## **UNIVERSITY COLLEGE LONDON**

## **EXAMINATION FOR INTERNAL STUDENTS**

MODULE CODE : PHASG426

ASSESSMENT : PHASG426C PATTERN

MODULE NAME: Advanced Quantum Theory

DATE : **13-May-15** 

TIME : 10:00

TIME ALLOWED : 2 Hours 30 Minutes

### 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:

$$e^{x} = \sum_{j=0}^{\infty} \frac{x^{j}}{j!}$$
  $\sin(x) = \sum_{j=0}^{\infty} (-1)^{j} \frac{x^{2j+1}}{(2j+1)!}$   $\cos(x) = \sum_{j=0}^{\infty} (-1)^{j} \frac{x^{2j}}{(2j)!}$ 

The Time-dependent Schrödinger Equation

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

#### Pauli operators

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

#### WKB Connection formulae

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

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

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

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

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

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:

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

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.

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(b) 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.

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.

- (c) Consider a particle of mass m and energy E < 0, subject to the potential V(x) = -c/x for x > 0 and  $V(x = 0) = \infty$  for x = 0. Here c > 0.
  - i. Sketch V(x) as a function of x and indicate the classical turning points.
  - ii. Write down the form of the eigenfunctions of the Hamiltonian for  $x \ge 0$ . Justify your answer in detail. You will find WKB connection formulae in the rubric at the beginning of this paper.
  - iii. Show that in this case the WKB approximation leads to the following quantization condition:

$$\int_0^a p(x')dx' = \hbar\pi\left(n + \frac{3}{4}\right),$$

where a is a classical turning point. Write down an expression for the classical turning point in terms of E.

iv. Using the quantization condition derived above, show that the allowed energies are given by

$$E = -\frac{c^2 m}{2\hbar^2 (n+3/4)^2} \,.$$

You may use the integral

$$\int_{0}^{1} dx \sqrt{-1 + \frac{1}{x}} = \frac{\pi}{2}.$$

- 2. (a) Let H be the total Hamiltonian of a quantum system and its environment and U(t) the unitary evolution associated to H. At time t=0 the total state of the system and environment is  $\rho(t=0)=\rho_s(0)\otimes\rho_B(0)$ , where the initial state of the environment is  $\rho_B(0)=|B_0\rangle\langle B_0|$ . Here the basis set  $|B_k\rangle$  spans the environment states.
  - i. Show that the reduced density matrix operator for the system  $\rho_s(t)$  takes the form

$$ho_s(t) = \sum_k S_k 
ho_s(0) S_k^{\dagger},$$

where  $S_k = \langle B_k | U(t) | B_0 \rangle$ .

- ii. Justify whether  $S_k$  is an operator acting on the system or on the environment and show that  $\sum_k S_k^{\dagger} S_k = 1$ . Discuss the physical implications of this result.
- (b) A two-level atom, with energy eigenstates  $|g\rangle$  with energy  $E_g=0$  and  $|e\rangle$  with  $E_e=\hbar\omega$ , is interacting with an environment such 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

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

Find a relation between  $\Gamma$  and  $\gamma$  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  $\omega$  and  $k_BT$ , where  $k_B$  is the Boltzmann constant. Recall that in thermal equilibrium, a system with Hamiltonian H is described by the density matrix operator  $\rho_{eq} = \frac{\exp(-H/k_BT)}{\text{Tr}[\exp(-H/k_BT)]}$ .

(c) The Markovian master equation for the density matrix  $\rho$  describing an open quantum system can be written in the following Lindblad form as

$$rac{\partial 
ho(t)}{\partial t} = rac{-i}{\hbar} \Big( H_{ ext{eff}} 
ho(t) - 
ho(t) H_{ ext{eff}}^{\dagger} \Big) + \sum_{j} L_{j} 
ho(t) L_{j}^{\dagger} \,,$$

where  $H_{\text{eff}} = H - (i\hbar/2) \sum_j L_j^{\dagger} L_j$ . Suppose that in the master equation above you neglect the term  $\sum_j L_j \rho(t) L_j^{\dagger}$ . What unphysical features will the resultant density matrix operator exhibit? Justify your answer with specific calculations.

(d) Consider a two-level atom, with energy eigenstates  $|g\rangle$  with energy  $E_g=0$  and  $|e\rangle$  with  $E_e=\hbar\omega$ . The atom is initially in the state  $|\psi(0)\rangle=a\,|e\rangle+b\,|g\rangle$ , where a and b are real numbers. The influence of an environment on this atom is described by the operator  $L=\alpha\,|e\rangle\,\langle e|$ . Show that the time-evolution of the coherence  $\rho_{eg}(t)=\langle e|\rho(t)|g\rangle$  takes the form

$$\rho_{eg}(t) = ab e^{-|\alpha|^2 t/2} e^{-i\omega t}.$$

Draw a sketch of the real part of  $\rho_{eg}(t)$ .

