46}$$

   and thus, the other irreps are of dimension 1. $(4+1+1+1+1 = 8$, because the trivial representation exists we need some irrep with dimension one.)

7. State a theorem that can help identify a groups 1D irreps. Hence identify the quaternion's groups 1D irreps.

   (Hint you will need to use the Cayley table to help find the irreps. You may also find that recalling the irreps of C3v helpful to guess.)

   (8 marks)

   1 point State (petite) orthogonality theorem. / grand/ any other that can be of use. People find clever wais of doing this.

1 point Trivial representation

1 point Identify + 1 point check $\{e, i, \bar{e}, \bar{i}\} \to 1$, $\{j, k, \bar{j}, \bar{k}\} \to -1$

1 point Identify + 1 point check $\{e, \bar{e}, j, \bar{j}\} \to 1$, $\{i, \bar{i}, k, \bar{k}\} \to -1$

1 point Identify + 1 point check $\{e, \bar{e}, k, \bar{k}\} \to 1$, $\{i, \bar{i}, j, \bar{j}\} \to -1$

Note:

- 1 point if they don't finish but explain the strategy good enough and/or find middle steps that can be helpful. I.e. they use previous results to say that $R(x) = R(\bar{x})$.

We can start by finding the trivial representation, i.e. all the elements are 1.

We will use the petite orthogonality theorem. For 1-D irreps is pretty useful.

$$\sum_{g \in G} \chi_a^*(g)\chi_b(g) = N\delta_{a,b} \tag{47}$$

where $\chi_R(g) = \text{Tr}[R(g)]$.

Due to the nature of the table, we can also see that if $\{e, i, \bar{e}, \bar{i}\} \to 1$, $\{j, k, \bar{j}, \bar{k}\} \to -1$, also fulfils the Cayley table. Using the petite orthogonality theorem we can see that this can also be an irrep. We do this by comparing it to the previous irreps. First to the trivial

$$\sum_{g \in G} \chi_a(g) = 4 - 4 = 0 \tag{48}$$

and also with the one from the previous exercise

$$\sum_{g \in G} \chi_a^*(g)\chi_b(g) = 2 - 2 = 0 \tag{49}$$

Applying the petite orthogonality theorem to this new irrep, we find that

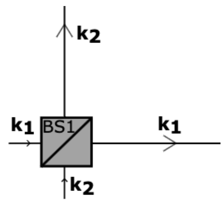
$$e = \bar{e} \tag{50}$$
$$e + \bar{e} + i + \bar{i} = 0 \tag{51}$$
$$j + \bar{j} + k + \bar{k} = 0 \tag{52}$$

therefore, another representation we can find is $\{e, \bar{e}, j, \bar{j}\} \to 1$, $\{i, \bar{i}, k, \bar{k}\} \to -1$. A different representation is switching j, k to find $\{e, \bar{e}, k, \bar{k}\} \to 1$, $\{i, \bar{i}, j, \bar{j}\} \to -1$. And with this we found the 4 irreps, i.e.

$$\{e, i, \bar{e}, \bar{i}, j, k, \bar{j}, \bar{k}\} \to 1 \tag{53}$$
$$\{e, i, \bar{e}, \bar{i}\} \to 1,\ \{j, k, \bar{j}, \bar{k}\} \to -1 \tag{54}$$
$$\{e, \bar{e}, j, \bar{j}\} \to 1,\ \{i, \bar{i}, k, \bar{k}\} \to -1 \tag{55}$$
$$\{e, \bar{e}, k, \bar{k}\} \to 1,\ \{i, \bar{i}, j, \bar{j}\} \to -1 \tag{56}$$

Question C - Quantum Bomb Testing

Let's start by getting familiar with a parameterized beamsplitter for the form sketched below:



The action of this parameterized beamsplitter on the mode operators $(a_1^\dagger, a_2^\dagger)$ is given by the unitary

$$U_{BS1} = U_{BS2}^\dagger = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

1. Find the output state for the case that the initial state contains: (i) 1 photon in mode $\mathbf{k}_1$, vacuum in mode $\mathbf{k}_2$ (ii) One photon in each mode (iii) Two photons in mode $\mathbf{k}_1$.

