Theoretical Physics V

SS 2014 **23.4.2014**
Assignment II **Due date 30.4.2014**

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Problem 1 *Green's functions*

a) Green's function $G^+(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1)$ can be defined as the solution of the inhomogenous differential equation

$$\left(i\hbar\frac{\partial}{\partial t_2} - H(\mathbf{r}_2, t_2)\right) G^+(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) = i\hbar\delta(t_2 - t_1)\delta(\mathbf{r}_2 - \mathbf{r}_1),$$
$$G^+(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) = 0, \quad \text{for } t_2 < t_1. \tag{1}$$

Here $H(\mathbf{r}_2, t_2)$ is a Hamiltonian that acts on the position and time coordinates $\mathbf{r}_2, t_2$ and δ is the Dirac delta distribution. Show that the time evolution of the wave function can be written in the form

$$\psi(\mathbf{r}_2, t_2) = \int G^+(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1)\psi(\mathbf{r}_1, t_1)d\mathbf{r}_1, \quad \text{for } t_2 > t_1$$
$$\psi(\mathbf{r}, t_2)_{|t_2=t_1} = \psi(\mathbf{r}, t_1), \tag{2}$$

i.e., show that $\psi(\mathbf{r}_2, t_2)$ satisfies the Schrödinger equation with the correct boundary condition

$$i\hbar\frac{\partial}{\partial t_2}\psi(\mathbf{r}_2, t_2) = H(\mathbf{r}_2, t_2)\psi(\mathbf{r}_2, t_2), \quad \text{for } t_2 > t_1$$
$$\psi(\mathbf{r}, t_2)_{|t_2=t_1} = \psi(\mathbf{r}, t_1). \tag{3}$$

(0.75 points)
Hint: Show that $G^+(\mathbf{r}_2, t; \mathbf{r}_1, t) = \delta(\mathbf{r}_2 - \mathbf{r}_1)$. *Operate on Eq. (2) with* $i\hbar\frac{\partial}{\partial t_2} - H(\mathbf{r}_2, t_2)$.

b) Let $H = H_0 + H_1$ be a decomposition of the Hamiltonian into the sum of two operators. Show that Eq. (1) can be written as an integral equation

$$G^+(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) = G_0^+(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) - \frac{i}{\hbar}\int_{-\infty}^{\infty} G_0^+(\mathbf{r}_2, t_2; \mathbf{r}_3, t_3)H_1(\mathbf{r}_3, t_3)G^+(\mathbf{r}_3, t_3; \mathbf{r}_1, t_1)d\mathbf{r}_3 dt_3, \tag{4}$$

where $G_0^+(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1)$ satisfies the equations

$$\left(i\hbar\frac{\partial}{\partial t_2} - H_0(\mathbf{r}_2, t_2)\right) G_0^+(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) = i\hbar\delta(t_2 - t_1)\delta(\mathbf{r}_2 - \mathbf{r}_1),$$
$$G_0^+(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) = 0, \quad \text{for } t_2 < t_1. \tag{5}$$

The equation (4) can be used to develop time-dependent perturbation theory. *(0.75 points)*
Hint: Operate on Eq. (4) with $i\hbar\frac{\partial}{\partial t_2} - H_0(\mathbf{r}_2, t_2)$.

c) Show that for a time-independent Hamiltonian H the Green's function can be written in the form

$$G^{+}(\mathbf{r}_2, t_2; \mathbf{r}_1, t_1) = \sum_n \psi_n(\mathbf{r}_2)\psi_n^*(\mathbf{r}_1)e^{-\frac{i}{\hbar}E_n(t_2-t_1)}, \tag{6}$$

where E_n, ψ_n are the eigenenergies and eigenstates of H, respectively.
Hint: Write the wave function in the form $\psi(\mathbf{r}_2, t_2) = \sum_n c_n(t_2)\psi_n(\mathbf{r}_2)$, solve $c_n(t_2)$ by using Schrödinger equation and the orthonormality of $\{\psi_n\}$, and compare the result with Eq. (2). *(1 point)*

d) Calculate Green's function for a free particle (in the absence of external potential) in one dimension. Use Eq. (6) as a starting point and replace the sum $\sum_n(\dots)$ by an integral $C\int dp(\dots)$ for the continuum limit. You need to derive the correct prefactor C and evaluate the integral. *(1.5 points)*
Hint: Consider free-particle states that are normalized in the interval of length L, i.e., $\int_0^L \psi_n\psi_n dx$=1. Apply periodic boundary conditions $\psi_n(x=0) = \psi_n(x=L)$. Then let $L \to \infty$. Find the possible wave numbers $\dots, \frac{p_n}{\hbar}, \frac{p_{n+1}}{\hbar}, \dots$ and the difference between adjacent wave numbers to obtain C.

