IMPERIAL

MATH70018

BSc, MSci and MSc EXAMINATIONS (MATHEMATICS)
May 2024

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

Quantum Mechanics 2

Date: Friday, May 17, 2024

Time: 10:00 – 12:30 (BST)

Time Allowed: 2.5 hours

This paper has 5 Questions.

Please Answer All Questions in 1 Answer Booklet

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

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

Any required additional material(s) will be provided.

Allow margins for marking.

Credit will be given for all questions attempted.

Each question carries equal weight.

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Formula Sheet

The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Connection to quantum information language: $X = \sigma_x$, $Y = \sigma_y$, $Z = \sigma_z$, $|\uparrow\rangle = |0\rangle$, $|\downarrow\rangle = |1\rangle$.

Useful relation:

$$e^{-i\mathbf{B}\cdot\boldsymbol{\sigma}} = \cos(B) - i\sin(B)\mathbf{e}_B \cdot \boldsymbol{\sigma}.$$

Results from non-degenerate perturbation theory:

$$E_n^{(1)} = \langle n| \hat{V} |n\rangle$$
$$E_n^{(2)} = \sum_{n' \neq n} \frac{|\langle n'| \hat{V} |n\rangle|^2}{\varepsilon_n - \varepsilon_{n'}}.$$

1. Shorter questions covering different aspects of the module. Derivations / proofs are not required unless explicitly stated.

(a) Let $\hat{a}$ be a bosonic annihilation operator. Evaluate and simplify $[\hat{a}, \hat{a}^\dagger \hat{a}]$.

(2 marks)

(b) Let $\hat{c}$ be a fermionic annihilation operator. Evaluate and simplify $[\hat{c}, \hat{c}^\dagger \hat{c} \hat{c}^\dagger]$. Express your result in terms of $\hat{n} = \hat{c}^\dagger \hat{c}$.

(3 marks)

(c) Suppose two Hermitian operators $\hat{A}$ and $\hat{B}$ commute. Suppose $\hat{B}$ has a doubly-degenerate eigenvalue. That is, there are two orthogonal states $|\phi_1\rangle$ and $|\phi_2\rangle$ for which $\hat{B}|\phi_1\rangle = b|\phi_1\rangle$ and $\hat{B}|\phi_2\rangle = b|\phi_2\rangle$. Will $|\phi_1\rangle$ and $|\phi_2\rangle$ be eigenstates of $\hat{A}$? Briefly explain.

(3 marks)

(d) As discussed in this module, time reversal when applied to the position and momentum operators does not affect the former but changes the sign of the latter. Deduce from this that the time reversal operator cannot be unitary.

(3 marks)

(e) Briefly describe at a qualitative level when the Heisenberg picture may be preferable to the Schrödinger picture for solving a problem in quantum mechanics. There is not a unique correct answer.

(3 marks)

(f) State the spin statistics theorem.

(2 marks)

(g) Suppose an anti-unitary operator operates on a two-state Hilbert space as $\hat{K}|0\rangle = i|1\rangle$ and $\hat{K}|1\rangle = -i|0\rangle$. Can $\hat{K}$ have an eigenstate, i.e. a state such that $\hat{K}|\phi\rangle = \lambda|\phi\rangle$? Why or why not?

(4 marks)

(Total: 20 marks)

2. Quantum circuits and measurement

(a) The swap gate acts on two-qubit states as $|\phi_1\phi_2\rangle \to |\phi_2\phi_1\rangle$ where $|\phi_1\rangle$ and $|\phi_2\rangle$ are arbitrary single qubit states. Denoting the swap operator as $\hat{S}$, this means $\hat{S}\,|\phi_1\phi_2\rangle = |\phi_2\phi_1\rangle$.

(i) Write down the computational basis that spans the Hilbert space of two qubits. This should have four states. Write out what the swap operation does to the computational basis.

(3 marks)

(ii) Deduce that the swap gate is a unitary operation.

(3 marks)

(iii) Find the eigenvalues and eigenvectors (expressed in terms of the computational basis) of the swap operator.

(3 marks)

(iv) Using the result of the Part (a iii) or otherwise deduce the following. For arbitrary single qubit states $|\phi_1\rangle$ and $|\phi_2\rangle$, the two-qubit state $|\phi_1\phi_2\rangle - |\phi_2\phi_1\rangle$ is proportional to the singlet state $\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$.

(3 marks)

(b) Quantum measurement.

(i) A two-qubit system is in the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$. The first qubit is measured in the $\hat{X}$ Pauli basis and the outcome is that it is an eigenstate with eigenvalue 1. What is the state of the two-qubit system after the measurement?

(4 marks)

(ii) A single qubit is in the state $|0\rangle$. It is first measured in the eigenbasis of $\hat{X}$. Next it is measured in the eigenbasis of $\hat{Z}$. What is the probability that the state is $|0\rangle$ after the final measurement?