   (10 marks)

   We first note that the beamsplitter transforms the mode operators as

$$a_1^\dagger \rightarrow \cos\theta a_1^\dagger + \sin\theta a_2^\dagger$$
$$a_2^\dagger \rightarrow \cos\theta a_2^\dagger - \sin\theta a_1^\dagger.$$

   We then state the initial states as (i) $|1\rangle|0\rangle = a_1^\dagger|0\rangle|0\rangle$, (ii) $|1\rangle|1\rangle = a_1^\dagger a_2^\dagger|0\rangle|0\rangle$, and (iii) $|2\rangle|0\rangle = \frac{1}{\sqrt{2}} a_1^\dagger a_1^\dagger|0\rangle|0\rangle$. Note the normalization in case (iii) due to the fact that $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$.

   Applying the unitary transformation to all the mode operators then yields

$$\text{(i):} \quad \left(\cos\theta a_1^\dagger + \sin\theta a_2^\dagger\right)|0\rangle|0\rangle = \cos\theta|1\rangle|0\rangle + \sin\theta|0\rangle|1\rangle$$

$$\text{(ii):} \quad \left(\cos\theta a_1^\dagger + \sin\theta a_2^\dagger\right)\left(\cos\theta a_2^\dagger - \sin\theta a_2^\dagger\right)|0\rangle|0\rangle$$
$$= \left[-\cos\theta\sin\theta a_1^\dagger a_1^\dagger + \left(\cos^2\theta - \sin^2\theta\right)a_1^\dagger a_2^\dagger + \cos\theta\sin\theta a_2^\dagger a_2^\dagger\right]|0\rangle|0\rangle$$
$$= -\sqrt{2}\cos\theta\sin\theta|2\rangle|0\rangle + \left(\cos^2\theta - \sin^2\theta\right)|1\rangle|1\rangle + \sqrt{2}\cos\theta\sin\theta|0\rangle|2\rangle$$
$$= \cos(2\theta)|1\rangle|1\rangle + \frac{1}{\sqrt{2}}\sin(2\theta)\left(|0\rangle|2\rangle - |2\rangle|0\rangle\right)$$

$$\text{(iii):} \quad \frac{1}{\sqrt{2}}\left(\cos\theta a_1^\dagger + \sin\theta a_2^\dagger\right)\left(\cos\theta a_1^\dagger + \sin\theta a_2^\dagger\right)|0\rangle|0\rangle$$
$$= \frac{1}{\sqrt{2}}\left(\cos^2\theta a_1^\dagger a_1^\dagger + 2\cos\theta\sin\theta a_1^\dagger a_2^\dagger + \sin^2\theta a_2^\dagger a_2^\dagger\right)|0\rangle|0\rangle$$
$$= \cos^2\theta|2\rangle|0\rangle + \sin^2\theta|0\rangle|2\rangle + \frac{1}{\sqrt{2}}\sin(2\theta)|1\rangle|1\rangle$$

2. Suppose you place photon detectors in both output modes of the beamsplitter. Would it be possible to determine which of the three initial states, (i) (ii) or (iii), you started with after a single run of the experiment?

   (2 marks)

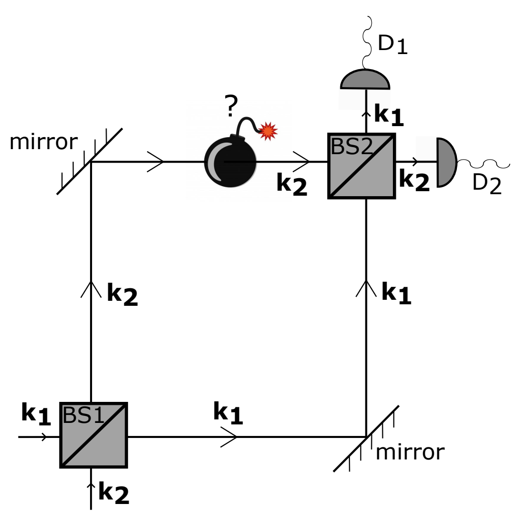
   We can immediately distinguish between the single photon case (i) and the two photon cases (ii) and (iii) just by counting the number of photons that are detected. Distinguishing between (ii) and (iii) is however not possible for arbitrary angles θ, as all three outcomes happen with non-vanishing probability for both initial states.

3. Would it be possible to determine which of the three initial states, (i) (ii) or (iii), you started with after many runs of the experiment?

