Cover-page

PHASM426/2014

Advanced Quantum Theory

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Answer THREE questions.

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per sub-section of a question.

The following formulae may be used if required:

$$e^x = \sum_{j=0}^{\infty} \frac{x^j}{j!} \quad \sin(x) = \sum_{j=0}^{\infty} (-1)^j \frac{x^{2j+1}}{(2j+1)!} \quad \cos(x) = \sum_{j=0}^{\infty} (-1)^j \frac{x^{2j}}{(2j)!} \quad \int_{-\infty}^{\infty} e^{-au^2} e^{-bu} du = \sqrt{\frac{\pi}{a}} e^{b^2/4a}$$

The Time-dependent Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

Pauli operators

$\sigma_z |\uparrow\rangle = |\uparrow\rangle$, $\sigma_z |\downarrow\rangle = -|\downarrow\rangle$; $\sigma_x |\uparrow\rangle = |\downarrow\rangle$, $\sigma_x |\downarrow\rangle = |\uparrow\rangle$; $\sigma_y |\uparrow\rangle = i|\downarrow\rangle$, $\sigma_y |\downarrow\rangle = -i|\uparrow\rangle$, where $\{|\uparrow\rangle, |\downarrow\rangle\}$ is the orthonormal basis for a spin-half quantum system.

Linear differential equations

A linear differential equation of the form $\frac{dy}{dx} + ay = b$ with a and b real numbers, has the general solution

$$y(x) = e^{-ax}\left(\frac{b}{a}e^{ax} + \kappa\right),$$

where κ is to be determined by initial conditions.

WKB Connection formulae

Right-hand barrier - with classical turning point at $x = a$:

$$\frac{2}{\sqrt{p(x)}} \cos\left(\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right) \quad \leftarrow \quad \frac{1}{\sqrt{q(x)}} \exp\left[-\int_a^x q(x')dx'/\hbar\right]$$

$$-\frac{1}{\sqrt{p(x)}} \sin\left(\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right) \quad \rightarrow \quad \frac{1}{\sqrt{q(x)}} \exp\left[+\int_a^x q(x')dx'/\hbar\right]$$

Left-hand barrier - with classical turning point at $x = a$:

$$\frac{1}{\sqrt{q(x)}} \exp\left[-\int_x^a q(x')dx'/\hbar\right] \quad \rightarrow \quad \frac{2}{\sqrt{p(x)}} \cos\left(\int_a^x p(x')dx'/\hbar - \frac{\pi}{4}\right)$$

$$\frac{1}{\sqrt{q(x)}} \exp\left[+\int_x^a q(x')dx'/\hbar\right] \quad \leftarrow \quad -\frac{1}{\sqrt{p(x)}} \sin\left(\int_a^x p(x')dx'/\hbar - \frac{\pi}{4}\right)$$

1. In order to derive the WKB wave-function in a classically-allowed region where $V(x) < E$, we use the ansatz $\psi(x) = A\exp[iS(x)/\hbar]$ and expand $S(x)$ as a power series in $\hbar$. The zeroth and first order solutions of $S(x)$ read as:

$$S_0(x) = \pm \int^x p(x')dx' + C \quad \text{and} \qquad S_1(x) = \frac{i}{2}\Big(\ln(p(x)) + D\Big)$$

where $p(x) = \sqrt{2m(E - V(x))}$ and C and D are constants.

(a) Derive the WKB wave-function in the classically-allowed region clearly stating the approximations made and the conditions under which they hold. **[4]**

(b) Comment on how the WKB wave-function compares with the probability distribution of a classical particle moving with momentum $p(x)$. **[2]**

(c) One can show that the second order term in the ansatz function $\psi(x)$ can be neglected when

$$\left|\frac{\hbar m}{p(x)^3}\frac{dV(x)}{dx}\right| \ll 1.$$

Show that this condition may equally be written in the form

$$\left|\frac{1}{2\pi}\frac{d\lambda(x)}{dx}\right| \ll 1\,,$$

where $\lambda(x) = h/p(x)$ is the local de Broglie wavelength. **[4]**

Hint: Notice that $\lambda(x)$ is a function of $p(x)$. You may want to write $V(x)$ as a function of $p(x)$ and consider the corresponding derivative $dV(x)/dx$.