Problem 2 *Limitations of perturbation theory*

Quantum mechanical two-level system interacting with electromagnetic radiation can be described by the Hamiltonian

$$\hat{H} = \frac{\hbar}{2}\begin{pmatrix} -\omega_{10} & W_{01}e^{i\omega t} \\ W_{01}^* e^{-i\omega t} & \omega_{10} \end{pmatrix} \equiv \hat{H}_0 + \hat{V}_S,$$

with

$$\hat{H}_0 = \frac{\hbar}{2}\begin{pmatrix} -\omega & 0 \\ 0 & \omega \end{pmatrix}, \quad \hat{V}_S = \frac{\hbar}{2}\begin{pmatrix} \Delta & W_{01}e^{i\omega t} \\ W_{01}^* e^{-i\omega t} & -\Delta \end{pmatrix}, \quad \Delta \equiv \omega - \omega_{10}.$$

Here the state $|0\rangle$ ($|1\rangle$) has the energy $-\hbar\omega_{10}/2$ ($\hbar\omega_{10}/2$). The interaction strength between the two-level system and radiation is characterized by W_{01}, and ω is the frequency of the driving field. The frequency difference $\Delta \equiv \omega - \omega_{10}$ is called detuning frequency. In rotating frame (interaction picture), the state vector obeys the equation

$$i\hbar\frac{d}{dt}|\psi_I(t)\rangle = \hat{V}_I|\psi_I(t)\rangle,$$

where

$$\hat{V}_I = e^{\frac{i\hat{H}_0 t}{\hbar}}\hat{V}_S e^{\frac{-i\hat{H}_0 t}{\hbar}}$$

is the Hamiltonian in rotating frame.

a) Show that

$$|\langle 1|\psi_S(t)\rangle|^2 = |\langle 1|\psi_I(t)\rangle|^2.$$

Here $|\psi_S(t)\rangle$ is the state vector in Schrödinger picture. Using this identity makes calculating the transition probabilities more convenient. *(0.5 points)*

b) Calculate the eigenenergies E_+ and E_- of $\hat{V}_I$. *(0.5 points)*

c) Two arbitrary orthogonal states for the two-state system can be written in the form

$$|\psi_0\rangle = \cos\left(\tfrac{\theta}{2}\right) e^{-i\phi/2}|0\rangle + \sin\left(\tfrac{\theta}{2}\right) e^{i\phi/2}|1\rangle,$$
$$|\psi_1\rangle = -\sin\left(\tfrac{\theta}{2}\right) e^{-i\phi/2}|0\rangle + \cos\left(\tfrac{\theta}{2}\right) e^{i\phi/2}|1\rangle, \quad 0 \le \theta \le \pi, \quad 0 \le \phi < 2\pi.$$

Calculate $\sin\theta$ in terms of W_{01} and Δ when $|\psi_0\rangle$ and $|\psi_1\rangle$ are eigenstates of $\hat{V}_I$. *(1 point)*

d) Assuming the system is initially in the state $|\psi_I(t=0)\rangle = |0\rangle$, calculate the occupation probability of the state $|1\rangle$ at time t

$$P_1(t) = |\langle 1|\psi_S(t)\rangle|^2 = |\langle 1|\psi_I(t)\rangle|^2.$$

Express the result in terms of the model parameters W_{01} and Δ.
Hint: Use the eigenequations $\hat{V}_I|\psi_0\rangle = E_-|\psi_0\rangle$ and $\hat{V}_I|\psi_1\rangle = E_+|\psi_1\rangle$ to simplify the matrix exponentials and the result of item c). *(1 point)*

e) Calculate an approximation of $P_1(t)$ using time-dependent first order perturbation theory. Is there a parameter region where the result given by first order perturbation theory and the exact result (item d) coincide?