(4 marks)

(Total: 20 marks)

3. Time-dependent unitary transformation

(a) Suppose $|\psi\rangle$ satisfies the time-dependent Schrödinger equation $\hat{\mathcal{H}}\,|\psi\rangle = i\hbar\partial_t\,|\psi\rangle$. Now introduce a new state $|\psi'\rangle = \hat{U}(t)\,|\psi\rangle$ where $\hat{U}(t)$ is a time-dependent unitary operator. Show that $|\psi'\rangle$ satisfies a time-dependent Schrödinger equation with transformed Hamiltonian $\hat{\mathcal{H}}' = \hat{U}\hat{\mathcal{H}}\hat{U}^\dagger - i\hbar\hat{U}\partial_t\hat{U}^\dagger$.

(4 marks)

(b) Let $\hat{\mathcal{U}}$ be the time-evolution operator for $\hat{\mathcal{H}}$ so that $|\psi(t)\rangle = \hat{\mathcal{U}}(t)\,|\psi(0)\rangle$. Denote the time-evolution operator for $\hat{\mathcal{H}}'$ as $\hat{\mathcal{U}}'$ so that $|\psi'(t)\rangle = \hat{\mathcal{U}}'(t)\,|\psi'(0)\rangle$. Show that

$$\hat{\mathcal{U}}(t) = \hat{U}^\dagger(t)\hat{\mathcal{U}}'(t)\hat{U}(0).$$

(4 marks)

(c) Consider the following Hamiltonian for a spin in a magnetic field:

$$\hat{\mathcal{H}} = \gamma(\cos(\omega t)\hat{\sigma}_x + \sin(\omega t)\hat{\sigma}_y).$$

Here, γ and ω are positive real parameters and $\hat{\sigma}_x$ and $\hat{\sigma}_y$ are operators corresponding to Pauli matrices, e.g. $\hat{\sigma}_x = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|$. What are the instantaneous eigen-energies of this Hamiltonian?

(4 marks)

(d) Determine a unitary transformation that removes the time dependence of this Hamiltonian. Hence, determine a transformed Hamiltonian $\hat{\mathcal{H}}'$ (see Part (a)) that has no time dependence. Hint: observe that (why?) $\hat{\mathcal{H}} = \gamma e^{-i\omega t\hat{\sigma}_z/2}\hat{\sigma}_x e^{i\omega\hat{\sigma}_z t/2}$.

(4 marks)

(e) Determine an explicit expression for the time-evolution operator for $\hat{\mathcal{H}}$ using the results of Part (b) and (d). When would you expect the adiabatic approximation to be valid for this system?

(4 marks)

(Total: 20 marks)

4. Perturbation theory.

In this problem, we consider a quantum pendulum described by

$$\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 - mgL\cos(\hat{x}/L).$$

In this, $\hat{x}$ and $\hat{p}$ are the usual position and momentum operators and m, g, and L are positive real parameters. We will focus on states that are tightly localised around $x = 0$.

(a) Expand the cosine in $\hat{\mathcal{H}}$ to fourth order in $\hat{x}$ to show that it can be approximately written as

$$\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - \gamma\hat{x}^4 - mgL.$$

where $\omega = \sqrt{g/L}$ and $\gamma = \frac{1}{4!}mg/L^3$.

(4 marks)

(b) We aim to treat the quartic $\hat{x}^4$ piece in the above Hamiltonian as a small perturbation. When might this approach be valid for finding an approximate ground state of the Schrödinger equation?

(4 marks)

(c) To proceed, it is useful to write the Hamiltonian of Part (b) in ladder operators $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\omega\hbar}}\hat{p}$. The resulting expression will have the form

$$\hat{\mathcal{H}} = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2) + B(\hat{a} + \hat{a}^\dagger)^4 + C.$$

Determine B and C in this expression. Hint: first express $\hat{p}$ and $\hat{x}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$ and insert into the Hamiltonian.

(6 marks)

(d) Split the Hamiltonian up as $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \lambda\hat{V}$ where $\hat{\mathcal{H}}_0 = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - mgL$, $\hat{V} = -\gamma\hat{x}^4$, and λ is our usual perturbative parameter (for bookkeeping). Determine the ground state energy of $\hat{\mathcal{H}}$ to first order in λ using first order perturbation theory. To do this, it may be easiest to use the result of part (c).

(6 marks)

(Total: 20 marks)

5. Central to the BCS theory of superconductivity is a Hamiltonian of the form

$$\hat{\mathcal{H}} = \xi(\hat{c}^\dagger\hat{c} + \hat{d}^\dagger\hat{d}) + \Delta(\hat{c}^\dagger\hat{d}^\dagger + \hat{d}\hat{c})$$

where $\hat{c}$ and $\hat{d}$ are Fermionic operators satisfying the usual anti-commutation relations (e.g. $\{\hat{d}, \hat{d}^\dagger\} = 1$) and ξ and Δ are positive real parameters.