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PHASG426/2015

3. (a) The interaction picture is employed to describe the dynamics of a system whose Hamiltonian has the form  $H = H_0 + V$ , where the eigenstates and eigenenergies of  $H_0$  are known. In this representation, operators take the form  $O_I(t) = U_0^{\dagger}(t)OU_0(t)$  with  $U_0(t) = \exp[-iH_0t/\hbar]$ . A Hamiltonian describing the interaction of a spin- $\frac{1}{2}$  particle and a quantum harmonic oscillator takes the form (for simplicity we omit the tensor product notation):

$$H = \frac{\hbar \epsilon}{2} \sigma_z + \hbar \omega \left( a^{\dagger} a + \frac{1}{2} \right) + \hbar g \sigma_z (a + a^{\dagger}).$$

i. Show that  $V_I(t) = \hbar g \sigma_z \left( e^{-i\omega t} a + e^{i\omega t} a^{\dagger} \right)$ . You may use the identity  $a = \sum_{n=0} \sqrt{n+1} |n\rangle \langle n+1|$ .

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- ii. Assume that the joint initial state of the spin and the harmonic oscillator is  $|\Psi\rangle = |\uparrow\rangle |0\rangle$ . Under the action of V(t), will the state of the spin change? Will the state of the harmonic oscillator change? Justify your answers with calculations.
- (b) For a quantum system subject to a weak time-dependent perturbation with associated Hamiltonian  $H(t) = H_0 + \lambda V(t)$ , 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  $H_0$ . Using the expansion  $c_j(t) = \sum_{n=0}^{\infty} \lambda^n c_j^{(n)}(t)$  one finds that the *n*th-order term satisfies the following equation:

$$\frac{\partial c_j^{(n)}(t)}{\partial t} = \frac{1}{i\hbar} \sum_k V_{jk}(t) \exp[i\omega_{jk}t] c_k^{(n-1)}(t).$$

- i. Explain what  $V_{jk}(t)$  and  $\omega_{jk}$  stand for. Assuming the system is initially in an eigenstate  $|\psi_m\rangle$ , write down general expressions for the first and second-order solutions  $c_j^{(1)}(t)$  and  $c_j^{(2)}(t)$ .
- ii. Consider a case where  $c_j^{(1)}(t)=0$  for  $j\neq m$ . Does this imply  $c_j^{(2)}(t)$  also vanishes? Justify your answer. [1]
- iii. Show that the energy of the system described by H(t) is not conserved. [3]
- (c) A quantum harmonic oscillator exposed to a weak perturbation has a Hamiltonian

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

where  $f(t) = \hbar A$  for  $0 \le t < \tau$ . At time t = 0 the state is  $|\Psi(0)\rangle = |n = 0\rangle$ . Show that the probability (to second order) of finding the system in the state  $|n = 2\rangle$  at  $\tau = \pi/2\omega$  is given by  $P_{n=2}^{(2)}(\tau = \pi/2) = A^4/\omega^4$ . [7]

4. (a) Two quantum systems a and b are prepared in a joint state  $|\Psi\rangle = |\psi_a\rangle |\psi_b\rangle$ . Let the set  $\{|\phi_k\rangle\}$  be a basis of states for system a,  $\{|\nu_j\rangle\}$  a basis for system b and A an operator on the Hilbert space of a with the following spectral decomposition:

$$A = \lambda_1 |\phi_1\rangle \langle \phi_1| + \lambda_2 \sum_{n=2}^{N} |\phi_n\rangle \langle \phi_n|.$$

i. Write down an expression for the projector acting on the total Hilbert space and which is associated to the measurement outcome  $\lambda_2$ . Derive an expression for the probability of obtaining  $\lambda_2$  in a measurement of A on the state  $|\Psi\rangle$ .

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- ii. Derive an expression for the state  $|\Psi'\rangle$  of the global system after the measurement. Has the state of the system b changed?
- iii. Discuss whether the predictions in (i) and (ii) would change depending of the choice of basis for the system b. Will the results of measurements on the systems a and b be correlated? Justify your answer.
- (b) Consider a spin- $\frac{1}{2}$  system whose Hamiltonian changes discontinuously as follows: for  $0 \le t \le t_1$  the dynamics is given by  $H_1 = \hbar g \sigma_x$  and for  $t > t_1$  the Hamiltonian is  $H_2 = \hbar \epsilon \sigma_z/2$ . 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  $U_1(t)=\exp\left[-i\frac{H_1t}{\hbar}\right]$  and  $U_2(t)=\exp\left[-i\frac{H_2t}{\hbar}\right]$ . Write down the time-evolved state  $|\Psi(t)\rangle$  for  $t>t_1$ , assuming  $|\Psi(0)\rangle=\frac{1}{\sqrt{2}}\big(|\uparrow\rangle+|\downarrow\rangle\big)$ . Simplify your answer as much as possible. 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  $\alpha$ .
- (c) Let  $\hat{A}$  and  $\hat{B}$  be two observables which, in the Schrödinger picture, satisfy  $[\hat{A}, \hat{B}] = \hat{C}$ . Show that the equivalent operators in the Heisenberg picture  $\hat{A}_H(t)$ ,  $\hat{B}_H(t)$  and  $\hat{C}_H(t)$  satisfy  $[\hat{A}_H(t), \hat{B}_H(t)] = \hat{C}_H(t)$ . Recall that in the Heisenberg picture  $\hat{O}_H(t) = U(t)^{\dagger} \hat{O}U(t)$ .
- (d) In the Heisenberg picture, the observable  $\hat{O}_H(t)$  satisfies the equation of motion

