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PHS 4201: Advanced Quantum Mechanics II

Assignment #1

Time dependent systems, decay width, WKB approximation, scattering theory

Date: *19th March 2021*
Due : *04th April 2021*

Instructions

- You are free to discuss the questions among yourselves if you choose to do so. However, you should write the answers independently at the end and submit them. You should be prepared to explain the steps and arguments in your answer if called upon to do so.

- Interpret the questions as a physicist and make reasonable assumptions when required and mention them.

- Your answers can be brief and to the point, giving just the essential algebraic steps and arguments. The marks for each of the questions are given on the right end of the question, in square brackets and boldface. Total marks: **100**.

- I have tried to keep the questions clear, consistent with the notation used in the class and error-free. But if you have any difficulties on these counts, feel free to email me.

USEFUL MATHEMATICAL RESULTS

1 Consider the following differential equation:

$$y''(z) \pm ia\, z\, y'(z) + b\, y(z) = 0; \qquad a, b \in \mathbb{R}$$

The general solution to this equations can be written as:

$$y(z) = e^{\mp \frac{iaz^2}{4}} \left[A\, D_{\pm \frac{ib}{a}} \left(e^{\mp i \frac{\pi}{4}} \sqrt{a} z \right) + B\, D_{-1 \mp \frac{ib}{a}} \left(-e^{\pm i \frac{\pi}{4}} \sqrt{a} z \right) \right]$$

where, $D_\nu(x)$ denotes the parabolic cylinder function.

2 You might need the following properties of parabolic cylinder functions:

$$D_\nu \left(-\frac{e^{\pm i \frac{\pi}{4}} \sqrt{\alpha} t}{\sqrt{\hbar}} \right) \sim e^{\frac{i\alpha t^2}{2\hbar}} e^{\pm i \frac{\pi\nu}{4}} \left(\frac{|t| \sqrt{\alpha}}{\sqrt{\hbar}} \right)^\nu; \qquad t \to -\infty$$

$$D_\nu \left(\frac{-e^{\pm i \frac{\pi}{4}} \sqrt{\alpha} t}{\sqrt{\hbar}} \right) \sim e^{\frac{i\alpha t^2}{2\hbar}} e^{\mp i \frac{3\pi\nu}{4}} \left(\frac{t \sqrt{\alpha}}{\sqrt{\hbar}} \right)^\nu \mp \frac{i\sqrt{2\pi}}{\Gamma(-\nu)} e^{\mp i \frac{\pi}{4}(\nu - 1)} e^{-\frac{i\alpha t^2}{2\hbar}} \left(\frac{t\sqrt{\alpha}}{\sqrt{\hbar}} \right)^{-(\nu+1)}; \quad t \to \infty$$

$$\frac{d}{dz} \left(e^{\mp \frac{z^2}{4}} D_\nu(z) \right) = -e^{\mp \frac{z^2}{4}} D_{\nu \pm 1}(z)$$

3 For simplifying results in Qn. 1 (d), you might need the following identify:

$$\left| \frac{1}{\Gamma(1 + i\beta)} \right|^2 = \frac{1}{\Gamma(1 + i\beta)\Gamma(1 - i\beta)} = \frac{\sinh(\pi\beta)}{\pi\beta} \quad ; \qquad \beta \in \mathbb{R} \tag{1}$$

4 The following limit may be useful for Qn 2:

$$\lim_{\epsilon \to 0} \frac{1}{x + i\epsilon} = \text{Pr.} \left(\frac{1}{x} \right) - i\pi\delta(x)$$

where, Pr. denotes the principle value.