   (3 marks)

   The outcome states for (ii) and (iii) are different, hence, by taking many runs of the experiment, we can compare the statistics with the expected outcomes. For example, in (ii) the probability of measuring two photons in D2 is equal to the probability of measuring two photons in D1. This is not the case for (iii) (except for $\theta = \frac{\pi}{4}$), where we can find other ways to distinguish the two states. Except for specific choices of θ, where the probability of measuring one outcome vanishes completely for one initial state, we can however only ever correctly determine the initial state up to some probability.

The Mach Zender interferometer is a variant on the double slit experiment where there are only two possible paths for a photon to take. Let's consider a version with a parameterized beamsplitter and a box that potentially contains a bomb in one arm as shown in the figure below. Can we use quantum trickery to test whether it contains a live bomb without actually setting the bomb off?



Assume a single photon enters the interferometer through the left hand arm (mode $\mathbf{k_1}$).

4. Assuming there is no bomb in the interferometer, what is the probability of measuring a photon at detectors 1 and 2 respectively?

   (1 marks)

   If there is no bomb, the total unitary acting on the mode operators is just $U_{BS2}U_{BS1} = U^{\dagger}_{BS1}U_{BS1} = I$. Hence, if a single photon enters through mode $\mathbf{k_1}$, the probability of measuring the photon at $D1$ is 1, while the probability of measuring it at $D2$ is 0.

Suppose now there is a bomb in the interferometer. If the bomb does not explode, then the photon is collapsed back into being definitely in the $\mathbf{k}_1$ arm of the interferometer.

There are three possible outcomes when a bomb is in the interferometer:

A) The bomb explodes.

B) The bomb does not explode but you can conclude with certainty that the interferometer does contain a bomb.

C) The bomb does not explode and you cannot tell whether or not there is a bomb.

5. What is the probability of the bomb exploding (i.e. option A) ?

   (3 marks)

   After the first beam splitter the photon is in a coherent superposition of being in either path:

$$|1\rangle_{\mathbf{k}_1}|0\rangle_{\mathbf{k}_2} = a^{\dagger}_{\mathbf{k}_1}|0\rangle \rightarrow BS1 \rightarrow (\cos\theta a^{\dagger}_{\mathbf{k}_1} + \sin\theta a^{\dagger}_{\mathbf{k}_2})|0\rangle|0\rangle = \cos\theta|1\rangle|0\rangle + \sin\theta|0\rangle|1\rangle$$

   The bomb now acts as a measurement after the first beamsplitter. From the above equation we see that the chance of the bomb exploding (i.e. the photon being in mode $\mathbf{k}_2$) is $\sin^2(\theta)$.

6. What is the probability of finding the photon at detectors 1 and 2 if there is a bomb but it does not explode?

   (3 marks)

   If the bomb does not explode, the state collapses into $a^{\dagger}_{\mathbf{k}_1}|0\rangle|0\rangle = |1\rangle|0\rangle$ before passing through the second beamsplitter. After passing through $BS2$, we find that the state is

$$|1\rangle_{\mathbf{k}_1}|0\rangle_{\mathbf{k}_2} = a^{\dagger}_{\mathbf{k}_1}|0\rangle \rightarrow BS2 \rightarrow (\cos\theta a^{\dagger}_{\mathbf{k}_1} - \sin\theta a^{\dagger}_{\mathbf{k}_2})|0\rangle|0\rangle = \cos\theta|1\rangle|0\rangle - \sin\theta|0\rangle|1\rangle$$

   The probability for measuring the photon in detector 1 in this case is thus $\cos^2(\theta)$, and for measuring it in detector 2 it's $\sin^2(\theta)$.

7. Hence, what are the probabilities of options B (you detect the bomb) and C (you cannot tell whether or not there is a bomb)?

(3 marks)

As discussed in point 3, if there is no bomb, the photon is always detected in detector 1. If we measure the photon in detector 1, we thus don't know whether there is a bomb or not. The probability of this happening is

$$p_C = p(\text{no explosion})p(D1|\text{no explosion}) = \cos^2(\theta)\cos^2(\theta).$$

Similarly, we find

$$p_B = p(\text{no explosion})p(D2|\text{no explosion}) = \cos^2(\theta)\sin^2(\theta) = \frac{1}{4}\sin^2(2\theta).$$