(d) For a quantum well with smooth sides, show that the WKB approximation leads to the following quantisation condition:

$$\int_{x_1}^{x_2} p(x')dx'/\hbar = \left(n + \frac{1}{2}\right)\pi\,,$$

where x_1 and x_2 are the positions of classical turning points and $n = 0, 1, 2, \ldots$ is a non-negative integer. You will find WKB connection formulae in the rubric at the beginning of this paper. **[6]**

(e) Show that the above quantisation condition gives the correct energy levels for all the states of the quantum harmonic oscillator with frequency ω and potential $V(x) = m\omega^2x^2/2$. You may use, without proof, the integral

$$\int_{-1}^{+1} dy\sqrt{1-y^2} = \frac{\pi}{2}\,.$$

[4]

2. (a) The combined state of a pair of two-level atoms, A and B, is given by the density matrix:

$$\rho = \frac{1}{2} |g_A, g_B\rangle \langle g_A, g_B| + \frac{1}{2} |g_A, e_B\rangle \langle g_A, e_B| \, .$$

i. Calculate the reduced density matrix operator for each of the two-level systems. **[2]**

ii. Calculate the purity of system A and indicate whether the state of the two atoms is a product or an entangled state. Justify your answer. **[2]**

(b) The Markovian master equation for an open quantum system can be written in the following Lindblad form

$$\frac{\partial \rho}{\partial t} = \frac{-i}{\hbar}\Big(H_{\text{eff}}\rho - \rho H_{\text{eff}}^{\dagger}\Big) + \sum_j L_j \rho L_j^{\dagger} \, ,$$

where $H_{\text{eff}} = H - (i\hbar/2)\sum_j L_j^{\dagger} L_j$.

i. Outline the key steps and assumptions made in the derivation of this master equation. **[4]**

ii. One can also rearrange the terms in the equation above to rewrite it as $\frac{\partial \rho}{\partial t} = \frac{-i}{\hbar}[H, \rho] + D[\rho]$ where the superoperator $D[\rho]$ becomes:

$$D[\rho] = \sum_j (L_j \rho L_j^{\dagger} - \frac{1}{2} L_j^{\dagger} L_j \rho - \frac{1}{2} \rho L_j^{\dagger} L_j).$$

Show that $\text{Tr}[D[\rho]] = 0$ where Tr denotes the trace operation. Comment on the physical significance of this result. **[2]**

(c) Consider a two-level atom with excited state $|e\rangle$ and ground state $|g\rangle$ such that its Hamiltonian is $H = \hbar\omega |e\rangle \langle e|$. The action of the environment interacting with the atom is described by the jump operators $L_1 = \Gamma |e\rangle \langle g|$ and $L_2 = \gamma |g\rangle\langle e|$.

i. Assuming that at $t = 0$ the state of the atom is $\rho(0) = |g\rangle \langle g|$, show that the probability of finding the atom in the excited state at time t , $\rho_{ee}(t) = \langle e| \rho(t)|e\rangle$, is given by

$$\rho_{ee}(t) = \frac{|\Gamma|^2}{|\gamma|^2 + |\Gamma|^2}\Big(1 - e^{-(|\gamma|^2 + |\Gamma|^2)t}\Big).$$

You will find an expression for the general solution of a linear differential equation in the rubric at the beginning of this paper. **[6]**

ii. Find a relation between Γ and γ such that in the long-time limit $\rho_{ee}(\infty)$ equals the probability of finding the atom in its excited state when it is in thermal equilibrium at temperature T. Express your answer as $|\Gamma|^2 = C|\gamma|^2$ and specify the value of C as a function of ω and $k_B T$ where k_B is the Boltzman constant. Recall that in thermal equilibrium, a system with Hamiltonian H is described by the density matrix operator $\rho_{eq} = \frac{\exp(-H/k_B T)}{\text{Tr}[\exp(-H/k_B T)]}$. **[4]**

3. The interaction picture is employed to describe the dynamics of a system whose Hamiltonian has the form $H = H_0 + V$ where H_0 is solved, i.e. its eigenstates $|\psi_j\rangle$ and its eigenenergies E_j are known. In this picture the state of a system satisfies the equation $i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle_I = V_I(t)|\Psi(t)\rangle_I$ where $V_I(t) = U_0^\dagger(t)VU_0(t)$ and $U_0(t) = \exp[-iH_0t/\hbar]$.