5 With suitable variable change, an integral required in Qn 3 can be evaluated using the following:

$$\int_{r_1}^{r_2} \frac{\sqrt{(r_1 - r)(r - r_2)}}{r} dr = \frac{\pi}{2} \left(-2\sqrt{r_1 r_2} + r_1 + r_2 \right); \qquad r_2 > r_1 > 0$$

6 The asymptotic expansion for Confluent Hypergeometric Function may be useful for Qn. 5(d):

$${}_1F_1(ia, 1, i\eta) = \frac{e^{-\frac{\pi}{2}a}}{\Gamma(ia)} \left[1 + \mathcal{O}(\eta^{-1}) \right] \frac{\eta^{ia} e^{i\eta}}{i\eta} + \frac{e^{-\frac{\pi a}{2}}}{\Gamma(1 - ia)} \left[1 + \frac{a^2}{i\eta} + \mathcal{O}(\eta^{-2}) \right] \eta^{-ia}; \qquad \eta \to \infty$$

where, a is a real constant.

QUESTIONS

1 Landau-Zener model: *In this question, we consider an exactly solvable, time-dependent two-state system. Assuming that the system is prepared in the ground state in the infinite past, the goal of this problem is to compute the probability of finding the system in the excited state in the infinite future. We will take a step-by-step approach; we will first consider a simple case and then progressively move to the exact solution.*

(a) The Hamiltonian of a certain time-dependent two-state quantum system is given by

$$\hat{H}_0(t) = \begin{bmatrix} \frac{1}{2}\alpha t & 0 \\ 0 & -\frac{1}{2}\alpha t \end{bmatrix} \tag{2}$$

where, $\alpha > 0$. **Find**:

(i) the instantaneous eigenvalues $E_g^{(0)}(t)$ and $E_e^{(0)}(t)$ of $\hat{H}_0(t)$, corresponding to the instantaneous ground state and excited state, respectively, for $t \neq 0$,

(ii) the solutions $|\psi_1(t)\rangle$ and $|\psi_2(t)\rangle$ of the time-dependent Schrödinger equation with the initial conditions $|\psi_1(0)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \equiv |1\rangle$ and $|\psi_2(0)\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \equiv |0\rangle$, respectively

(iii) the probability of finding the system in the instantaneous excited state at $t \to \infty$, if the system was initially in the instantaneous ground state at $t \to -\infty$. **[3]**

(b) Now, consider the scenario in which a time-independent potential is introduced into the system, so that the new Hamiltonian is given by

$$\hat{H}(t) = \hat{H}_0(t) + \begin{bmatrix} 0 & \epsilon \\ \epsilon & 0 \end{bmatrix} \tag{3}$$

where, ϵ is a positive real constant. Find the instantaneous eigenvalues $E_g^{(\epsilon)}(t)$ and $E_e^{(\epsilon)}(t)$ of $\hat{H}(t)$, corresponding to the instantaneous ground state and excited state, respectively. It is convenient to express a general time-dependent state $|\phi(t)\rangle$ of this system in the following form.

$$|\phi(t)\rangle = c_1(t)\,|\psi_1(t)\rangle + c_2(t)\,|\psi_2(t)\rangle \tag{4}$$

where, $c_{1,2}(t)$ are complex functions. In the adiabatic approximation, find the approximate expressions for $c_{1,2}(t)$, when the system is prepared in the instantaneous ground state at $t \to -\infty$. In this case, what is the probability of finding the system in the instantaneous excited state at $t \to \infty$? **[5]**

(c) Let us now look at the general case, where we do not impose adiabatic approximation. Show that the time-dependent Schrödinger equation implies the following coupled differential equations for the functions $c_{1,2}(t)$:

$$i\hbar \begin{bmatrix} \dot{c}_1 \\ \dot{c}_2 \end{bmatrix} = \begin{bmatrix} 0 & \epsilon e^{\frac{i\alpha t^2}{2\hbar}} \\ \epsilon e^{-\frac{i\alpha t^2}{2\hbar}} & 0 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} \tag{5}$$

where the over-dot denotes derivative with respect to time t. Take the time derivative of Eq.(5) and simplify to show that $c_{1,2}(t)$ satisfy the following uncoupled differential equations:

$$\ddot{c}_1 - \left(\frac{i\alpha t}{\hbar}\right)\dot{c}_1 + \left(\frac{\epsilon}{\hbar}\right)^2 c_1 = 0; \qquad \ddot{c}_2 + \left(\frac{i\alpha t}{\hbar}\right)\dot{c}_2 + \left(\frac{\epsilon}{\hbar}\right)^2 c_2 = 0 \tag{6}$$

If we had assumed that ϵ is a function of time, how would Eq.(5) and Eq.(6) modify?