$$\frac{\partial}{\partial t}\hat{O}_{H}(t) = \frac{i}{\hbar}[H_{H}(t), \hat{O}_{H}(t)] + \left(\frac{\partial}{\partial t}\hat{O}(t)\right)_{H}.$$

Consider a free particle of mass m described by the Hamiltonian  $H = \hat{p}^2/2m$ .

i. Using the above equation, show that the position operator in the Heisenberg picture becomes

$$\hat{x}_H(t) = \hat{x}_H(0) + \frac{t}{m}\hat{p}_H.$$

You may use the relationship  $[\hat{x}, \hat{p}^2] = 2i\hbar\hat{p}$  and the result of part 4(c).

ii. Show that the commutator  $[\hat{x}_H(0), \hat{x}_H(t)] = i\hbar t/m$ . You may use the relationship  $[\hat{x}, \hat{p}] = i\hbar \mathbb{I}$ .

- 5. (a) Let K be the operator defined as  $K = |\phi\rangle\langle\psi|$ , where  $|\phi\rangle$  and  $|\psi\rangle$  are two vectors of the Hilbert space of a system.
  - i. Show that K is a linear operator. [1]
  - ii. Under which condition is K Hermitian? [1]
  - iii. Under which condition is K a projector? [1]
  - iv. Show that K can always be written in the form  $K = \lambda P_{\phi}P_{\psi}$ , where  $\lambda$  is a constant and  $P_{\phi}$  and  $P_{\psi}$  are the projector operators associated to  $|\phi\rangle$  and  $|\psi\rangle$ .
  - (b) Consider two distinct sets of complete orthonormal basis vectors  $\{|u_j\rangle\}$  and  $\{|v_k\rangle\}$ . By defining the trace of an operator A with respect to each of these basis sets, show that the trace of an operator is basis invariant. [2]
  - (c) The position states  $|x\rangle$  and the momentum states  $|p\rangle$  satisfy, respectively, the closure relationships  $\mathbb{1} = \int_{-\infty}^{\infty} dx |x\rangle \langle x|$  and  $\mathbb{1} = \int_{-\infty}^{\infty} dp |p\rangle \langle p|$ .
    - i. Let A be an operator on the Hilbert space of a quantum system and  $\tilde{A}$  its representation in the position basis. Using the relationship  $\langle x|p\rangle=(2\pi\hbar)^{-1/2}e^{ipx/\hbar}$ , show that  $\tilde{p}=\frac{\hbar}{i}\frac{\partial}{\partial x}$ . [1]
    - ii. Show that  $\langle x|p|\psi\rangle=\tilde{p}\psi(x)$ , where  $\psi(x)=\langle x|\psi\rangle$ . [2]
    - iii. Derive an expression for  $\langle x|xp|\psi\rangle$  in terms of  $\psi(x)$ . [2]
  - (d) i. Let A and B be two observables. Prove that the product AB can be written as AB = X + iY, where X and Y are Hermitian and are given by

$$X = \frac{1}{2}(AB + BA)$$
 and  $Y = \frac{1}{2i}[A, B]$ .

ii. Using the above result, show that the observables A and B satisfy the uncertainty relation

$$\Delta A \Delta B \ge \frac{|\langle [A,B] \rangle|}{2},$$

where  $\Delta M = \sqrt{\langle M^2 \rangle - \langle M \rangle^2}$  and  $\langle M \rangle = \langle \Psi | M | \Psi \rangle$ .

Hint: You may want to start your proof by defining two vectors  $|\phi_A\rangle = (A - \langle A\rangle) |\Psi\rangle$  and  $|\phi_B\rangle = (B - \langle B\rangle) |\Psi\rangle$  and considering the product  $\langle \phi_A | \phi_A \rangle \langle \phi_B | \phi_B \rangle$ . This is turn can be bound using, without proof, the Cauchy-Schwartz inequality  $|\langle \phi_1 | \phi_2 \rangle|^2 \leq \langle \phi_1 | \phi_1 \rangle \langle \phi_2 | \phi_2 \rangle$ .

PHASG426/2015

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# PHASM426 and PHASG426: Advanced Quantum Theory - Addendum

Correction to Q3 (c) The final part of this question should read as follows: Show that the probability (to second order) of finding the system in the state  $|n=2\rangle$  at  $\tau = \pi/2\omega$  is given by  $P_{n=2}^{(2)}(\tau = \pi/2) = 2A^4/\omega^4$ .