(0.5 points)

f) Calculate the transition rate $\frac{dP_1(t)}{dt}$ by using Fermi's golden rule. Is there a parameter region where the result given by Fermi's golden rule and the exact result coincide?

(0.5 points)

Problem 3 *Photoelectric effect*

Consider a hydrogen atom in its ground state placed in a light wave. If the wavelength of the light is much larger than the Bohr radius a, then the perturbation Hamiltonian depends only on the electric field at the location of the atom, which for plane polarization in the z direction takes the form

$$\mathbf{E}(t) = \mathcal{E}\exp(-i\omega t)\hat{z} + \mathcal{E}^*\exp(i\omega t)\hat{z}, \tag{7}$$

with $\mathcal{E}$ constant. The perturbation Hamiltonian is then $V(t) = e\mathbf{E}(t)\cdot\mathbf{X}$. Let us work out the ionization rate, i.e., the rate at which the monochromatic light field mediates a transition from a bounded to a free electronic state.

a) With the binding energy of the hydrogen atom and the recoil energy of the hydrogen nucleus neglected, the normalized wave functions for the ground and free electronic states are given by

$$\Psi_{1s}(\mathbf{x}) = \frac{\exp(-r/a)}{\sqrt{\pi a^3}}, \tag{8}$$

$$\Psi_e(\mathbf{x}) = \frac{\exp(i\mathbf{k}_e \cdot \mathbf{x})}{\sqrt{(2\pi\hbar)^3}}. \tag{9}$$

Find the matrix element of the perturbation Hamiltonian between these wave functions. *(2 point)*

b) Show that the differential ionization rate is given by

$$\frac{d\Gamma(1s \to e)}{d\Omega} = \frac{256 e^2 \mathcal{E}^2 m_e \cos^2\theta}{\pi \hbar^3 k_e^9 a^5}, \tag{10}$$

where m_e is the electron mass and θ is the angle between $\mathbf{k}_e$ and the light polarization direction (taken to be the z direction). *(2 point)*

Problem 4 *Irreversible decay*

Let us examine the problem of a single discrete state $|\phi_i\rangle$ resonantly coupled to a continuum of final states. The spectrum of the unperturbed Hamiltonian includes:

- a discrete, non-degenerate, state $|\phi_i\rangle$:

$$H_0 |\phi_i\rangle = E_i |\phi_i\rangle \tag{11}$$

- and a set of orthonormal states $|\alpha\rangle$ forming a continuum:

$$H_0 |\alpha\rangle = E |\alpha\rangle, \tag{12}$$

where $E \geq 0$ and each state of the continuum can be characterized by its energy and a set of parameters β, i.e., $|\alpha\rangle \equiv |\beta, E\rangle$. Assuming that the coupling Hamiltonian W has no diagonal elements and cannot couple two states of the continuum, the probability density for finding the system in ANY of the final states $|\alpha\rangle$ is found by integrating Fermi's Golden Rule over ALL final states, $\Gamma = \frac{2\pi}{\hbar} K(E = E_i)$, where

$$K(E) = \int d\beta \, |\langle \beta, E| W |\phi_i\rangle|^2 \rho(\beta, E), \tag{13}$$

and $\rho(\beta, E)$ is the density of final states.

a) The state at any time t can be expanded as

$$|\psi(t)\rangle = b_i(t)\, e^{-iE_i t/\hbar} |\phi_i\rangle + \int d\alpha \, b(\alpha, t)\, e^{-iEt/\hbar} |\alpha\rangle. \tag{14}$$

Using the assumptions above and as initial conditions $b_i(0) = 1$ and $b(\alpha, 0) = 0$, obtain an integrodifferential equation involving only b_i. *(1 point)*

b) For very short times, i.e., if $b_i(t) \simeq b_i(0)$, we can replace $b_i(t')$ by $b_i(0)$ inside the integral part of the equation found above. For this case, find the solution $b_i(t)$ and show that it contains real and imaginary parts. *(1 point)*

c) A better approximation consists of replacing $b_i(t')$ by $b_i(t)$ rather than by $b_i(0)$. Find the solution $b_i(t)$ in this case. *(1 point)*

d) Show that the probability of finding the system in the discrete state decays irreversibly approaching zero as $t \to \infty$ and that the coupling with the continuum is responsible for a shift in the discrete state energy. *(1 point)*