[6]

(d) Let us once again restrict ourselves to the case of constant ϵ. Solve for the functions $c_{1,2}(t)$, corresponding to the initial condition that the system is prepared in the instantaneous ground state at $t \to -\infty$. In this case, what is the probability of finding the system in the instantaneous excited state at $t \to \infty$? In what limit does this result reduce to the probabilities computed in **(a)** and **(b)**.

[6]

2 Decay width: *In the presence of a perturbation, a system initially prepared in a given eigenstate of the unperturbed Hamiltonian will evolve to a state which is, in general, a linear combination of all the energy eigenstates. Therefore, in the infinite future, the probability to find the system in the initial eigenstate can be less that one.*

(a) Let us consider a system described by the following Hamiltonian:

$$\hat{H}(t) = \hat{H}_0 + \lambda e^{\eta t}\hat{V} \tag{7}$$

where, $\lambda \ll 1$. Therefore, $\hat{H}_0$ is the 'unperturbed' Hamiltonian and $\lambda e^{\eta t}\hat{V}$ is the perturbation. Let us denote the eigenstates and the corresponding eigenvalues of $\hat{H}_0$ by $|n\rangle$ and E_n, respectively, where $n = 0, 1, 2....$ Let $|\psi_n(t)\rangle_I$ denote the state ket in the interaction picture with the initial condition $|\psi_n(-\infty)\rangle_I = |n\rangle$. Show that, up to second order in λ, the amplitude $c_n(t) \equiv \langle n|\psi_n(t)\rangle_I$ is given by the following:

$$c_n(t) \approx 1 - \frac{i\lambda}{\hbar\eta}V_{nn}e^{\eta t} + \frac{1}{2}\left(\frac{-i\lambda}{\hbar\eta}\right)^2 |V_{nn}|^2 e^{2\eta t} + \left(\frac{-i\lambda^2}{\hbar}\right)\sum_{m\neq n}\frac{|V_{mn}|^2 e^{2\eta t}}{2\eta\left(E_n - E_m + i\hbar\eta\right)} \tag{8}$$

where, $V_{mn} \equiv \langle m|\hat{V}|n\rangle$ **[7]**

(b) Find the expression for $\frac{\dot{c}_n}{c_n}$, upto $\mathcal{O}(\lambda^2)$. Then evaluate the following limit

$$\lim_{\eta\to 0}\frac{\dot{c}_n}{c_n} \equiv \frac{-i}{\hbar}\Delta_n \tag{9}$$

Does Δ_n depend on time?

***(Caution**: You might want to look at item 3 of mathematical results given in the beginning)*

[4]

(c) Argue that, in the Schrödinger picture, we can write:

$$\langle n|\psi_n(t)\rangle = \langle n|\psi_n(0)\rangle\, e^{-\frac{i}{\hbar}(E_n+\Delta_n)t} \tag{10}$$

Further, show that the probability to find the system in $|n\rangle$, namely, $|\,\langle n|\psi_n(t)\rangle\,|^2$ decays with time as

$$|\,\langle n|\psi_n(t)\rangle\,|^2 \propto e^{-\gamma_n t}. \tag{11}$$

[3]

(d) The quantity $\Gamma_n \equiv \hbar\gamma_n$ is called the decay 'width'. To see why, first evaluate the following Fourier transform

$$f(E) \equiv \int_0^\infty \langle n|\psi_n(t)\rangle\, e^{\frac{i}{\hbar}Et} dt \tag{12}$$

Show that $|f(E)|^2$ is has a Lorentzian profile. What is the full width at half maximum (FWHM) of $|f(E)|^2$. **[4]**

(e) Let $\Delta t \equiv \gamma_n^{-1}$ denote the mean life time of the state $|n\rangle$ in the presence of the perturbation and ΔE denote the FWHM of $|f(E)|^2$. Find $\Delta t \Delta E$. What does the final result signify? **[2]**