(a) An important aspect of BCS superconductivity is that the particle number is not a conserved quantity. Explicitly demonstrate this by showing that $[\hat{N}, \hat{\mathcal{H}}]\,|0\rangle$ is generally nonzero. Here $\hat{N} = \hat{c}^\dagger\hat{c} + \hat{d}^\dagger\hat{d}$ and $|0\rangle$ is the vacuum state. Hint: it might be easiest to directly act with $\hat{N}$ and $\hat{\mathcal{H}}$ on $|0\rangle$ instead of directly evaluating the commutator.

(4 marks)

(b) A strategy for simplifying the Hamiltonian is to introduce the operators $\hat{\gamma}_1 = u\hat{c} + v\hat{d}^\dagger$ and $\hat{\gamma}_2 = -v\hat{c}^\dagger + u\hat{d}$ where u and v are real parameters. These operators are unusual because they can make a superposition of a particle and a "hole". We require that these new operators satisfy Fermionic anti-commutation relations: $\{\hat{\gamma}_1, \hat{\gamma}_1^\dagger\} = 1$, $\{\hat{\gamma}_2, \hat{\gamma}_2^\dagger\} = 1$, and $\{\hat{\gamma}_1, \hat{\gamma}_2\} = \{\hat{\gamma}_1, \hat{\gamma}_2^\dagger\} = 0$. What constraint(s) does this place on the u and v parameters?

(4 marks)

(c) Invert the relations found in (b) to show that $\hat{c} = u\hat{\gamma}_1 - v\hat{\gamma}_2^\dagger$ and $\hat{d} = v\hat{\gamma}_1^\dagger + u\hat{\gamma}_2$. The strategy is then to insert these expressions into $\hat{\mathcal{H}}$ and choose u and v such that "off diagonal" terms (e.g. terms proportional to $\hat{\gamma}_1\hat{\gamma}_2$) vanish. The result is

$$\hat{\mathcal{H}} = E(\hat{\gamma}_1^\dagger\hat{\gamma}_1 + \hat{\gamma}_2^\dagger\hat{\gamma}_2) + \xi - E$$

where E is positive, real, and can be expressed in terms of ξ and Δ. What is E?

Hint: you are <u>not</u> being asked to find explicit expressions for u and v. It might be helpful to write the Hamiltonian as $\hat{\mathcal{H}} = \hat{\Psi}^\dagger M \hat{\Psi} + \xi$ where M is a 2 by 2 matrix and $\hat{\Psi}$ is a column vector with entries $\hat{c}$ and $\hat{d}^\dagger$. Then introduce the γ operators through $\hat{\Psi} = U\hat{\Phi}$ where U is a 2 by 2 unitary matrix and $\hat{\Phi}$ is a column vector with entries $\hat{\gamma}_1$ and $\hat{\gamma}_2^\dagger$. Choose U strategically.

(6 marks)

(d) The ground state of the Hamiltonian from Part (c) is the vacuum state of the γ Fermions we found. That is, it is the state $|\phi\rangle$ that satisfies $\hat{\gamma}_1\,|\phi\rangle = \hat{\gamma}_2\,|\phi\rangle = 0$.

Consider the state $\left|\tilde{\phi}\right\rangle = \hat{\gamma}_1\hat{\gamma}_2\,|0\rangle$ where $|0\rangle$ is the usual (normalised) vacuum state of the original $\hat{c}$ and $\hat{d}$ Fermions. Show that acting with $\hat{\gamma}_1$ or $\hat{\gamma}_2$ on $\left|\tilde{\phi}\right\rangle$ gives zero. We can identify $\left|\tilde{\phi}\right\rangle$ with the desired vacuum state of the γ Fermions. But it is not normalised.

Normalise $\left|\tilde{\phi}\right\rangle$ and simplify to show that the desired ground state can be written as

$$|\phi\rangle = (a + b\hat{d}^\dagger\hat{c}^\dagger)\,|0\rangle$$

where explicit expressions for a and b in terms of u and v are to be found.

(6 marks)

(Total: 20 marks)

Solutions for Quantum Mechanics II Exam, 2024

1. Shorter questions covering different aspects of the module. Derivations / proofs are not required unless explicitly stated.

   (a) Let $\hat{a}$ be a bosonic annihilation operator. Evaluate and simplify $[\hat{a}, \hat{a}^\dagger \hat{a}]$.

   Seen. Use $[A, BC] = [A, B]C + B[A, C]$ to find $[\hat{a}, \hat{a}^\dagger \hat{a}] = \hat{a}$.

   (b) Let $\hat{c}$ be a fermionic annihilation operator. Evaluate and simplify $[\hat{c}, \hat{c}^\dagger \hat{c}\hat{c}^\dagger]$. Express your result in terms of $\hat{n} = \hat{c}^\dagger \hat{c}$.

   Similar seen. First, we can simplify one of the pieces: $\hat{c}^\dagger \hat{c}\hat{c}^\dagger = \hat{c}^\dagger(\{\hat{c}, \hat{c}^\dagger\} - \hat{c}^\dagger \hat{c}) = \hat{c}^\dagger$.