   (a) In the dipole approximation, the Hamiltonian describing the interaction of an atom with states $|e\rangle$ and $|g\rangle$ and quantised light takes the form

$$H = \hbar\epsilon\,|e\rangle\langle e| + \hbar\omega\Big(a^\dagger a + \frac{1}{2}\Big) + \hbar g\Big(\,|g\rangle\langle e| + |e\rangle\langle g|\,\Big)\Big(a + a^\dagger\Big).$$

   For simplicity we have omitted the tensor product notation.

   i. Show that in this case $V_I(t)$ reads

$$V_I = \hbar g\Big(e^{-i\epsilon t}\,|g\rangle\langle e| + e^{i\epsilon t}\,|e\rangle\langle g|\,\Big)\Big(e^{-i\omega t}a + e^{i\omega t}a^\dagger\Big).$$

   You may use the identity $a = \sum_{n=0}\sqrt{n+1}\,|n\rangle\langle n+1|$ and the closure relation $\mathbb{1} = |e\rangle\langle e| + |g\rangle\langle g|$. **[4]**

   ii. Derive the form $V_I(t)$ takes after making the rotating wave approximation and assuming $\epsilon = \omega$. **[2]**

   (b) For a quantum system subject to a weak time-dependent perturbation with associated Hamiltonian $H = H_0 + \lambda V(t)$, its state in the interaction picture can be written as $|\Psi(t)\rangle_I = \sum_j c_j(t)\,|\psi_j\rangle$ where $|\psi_j\rangle$ are eigenstates of H_0. Show that the coefficients $c_j(t)$ satisfy the equations of motion,

$$\dot{c}_j(t) = \frac{\lambda}{i\hbar}\sum_k c_k(t)\exp\left[i\omega_{jk}t\right]V_{jk}(t)\,.$$

   [4]

   (c) Expanding $c_j(t)$ as a power series in λ, explain why the mth order terms in this expansion satisfy the following expressions (for $m = 1, 2, 3, \dots$): **[2]**

$$\dot{c}_j^{(0)}(t) = 0 \qquad\qquad \dot{c}_j^{(m)}(t) = \frac{1}{i\hbar}\sum_k \exp[i\omega_{jk}t]V_{jk}(t)c_k^{(m-1)}(t)\,.$$

   (d) A quantum harmonic oscillator is exposed to a weak time-dependent perturbation. The Hamiltonian of the system is given by

$$H = \hbar\omega\Big(a^\dagger a + \frac{1}{2}\Big) + f(t)(a + a^\dagger)\,,$$

   where $f(t) = Ae^{-t^2/\tau^2}$. At time $t = -\infty$ the state is $|\Psi(-\infty)\rangle = |n = 0\rangle$.

   i. Derive the probability (to first order) of finding the system in state $|n = 1\rangle$ at $t = \infty$. For which value of τ (in units of ω) is this probability maximised? You will find Gaussian integral definitions in the rubric at the beginning of this paper. **[6]**

   ii. Which is the minimum order that we need to consider to compute a non-vanishing probability of finding the system in state $|n = 2\rangle$? Justify your answer. **[2]**

4. (a) The evolution operator $U(t)$ transforms a state of a system at time 0, $|\psi(0)\rangle$ to the state of the system at time t, $|\psi(t)\rangle$, i.e. $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$. Show that for a time-independent Hamiltonian H, the evolution operator can be written:

$$U(t) = \exp\left[-i\frac{Ht}{\hbar}\right].$$

You may assume the identity $\frac{\partial}{\partial t}\exp[At] = A\exp[At]$ for a time-independent linear operator A. **[2]**

(b) Consider a spin-half system whose Hamiltonian changes discontinuously as follows: for $0 \leq t \leq t_1$ the dynamics is given by $H_1 = g\sigma_x$ and for $t > t_1$ the dynamics is given by $H_2 = \frac{\epsilon}{2}\sigma_z$.

i. Show that the state of the system at time $t > t_1$ is given by

$$|\Psi(t)\rangle = U_2(t-t_1)U_1(t_1)\,|\Psi(0)\rangle\,,$$

where $U_1(t) = \exp\left[-i\frac{H_1 t}{\hbar}\right]$ and $U_2(t) = \exp\left[-i\frac{H_2 t}{\hbar}\right]$. **[2]**

ii. Write down the time-evolved state $|\Psi(t)\rangle$ for $t > t_1$, assuming $|\Psi(0)\rangle = |\uparrow\rangle$. You may use, without proof, the identity $\exp[iA\alpha] = \cos(\alpha)\mathbb{1} + i\sin(\alpha)A$, which holds for all self-inverse linear operators A and scalars α. **[4]**