3 WKB approximation: *When exact solutions are difficult or unavailable, the Schrödinger equation can be solved using WKB approximation. We will see some examples that illustrate the effectiveness of this approximation.*

(a) Consider a particle in a one-dimensional 'inverted' harmonic oscillator potential $V(x)$ given by:

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2(L^2 - x^2) & ; \quad x^2 < L^2 \\ 0 & ; \quad x^2 > L^2 \end{cases} \tag{13}$$

Find the WKB wavefunction corresponding to an energy E, such that $0 < E \ll (1/2)m\omega^2 L^2$. Assume that for $x \to -\infty$, the wavefunction has the form:

$$\psi(x) \propto e^{-\frac{i}{\hbar}px} \quad ; x \to -\infty \tag{14}$$

where p is a real constant. Find the reflection and transmission coefficients, in the WKB approximation. **[8]**

(b) **(i)** The radial part of the energy eigenfunction for an electron in Hydrogen atom (in the non-relativistic limit, neglecting spin) satisfies the following Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_\ell}{dr^2} + \left(-\frac{e^2}{r} + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)\psi_\ell = E\psi_\ell \tag{15}$$

Is the WKB approximation reliable near $r \to 0$ for this equation? Justify your answer. **[4]**

(ii) Let us define two news variables x and $\phi_\ell(x)$ as follows:

$$r = e^x \tag{16}$$

$$\phi_\ell(x) = e^{\frac{x}{2}}\psi_\ell(e^x) \tag{17}$$

Show that Eq.(15) can be rewritten as

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_\ell}{dx^2} + V_{\ell,E}(x)\phi_\ell(x) = 0 \tag{18}$$

where, $V_{\ell,E}(x)$ is a real function. Is the WKB approximation reliable near $x \to -\infty$ for this equation. Use the WKB quantization condition for bound states to determine the energy levels of Hydrogen atom. How does this compare with the exact result? **[8]**

4 Green's function: *A general solution to the time-independent Schrödinger equation for a particle in a potential can be formally written in terms of the appropriate Green's function $G(\mathbf{r};\mathbf{r}')$ and a solution of the free-particle Schrödinger equation $\psi_0(\mathbf{r})$. Hence, Green's functions are very useful mathematical tools in quantum mechanics.*

(a) The Green's function for the free-particle Schrödinger equation is defined by the following differential equation:

$$\left(\nabla^2 + k^2\right) G(\mathbf{r}) = \delta^3(\mathbf{r}) \tag{19}$$

where, $k = \hbar^{-1}\sqrt{2mE}$ and E is the energy. Show that the wavefunction $\psi(\mathbf{r})$, given by

$$\psi(\mathbf{r}) = e^{i\mathbf{k}.\mathbf{r}} + \int G(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')\,\psi(\mathbf{r}')\,d^3\mathbf{r}' \tag{20}$$

where $|\mathbf{k}| = k$, satisfies the time-independent Schrödinger equation for a particle in the potential $V(\mathbf{r})$, with energy $E = \frac{\hbar^2}{2m}k^2$. **[5]**

(b) Let us define the Fourier transform of $G(\mathbf{r})$ via:

$$\tilde{G}(\mathbf{q}) = \int e^{-i\mathbf{q}.\mathbf{r}}G(\mathbf{r})d^3\mathbf{r} \tag{21}$$

Show that Eq.(19) implies that $\tilde{G}(\mathbf{q})$ is given by

$$\tilde{G}(\mathbf{q}) = \frac{1}{k^2 - q^2} \tag{22}$$

where $q = |\mathbf{q}|$. **[5]**

(c) Show that the Green's function can be written as:

$$G(\mathbf{r}) = \frac{1}{4\pi^2 r} \int_{-\infty}^{\infty} \frac{q\sin(qr)}{k^2 - q^2} dq \tag{23}$$

where $r = |\mathbf{r}|$. **[5]**

(d) Notice that the integrand in the right-hand-side of Eq.(23) has two simple poles, at $q = \pm k$. Hence, we need a prescription to 'go around' the poles while performing the q integration. Independently evaluate $G(\mathbf{r})$ using the following two prescriptions for deforming the original real line integration contour:

(i) go around the poles at $q = -k$ *above* the real axis, while for the pole at $q = k$, go around *below* the real axis

(ii) evade both the poles by going around *above* the real axis.