   So $[\hat{c}, \hat{c}^\dagger \hat{c}\hat{c}^\dagger] = [\hat{c}, \hat{c}^\dagger] = 1 - 2\hat{n}$.

   (c) Suppose two Hermitian operators $\hat{A}$ and $\hat{B}$ commute. Suppose $\hat{B}$ has a doubly-degenerate eigenvalue. That is, there are two orthogonal states $|\phi_1\rangle$ and $|\phi_2\rangle$ for which $\hat{B}|\phi_1\rangle = b|\phi_1\rangle$ and $\hat{B}|\phi_2\rangle = b|\phi_2\rangle$. Will $|\phi_1\rangle$ and $|\phi_2\rangle$ be eigenstates of $\hat{A}$?

   Similar seen. Only if we are lucky. In general, we need to diagonalise $\hat{A}$ within this subspace of degenerate states.

   (d) As discussed in this module, time reversal when applied to the position and momentum operators does not affect the former but changes the sign of the latter. Deduce from this that the time reversal operator cannot be unitary.

   Seen. Suppose time reversal is achieved by a unitary: $\hat{U}\hat{x}\hat{U}^\dagger = \hat{x}$ and $\hat{U}\hat{p}\hat{U}^\dagger = -\hat{p}$. Using this we reach a contradiction:

$$i\hbar = [\hat{x}, \hat{p}] = [\hat{U}\hat{x}\hat{U}^\dagger, -\hat{U}\hat{p}\hat{U}^\dagger] = \hat{U}[\hat{x}, -\hat{p}]\hat{U}^\dagger = \hat{U}(-i\hbar)\hat{U}^\dagger = -i\hbar.$$

   (e) Briefly describe at a qualitative level when the Heisenberg picture may be preferable to the Schrödinger picture for solving a problem in quantum mechanics. There is not a unique correct answer.

   Unseen. Answers will vary. Looking for an understanding of the two pictures and thoughts. Sometimes finding the full spectrum of a Hamiltonian is not possible or difficult. For such cases, the Heisenberg picture often is preferable. An example we considered is the dynamics of a particle under a linear potential. The eigenstates are complicated Airy functions, yet we found simple motion by using the Heisenberg approach. The full wavefunction sometimes contains a lot of irrelevant information for the problem at hand. The Heisenberg picture exploits this and focuses only on the dynamics of operators of interest. On the other hand, if you require full information about the dynamics of a system, the Schrödinger picture probably is the way to go because it focuses directly on computing the full wavefunction.

   (f) State the spin statistics theorem.

   Seen. Bosons have integer spin while Fermions have half-integer spin.

(g) Suppose an anti-unitary operator operates on a two-state Hilbert space as $\hat{K}|0\rangle = i|1\rangle$ and $\hat{K}|1\rangle = -i|0\rangle$. Can $\hat{K}$ have an eigenstate, i.e. a state such that $\hat{K}|\phi\rangle = \lambda|\phi\rangle$? Why or why not?

Unseen. A little tricky. Apply $\hat{K}$ to the first relation and use the second relation to get $\hat{K}^2|0\rangle = -i\hat{K}|1\rangle = (-i)(-i)|0\rangle = -|0\rangle$. A similar manipulation on the second relation gives $\hat{K}^2|1\rangle = -|1\rangle$. It therefore follows that $\hat{K}^2 = -1$.

Now suppose that it has and eigenstate: $\hat{K}|\phi\rangle = \lambda|\phi\rangle$. Apply $\hat{K}$ to this equation to reach a contradiction: $-|\phi\rangle = \lambda^*\hat{K}|\phi\rangle = |\lambda|^2|\phi\rangle$ which means $|\lambda|^2 = -1$ which can't be true.

So there is not such an eigenstate.

2. Quantum circuits and measurement

(a) The swap gate acts on two-qubit states as $|\phi_1\phi_2\rangle \to |\phi_2\phi_1\rangle$ where $|\phi_1\rangle$ and $|\phi_2\rangle$ are arbitrary single qubit states. Denoting the swap operator as $\hat{S}$, this means $\hat{S}|\phi_1\phi_2\rangle = |\phi_2\phi_1\rangle$.

i. Write down the computational basis that spans the Hilbert space of two qubits. This should have four states. Write out what the swap operation does to the computational basis.

Seen. Computational basis is $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. Also $\hat{S}|00\rangle = |00\rangle$, $\hat{S}|01\rangle = |10\rangle$, $\hat{S}|10\rangle = |01\rangle$, $\hat{S}|11\rangle = |11\rangle$.

ii. Deduce that the swap gate is a unitary operation.

Seen. To do this you can write out $\hat{S}$ in matrix form in the computational basis using the result from the previous part. Then you can explicitly show that this matrix is unitary: multiplying it by its adjoint gives the identity matrix.

iii. Find the eigenvalues and eigenvectors (expressed in terms of the computational basis) of the swap operator.