(c) Consider a two-level atom interacting with a quantum harmonic oscillator according to the following Hamiltonian:

$$H = \hbar\epsilon\,|e\rangle\langle e| \otimes \mathbb{1}_{osc} + \mathbb{1}_{atom} \otimes \hbar\omega\Big(a^\dagger a + \frac{1}{2}\Big) + \hbar g\,|e\rangle\langle e| \otimes \Big(a^\dagger a + \frac{1}{2}\Big).$$

Assume that at time $t = 0$ the state of the atom-oscillator system is $|\Psi(0)\rangle = |e\rangle \otimes |n\rangle$ where $|n\rangle$ is an eigenstate of the operator $a^\dagger a$. Indicate whether it is possible to compute analytically the time-evolved state of the compound system without the use of any approximation. Justify your answer. **[3]**

(d) $M = (\hbar\epsilon - i\gamma)\,|e\rangle\langle e|$ is a non-Hermitian operator associated with a two-state atom with excited state $|e\rangle$. If you attempt to compute the time-evolved state of the atom as $|\Psi(t)\rangle = \exp\left[-i\frac{Mt}{\hbar}\right]|\Psi(0)\rangle$ what unphysical features will this state exhibit? Justify your answer with specific calculations using the operator given. **[5]**

(e) In the following, the subscript H indicates operators in the Heisenberg picture and the subscript S denotes the Schrödinger picture. In the Heisenberg picture, time evolution is carried by operators, $\hat{O}_H(t) = U(t)^\dagger\hat{O}_S U(t)$. Consider an operator in the Schrödinger picture that is explicitly time-dependent, i.e. $\hat{O}_S(t)$. Show that, in the Heisenberg picture, the observable $\hat{O}_H(t)$ satisfy the following equation of motion:

$$\frac{\partial}{\partial t}\hat{O}_H(t) = \frac{i}{\hbar}[H_H(t), \hat{O}_H(t)] + \Big(\frac{\partial}{\partial t}\hat{O}_S(t)\Big)_H.$$

[4]

5. (a) Consider a Hermitian operator A and prove that the eigenvectors corresponding to two different eigenvalues are orthogonal. **[2]**

(b) Show that any linear operator A can be expressed as $A = B + iC$ where B and C are Hermitian operators. **[2]**

(c) Now assume that $B = \sigma_x$ and $C = \sigma_y$ and show that $A^2 = 0$. **[2]**

(d) The position basis states $|x\rangle$ represent continuous variable states and they satisfy the closure relationship $\mathbb{1} = \int_{-\infty}^{\infty} dx\, |x\rangle \langle x|$.

i. A is an operator on the Hilbert space of a quantum system and $\tilde{A}$ its representation in the position basis. These operators are related by the identity $\langle x|A|\psi\rangle = \tilde{A}\langle x|\psi\rangle = \tilde{A}\psi(x)$. Based on this, derive an expression for the expected value $\langle\psi|A|\psi\rangle$ in the position representation. **[3]**

ii. The operator $T(a)$ translates a system a distance a along the $x-$axis. The action of this operator over the position states $|x\rangle$ is defined by

$$T(a)\,|x\rangle = |x + a\rangle\,.$$

Consider a general quantum state $|\psi\rangle$ and show that $\langle x|\, T(a)\,|\psi\rangle = \psi(x - a)$. **[3]**

(e) Consider two arbitrary vectors $|\phi_1\rangle$ and $|\phi_2\rangle$ belonging to the inner product space $\mathcal{H}$. Show that these vectors satisfy the following inequalities:

i.

$$\langle\phi_1|\phi_1\rangle + \langle\phi_2|\phi_2\rangle \geq 2\mathrm{Re}(\langle\phi_1|\phi_2\rangle)\,.$$

You may start this proof by considering the vector $|\Psi\rangle = |\phi_1\rangle - |\phi_2\rangle$. **[3]**

ii.

$$||\,|\phi_1\rangle + |\phi_2\rangle\,|| \leq ||\,|\phi_1\rangle\,|| + ||\,|\phi_2\rangle\,||$$

where $||\,|v\rangle\,|| = \sqrt{\langle v|v\rangle}$ denotes the norm of vector $|v\rangle$. This is known as the triangle inequality. You may use, without proof, the fact that these vectors satisfy the Cauchy-Schwartz inequality i.e. $|\langle\phi_1|\phi_2\rangle|^2 \leq \langle\phi_1|\phi_1\rangle \times \langle\phi_2|\phi_2\rangle$. **[5]**

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