Let us denote the Green's functions hence obtained as $G_{\text{(i)}}(\mathbf{r})$ and $G_{\text{(ii)}}(\mathbf{r})$, respectively. Are there any other prescriptions which are linearly independent to $G_{\text{(i)}}(\mathbf{r})$ and $G_{\text{(ii)}}(\mathbf{r})$? **[5]**

5 Scattering amplitude and cross-section: *One of the most efficient ways of understanding fundamental interactions experimentally is by studying scattering processes. Specifically, the scattering cross-section is often the most convenient quantity that we can 'observe' and hence, is a concept of great significance in physics.*

(a) The scattering amplitude, in a spherically symmetric potential $V(r)$, in the first-order Born approximation is given by

$$f(\theta) = -\frac{2m}{\hbar^2\kappa} \int_0^{\infty} rV(r)\sin(\kappa r)dr \quad ; \quad \text{(1st order Born approx.)} \tag{24}$$

where, $\kappa = 2k\sin(\theta/2)$ and the energy is given by $E = \hbar^2 k^2/2m$. It is convenient to define the Fourier transform of a potential $V(\mathbf{r})$ as follows:

$$\tilde{V}(\mathbf{q}) = \int e^{i\mathbf{q}.\mathbf{r}} V(\mathbf{r}) d^3\mathbf{r} \tag{25}$$

Show that the scattering amplitude can be rewritten in the following way:

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \tilde{V}(\mathbf{k}_i - \mathbf{k}_s) \tag{26}$$

where, $\hbar\mathbf{k}_i$ corresponds to the momentum of an incident particle, while $\hbar\mathbf{k}_s$ corresponds to that of a scattered particle. **[5]**

(b) Let us consider the special case of a Yukawa potential, which is defined as

$$V_Y(r) = \beta \frac{e^{-\mu r}}{r} \tag{27}$$

where, β and μ are constants. This potential can be used to approximately describe nuclear binding force. Show that the scattering amplitude, in the Born approximation, for this potential is given by

$$f(\theta) = -\frac{2m\beta}{\hbar^2(\mu^2 + \kappa^2)} \tag{28}$$

Find the differential and total cross sections. **[5]**

(c) Let us now consider the Coulomb potential, defined as:

$$V_C = \frac{e_i e_s}{r^2} \tag{29}$$

where e_i and e_s are, respectively, the charges of the incident particle and the scatterer. What is the scattering amplitude in this case? Also, find the differential cross-section. How does your final result compare with that of classical Rutherford scattering? **[2]**

(d) It turns out that the *exact* wavefunction describing the scattering of particles incident along a given direction, say the negative z-axis, to a scatterer at the origin can be solve in the case of Coulomb potential. This solution is given by:

$$\psi(\mathbf{r}) = e^{-\frac{\pi}{\xi}}\Gamma(1 + i\xi)e^{ikz}\ {}_1F_1(-i\xi, 1, ik(r - z)) \tag{30}$$

where, ${}_1F_1(a, b, z)$ denotes the Confluent Hypergeometric function and $\xi = \left(\frac{me_ie_s}{\hbar^2 k}\right)$. Show that the asymptotic expansion of $\psi(\mathbf{r})$, for $r \to \infty$ gives

$$\psi(\mathbf{r}) = \left[1 + \frac{\xi^2}{ikr(\cos\theta)}\right] e^{ikz + i\xi\log(kr - kr\cos\theta)} + \frac{f_{\text{ex}}(\theta)}{r}e^{ikr - i\xi\log(2kr)} + \mathcal{O}(r^{-2}) \tag{31}$$

Therefore, $f_{\text{ex}}(\theta)$ can be read off as the *exact* scattering amplitude in the Coulomb potential. Find the corresponding differential cross-section. How does your result compare with that in part **(c)** and the classical Rutherford scattering? **[8]**