Unseen. From (a) we see that we have already found two eigenstates: $|00\rangle$ and $|11\rangle$ which both have eigenvalue of 1. Next we can diagonalise $\hat{S}$ within the subspace of the remaining states. One finds the following two eigenstates: $\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$ with eigenvalue 1 and $\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ with eigenvalue -1.

iv. Using the result of the Part (a iii) or otherwise deduce the following. For arbitrary single qubit states $|\phi_1\rangle$ and $|\phi_2\rangle$, the two-qubit state $|\phi_1\phi_2\rangle - |\phi_2\phi_1\rangle$ is proportional to the singlet state $\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$.

Unseen. The long way of doing this is to parametrise the individual qubit states, multiply everything out, apply the swap and show directly by brute force.

The shorter way is to recognise that both of the states have swap eigenvalue -1. Since this is a non-degenerate eigenvalue (see previous part) it must be that they are proportional to one another.

(b) Quantum measurement.

i. A two-qubit system is in the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$. The first qubit is measured in the $\hat{X}$ Pauli basis and the outcome is that it is an eigenstate with eigenvalue 1. What is the state after the measurement?

Similar seen. First one needs to find the X Pauli basis states. They are $|\phi_+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $|\phi_-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. The first state has eignevalue 1 while the second state has eigenvalue -1. Using measurement postulates, the (un-normalised) state after the measurement is $\hat{P}_+ \otimes \mathbb{1} |\psi\rangle$ (see Appendix 4.A of notes). Working this out and normalising, we find:

$$|\psi'\rangle = |\phi_+\rangle |\phi_+\rangle$$

is the state after the measurement.

ii. A single qubit is in the state $|0\rangle$. It is first measured in the eigenbasis of $\hat{X}$. Next it is measured in the eigenbasis of $\hat{Z}$. What is the probability that the state is $|0\rangle$ after the final measurement?

Unseen. An important aspect here is that the outcome of the first measurement is not specified. Let the two eigenstates of Pauli X be $|\phi_+\rangle$ and $|\phi_-\rangle$. For the first measurement, the probability of measuring $+X$ is $|\langle\phi_+|0\rangle|^2 = 1/2$ and the probability of measureing $-X$ is also $1/2$.

After the first measurement the system will be in either $|\phi_+\rangle$ or $|\phi_-\rangle$. Then with these states, you can determine the probability of measuring $+Z$ – it's half for both cases!

So we see that there are four possibilities:
Measure $+X$ then measure $+Z$: $P = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$.
Measure $+X$ then measure $-Z$: $P = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$.
Measure $-X$ then measure $+Z$: $P = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$.
Measure $-X$ then measure $-Z$: $P = \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}$.
The probability of the final measurement giving $+Z$ (or the final state being $|0\rangle$) is therefore $P = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$ where we have added the probabilities of the first and third cases above.

3. Time-dependent unitary transformation and adiabatic theory

(a) Suppose $|\psi\rangle$ satisfies the time-dependent Schrödinger equation $\hat{\mathcal{H}}|\psi\rangle = i\hbar\partial_t|\psi\rangle$. Now introduce a new state $|\psi'\rangle = \hat{U}(t)|\psi\rangle$ where $\hat{U}(t)$ is a time-dependent unitary operator. Show that $|\psi'\rangle$ satisfies a Schrödinger equation with transformed Hamiltonian $\hat{\mathcal{H}}' = \hat{U}\hat{\mathcal{H}}\hat{U}^\dagger - i\hbar\hat{U}\partial_t\hat{U}^\dagger$.

Seen. The answer follows from inserting $|\psi\rangle = \hat{U}^\dagger|\psi'\rangle$ into the Schrödinger equation, using the product rule for differentiation, and rearrangement. Note that $\hat{\mathcal{H}}'$ will be Hermitian.

(b) Let $\hat{\mathcal{U}}$ be the time-evolution operator for $\hat{\mathcal{H}}$ so that $|\psi(t)\rangle = \hat{\mathcal{U}}(t)|\psi(0)\rangle$. Denote the time-evolution operator for $\hat{\mathcal{H}}'$ as $\hat{\mathcal{U}}'$ so that $|\psi'(t)\rangle = \hat{\mathcal{U}}'(t)|\psi'(0)\rangle$. Show that

$$\hat{\mathcal{U}}(t) = \hat{U}^\dagger(t)\hat{\mathcal{U}}'(t)\hat{U}(0).$$

Unseen. Put $|\psi'\rangle = \hat{U}\,|\psi\rangle$ for $|\psi'\rangle$ at times t and 0 into $|\psi'(t)\rangle = \hat{\mathcal{U}}'(t)\,|\psi'(0)\rangle$ to get

$$\hat{U}(t)\,|\psi(t)\rangle = \hat{\mathcal{U}}'(t)\hat{U}(0)\,|\psi(0)\rangle$$

or

$$|\psi(t)\rangle = \hat{U}^\dagger(t)\hat{\mathcal{U}}'(t)\hat{U}(0)\,|\psi(0)\rangle\,.$$

Next we note that the unique time evolution operator satisfies $|\psi(t)\rangle = \hat{\mathcal{U}}(t)\,|\psi(0)\rangle$. So it must be that

$$\hat{\mathcal{U}}(t) = \hat{U}^\dagger(t)\hat{\mathcal{U}}'(t)\hat{U}(0).$$

(c) Consider the following Hamiltonian for a spin in a magnetic field:

$$\hat{\mathcal{H}} = \gamma(\cos(\omega t)\hat{\sigma}_x + \sin(\omega t)\hat{\sigma}_y).$$

Here, γ and ω are positive real parameters and $\hat{\sigma}_x$ and $\hat{\sigma}_y$ are operators corresponding to Pauli matrices, e.g. $\hat{\sigma}_x = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|$. What are the instantaneous eigen-energies of this Hamiltonian?

Unseen. You can write out the matrix form of the Hamiltonian in the spin basis and diagonalise. Or you can recall the discussed Pauli matrix identities. The instantaneous eigenvalues are $\pm\gamma$.

(d) Determine a unitary transformation that removes the time dependence of this Hamiltonian. Hence, determine a transformed Hamiltonian $\hat{\mathcal{H}}'$ that has no time dependence. Hint: try a unitary of the form $\hat{U} = e^{if(t)\hat{\sigma}_z}$ where f is a function to be determined.

Unseen. There are a few ways of approaching this. One way is to observe that

$$\hat{\mathcal{H}} = \gamma e^{-i\omega t\hat{\sigma}_z/2}\hat{\sigma}_x e^{i\omega\hat{\sigma}_z t/2}$$

This suggests that we use $\hat{U} = e^{i\omega\hat{\sigma}_z t/2}$. Trying this we find

$$\hat{\mathcal{H}}' = \gamma\sigma_x - \frac{\hbar\omega}{2}\hat{\sigma}_z.$$

(e) Determine an explicit expression for the time-evolution operator for $\hat{\mathcal{H}}$ using the results of Part (b) and (d). When would you expect the adiabatic approximation to be valid for this system?

Unseen. For adiabatic theory to apply we require the energy spacing of eigenstates to be large compared to (hbar times) the rate of variation of the Hamiltonian. So we require (using the result from c)

$$\hbar\omega \ll \gamma.$$

In finding the time-evolution operator, we use the result of (b). Since $\hat{\mathcal{H}}'$ has no time dependence finding $\hat{\mathcal{U}}'$ is easier. It is $\hat{\mathcal{U}}' = e^{-it\hat{\mathcal{H}}'/\hbar}$. So we have

$$\hat{\mathcal{U}}(t) = e^{-i\omega\hat{\sigma}_z t/2} e^{-it(\gamma\sigma_x - \frac{\hbar\omega}{2}\hat{\sigma}_z)/\hbar}$$

4. Perturbation theory.

In this problem, we consider a quantum pendulum described by

$$\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 - mgL\cos(\hat{x}/L).$$

In this, $\hat{x}$ and $\hat{p}$ are the usual position and momentum operators and m, g, and L are positive real parameters. We will focus on states that are tightly localised around $x = 0$.

(a) Expand the cosine in $\hat{\mathcal{H}}$ to fourth order in $\hat{x}$ to show that it can be approximately written as

$$\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - \gamma\hat{x}^4 - mgL.$$

where $\omega = \sqrt{g/L}$ and $\gamma = \frac{1}{4!}mg/L^3$.

Unseen. Use the cosine expansion $\cos(x) = 1 - \frac{1}{2}x^2 + \frac{1}{4!}x^4 + \ldots$ and the given expression for ω to get the answer.

(b) We aim to treat the quartic $\hat{x}^4$ piece in the above Hamiltonian as a small perturbation. When might this approach be valid for finding an approximate ground state of the Schrödinger equation?

Unseen. Answers will vary. Intuitively, we are applying the small angle approximation to the pendulum, so we require that the wavefunction will be very small except when $|x| \ll L$. To be more quantitative: we can recall or derive that the ground state of the Harmonic oscillator has variance $\sigma_x^2 = \ell^2$ where $\ell = \sqrt{\frac{\hbar}{2m\omega}}$. Then we expect that the quartic term will be a small correction when $\ell \ll L$. Indeed, we can write the position dependent potential in a revealing way

$$\frac{1}{2}m\omega^2 x^2 - \gamma x^4 = \frac{\hbar\omega}{4}\left[\left(\frac{x}{\ell}\right)^2 - \frac{1}{12}\left(\frac{\ell}{L}\right)^2\left(\frac{x}{\ell}\right)^4\right].$$

Due to the term factor $(\ell/L)^2$, the quartic piece will give a small correction to the quadratic piece in regions where the wave function is not vanishingly small.

(c) To proceed, it is useful to write the Hamiltonian of Part (b) in ladder operators $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\omega\hbar}}\hat{p}$. The resulting expression will have the form

$$\hat{\mathcal{H}} = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2) + B(\hat{a} + \hat{a}^\dagger)^4 + C.$$

Determine B and C in this expression. Hint: first express $\hat{p}$ and $\hat{x}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$ and insert into the Hamiltonian.

Similar seen. We can invert the equations for $\hat{a}$ and $\hat{a}^\dagger$ to find

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger)$$
$$\hat{p} = -i\sqrt{\frac{m\omega\hbar}{2}}(\hat{a} - \hat{a}^\dagger)$$

Then after subbing in and some manipulation we find

$$\hat{\mathcal{H}} = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2) - \gamma\left(\frac{\hbar}{2m\omega}\right)^2(\hat{a} + \hat{a}^\dagger)^4 - mgL.$$

(d) Split the Hamiltonian up as $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \lambda\hat{V}$ where $\frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 - mgL$, $\hat{V} = -\gamma\hat{x}^4$, and λ is our usual perturbative parameter (for bookkeeping). Determine the ground state energy of $\hat{\mathcal{H}}$ to first order in λ using first order perturbation theory. To do this, it may be easiest to use the result of part (c).

Unseen. Using our normal notation, we denote eigenstates of the Harmonic oscillator as $|n\rangle$. The ground state of $\hat{\mathcal{H}}_0$ is $|0\rangle$ with energy $\hbar\omega/2 - mgL$. Using first order perturbation theory requires evaluating $\langle 0|\,\hat{x}^4\,|0\rangle = \left(\frac{\hbar}{2m\omega}\right)^2\langle 0|\,(\hat{a} + \hat{a}^\dagger)^4\,|0\rangle$. Let $|\phi\rangle = (\hat{a} + \hat{a}^\dagger)^2\,|0\rangle$. Expanding we find

$$|\phi\rangle = |0\rangle + \sqrt{2}\,|2\rangle\,.$$

From this we see $\langle\phi|\,\phi\rangle = 1 + 2 = 3$ and so $\langle 0|\,\hat{x}^4\,|0\rangle = 3\left(\frac{\hbar}{2m\omega}\right)^2$.

Putting everything together, we have the first order expression for the ground state energy:

$$E = \hbar\omega/2 - mgL - \lambda\gamma 3\left(\frac{\hbar}{2m\omega}\right)^2.$$

5. Central to the BCS theory of superconductivity is a Hamiltonian of the form

$$\hat{\mathcal{H}} = \xi(\hat{c}^\dagger\hat{c} + \hat{d}^\dagger\hat{d}) + \Delta(\hat{c}^\dagger\hat{d}^\dagger + \hat{d}\hat{c})$$

where $\hat{c}$ and $\hat{d}$ are Fermionic operators satisfying the usual anti-commutation relations (e.g. $\{\hat{d}, \hat{d}^\dagger\} = 1$) and ξ and Δ are positive real parameters.

(a) An important aspect of BCS superconductivity is that the particle number is not a conserved quantity. Explicitly demonstrate this by showing that $[\hat{N}, \hat{\mathcal{H}}]\,|0\rangle$ is generally nonzero. Here $\hat{N} = \hat{c}^\dagger\hat{c} + \hat{d}^\dagger\hat{d}$ and $|0\rangle$ is the vacuum state. Hint: it might be easiest to directly act with $\hat{N}$ and $\hat{\mathcal{H}}$ on $|0\rangle$ instead of directly evaluating the commutator.

Unseen. We find $\hat{\mathcal{H}}\,|0\rangle = \Delta\hat{c}^\dagger\hat{d}^\dagger\,|0\rangle$ and $\hat{N}\,|0\rangle = 0$. So $[\hat{N}, \hat{\mathcal{H}}]\,|0\rangle = \hat{N}\hat{\mathcal{H}}\,|0\rangle = \hat{N}\hat{c}^\dagger\hat{d}^\dagger\,|0\rangle = 2\hat{c}^\dagger\hat{d}^\dagger\,|0\rangle$.

(b) A strategy for simplifying the Hamiltonian is to introduce the operators $\hat{\gamma}_1 = u\hat{c} + v\hat{d}^\dagger$ and $\hat{\gamma}_2 = -v\hat{c}^\dagger + u\hat{d}$ where u and v are real parameters. These operators are unusual because they can make a superposition of a particle and a "hole". We require that these new operators satisfy Fermionic anti-commutation relations: $\{\hat{\gamma}_1, \hat{\gamma}_1^\dagger\} = 1$, $\{\hat{\gamma}_2, \hat{\gamma}_2^\dagger\} = 1$, and $\{\hat{\gamma}_1, \hat{\gamma}_2\} = \{\hat{\gamma}_1, \hat{\gamma}_2^\dagger\} = 0$. What constraint(s) does this place on the u and v parameters?

Unseen. We can check each of the four given relations. The first two give $u^2 + v^2 = 1$ while the last two are automatically satisfied. So the constraint is $u^2 + v^2 = 1$.

(c) Invert the relations found in (b) to show that $\hat{c} = u\hat{\gamma}_1 - v\hat{\gamma}_2^\dagger$ and $\hat{d} = v\hat{\gamma}_1^\dagger + u\hat{\gamma}_2$. The strategy is then to insert these expressions into $\hat{\mathcal{H}}$ and choose u and v such that "off diagonal" terms (e.g. terms proportional to $\hat{\gamma}_1\hat{\gamma}_2$) vanish. The result is

$$\hat{\mathcal{H}} = E(\hat{\gamma}_1^\dagger\hat{\gamma}_1 + \hat{\gamma}_2^\dagger\hat{\gamma}_2) + \xi - E$$

where E is positive, real, and can be expressed in terms of ξ and Δ. What is E? Hint: you are <u>not</u> being asked to find explicit expressions for u and v. It might be helpful to write the Hamiltonian as $\hat{\mathcal{H}} = \hat{\Psi}^\dagger M \hat{\Psi} + \xi$ where M is a 2 by 2 matrix and $\hat{\Psi}$ is a column vector with entries $\hat{c}$ and $\hat{d}^\dagger$. Then introduce the γ operators through $\hat{\Psi} = U\hat{\Phi}$ where U is a 2 by 2 unitary matrix and $\hat{\Phi}$ is a column vector with entries $\hat{\gamma}_1$ and $\hat{\gamma}_2^\dagger$. Choose U strategically.

Unseen. The inversion is fairly direct, and uses the condition $u^2 + v^2 = 1$. For the next part, let's follow the hint and write

$$\hat{\mathcal{H}} = \begin{pmatrix} \hat{c}^\dagger & \hat{d} \end{pmatrix} \begin{pmatrix} \xi & \Delta \\ \Delta & -\xi \end{pmatrix} \begin{pmatrix} \hat{c} \\ \hat{d}^\dagger \end{pmatrix} + \xi = \Psi^\dagger M \Psi + \xi.$$

We note that M given here is a Hermitian matrix and so is diagonalised by a unitary transformation. Furthermore it is real and so its eigenvectors can be taken to be real. We choose u and v so that our 2 by 2 unitary U diagonalises M. The eigenvalues of M are $\pm E$ where $E = \sqrt{\xi^2 + \Delta^2}$. This is the E entering the desired expression.

(d) The ground state of the Hamiltonian from Part (c) is the vacuum state of the γ Fermions we found. That is, it is the state $|\phi\rangle$ that satisfies $\hat{\gamma}_1|\phi\rangle = \hat{\gamma}_2|\phi\rangle = 0$. Consider the state $\left|\tilde{\phi}\right\rangle = \hat{\gamma}_1\hat{\gamma}_2|0\rangle$ where $|0\rangle$ is the usual (normalised) vacuum state of the original $\hat{c}$ and $\hat{d}$ Fermions. Show that acting with $\hat{\gamma}_1$ or $\hat{\gamma}_2$ on $\left|\tilde{\phi}\right\rangle$ gives zero. We can identify $\left|\tilde{\phi}\right\rangle$ with the desired vacuum state of the γ Fermions. But it is not normalised.
Normalise $\left|\tilde{\phi}\right\rangle$ and simplify to show that the desired ground state can be written as

$$|\phi\rangle = (a + b\hat{d}^\dagger\hat{c}^\dagger)|0\rangle$$

where explicit expressions for a and b in terms of u and v are to be found.

Unseen. The first part follows from observing that $\hat{\gamma}_1\hat{\gamma}_1\hat{\gamma}_2 = 0$ since $(\hat{\gamma}_1)^2 = 0$. Also we observe that $\hat{\gamma}_2\hat{\gamma}_1\hat{\gamma}_2 = -\hat{\gamma}_1(\hat{\gamma}_2)^2 = 0$. So both $\hat{\gamma}_1$ and $\hat{\gamma}_2$ give zero when acting on $\left|\tilde{\phi}\right\rangle$.

Next expand out $\left|\tilde{\phi}\right\rangle$ and simplify:

$$\left|\tilde{\phi}\right\rangle = (u\hat{c} + v\hat{d}^\dagger)(-v\hat{c}^\dagger + u\hat{d})\left|0\right\rangle = (-uv - v^2\hat{d}^\dagger\hat{c}^\dagger)\left|0\right\rangle = -v(u + v\hat{d}^\dagger\hat{c}^\dagger)\left|0\right\rangle.$$

Finally, normalising we find

$$\left|\phi\right\rangle = (u + v\hat{d}^\dagger\hat{c}^\dagger)\left|0\right\rangle.$$

MATH60018 Quantum Mechanics 2

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