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Exam in TFY4205 Quantum Mechanics

December 4, 2009
09:00–13:00

Allowed help: Alternativ C
Approved calculator
K. Rottman: *Matematisk formelsamling*
Barnett and Cronin: *Mathematical formulae*

Some relations that might be useful are given at the end of this exam.

This problem set consists of 9 pages.

Problem 1. Time-dependent perturbation theory

Consider the initially unperturbed system described by the Hamiltonian $H_0(\vec{r})$, and the stationary, orthonormal eigenstates $\Psi_n^0(\vec{r},t)$:

$$\Psi_n^0(\vec{r},t) = \psi_n(\vec{r})\mathrm{e}^{-\mathrm{i}E_n t/\hbar}, \tag{1}$$

where

$$H_0(\vec{r})\psi_n(\vec{r}) = E_n\psi_n(\vec{r}). \tag{2}$$

We introduce the time-dependent perturbation $V(\vec{r},t)$, so that the total Hamiltonian is

$$H(\vec{r},t) = H_0(\vec{r}) + V(\vec{r},t). \tag{3}$$

a) We let $\Psi(\vec{r},t)$ be eigenstates of the total Hamiltonian $H(\vec{r},t)$, and expand them in terms of the known stationary states:

$$\Psi(\vec{r},t) = \sum_k a_k(t)\Psi_k^0(\vec{r},t). \tag{4}$$

What is the physical interpretation of the expansion coefficients $a_k(t)$?

Solution: $a_k(t)$ is the probability ampitude for finding the system in the state $\Psi_k^0(\vec{r},t)$ at time t. The probability of finding the system in the state k at time t is given by

$$P_k(t) = |a_k(t)|^2.$$

In the rest of this problem, we will restrict ourselves to first-order time-dependent perturbation theory. If we assume that our unperturbed system was in the state described by $\Psi_i^0(\vec{r},t)$ at $t \to -\infty$, one can show that

$$a_n(t) = \delta_{n,i} + \frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t} \mathrm{d}t'\, V_{ni}(t')\mathrm{e}^{\mathrm{i}\omega_{ni}t'}, \tag{5}$$

where

$$V_{ni}(t) = \int \mathrm{d}\vec{r}\ (\psi_n(\vec{r}))^* V(\vec{r},t)\psi_i(\vec{r}) = \langle n|V(\vec{r},t)|i\rangle, \tag{6a}$$

and

$$\omega_{ni} = \frac{E_n - E_i}{\hbar}. \tag{6b}$$

b) Consider an electron, moving in the x-direction, in a one dimensional harmonic oscillator potential:

$$H_0(x) = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{7}$$

The electron is in the ground state at $t \to -\infty$. The electron is then subject to a time-dependent electric field $\mathcal{E}(t)$, so that the perturbation reads

$$V(x,t) = -e\mathcal{E}(t)x = e\mathcal{E}_0 x \mathrm{e}^{-t^2/\tau^2}. \tag{8}$$

In which excited states is it possible to find the electron as $t \to +\infty$?

Solution: We introduce the ladder operators

$$x = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right),$$

and write

$$V_{n,i=0}(t) = \langle n|V(x,t)|0\rangle = -e\mathcal{E}(t)\sqrt{\frac{\hbar}{2m\omega}}\langle n|\hat{a} + \hat{a}^\dagger|0\rangle = -e\mathcal{E}(t)\sqrt{\frac{\hbar}{2m\omega}}\delta_{n,1}.$$

Thus, to first order in V, the only non-zero expansion coefficients are $a_0(t)$ and $a_1(t)$, and the only possible excited state is the *first* excited state $|1\rangle$.

c) Show that the probability P of finding the electron in an excited state as $t \to +\infty$ can be written

$$P = \frac{\pi e^2 \mathcal{E}_0^2 \tau^2}{2m\hbar\omega}\exp\left(-\frac{\omega^2\tau^2}{2}\right). \tag{9}$$

You might find the following integral useful:

$$\int_{-\infty}^{\infty} \mathrm{d}t \exp\left(-\frac{t^2}{\tau^2} + \mathrm{i}\omega t\right) = \tau\sqrt{\pi}\exp\left[-\left(\frac{\omega\tau}{2}\right)^2\right].$$

Solution: Since the only possible excited state is the first excited one, P is given by

$$P = |a_1(\infty)|^2 = \frac{e^2\mathcal{E}_0^2}{2m\hbar\omega}\left|\int_{-\infty}^{\infty} \mathrm{d}t' \exp\left(-\frac{t'^2}{\tau^2} + \mathrm{i}\omega t'\right)\right|^2,$$

where we have used that $\omega_{10} = (E_1 - E_0)/\hbar = \omega$. Making use of the integral given in the text, we obtain the desired expression for P.

d) How should we choose τ in order to maximize the transition probability? Call the maximum transition probability $P_{\max}$, and derive an expression for $P_{\max}$.

Solution: We consider the partial derivative:

$$\left.\frac{\partial P}{\partial \tau}\right|_{\tau=\tau_m} = 0 = \frac{\pi e^2 \mathcal{E}_0^2}{2m\hbar\omega} \exp\left[-\frac{\omega^2\tau_m^2}{2}\right](2\tau_m - \tau_m^3\omega^2).$$

Setting the final parenthesis to zero yields

$$\tau_m = \frac{\sqrt{2}}{\omega}.$$

Thus, the maximum transition probability is

$$P_{\max} = \frac{\pi e^2 \mathcal{E}_0^2 \tau_m^2}{2m\hbar\omega} \exp\left[-\frac{\omega^2\tau_m^2}{2}\right] = \frac{\pi e^2 \mathcal{E}_0^2}{m\hbar\omega^3} \exp(-1).$$

e) What happens to $P_{\max}$ when $\mathcal{E}_0$, the amplitude of the electric field, is increased towards $+\infty$? Derive an expression describing the validity of $P_{\max}$.

(*Comment:* If you did not find an expression for $P_{\max}$ in 1 **d)**, you can solve this problem by instead using P from Eq. (9), with τ as a positive constant.)

Solution: This is only first-order perturbation theory, so we demand that the transition probability is much smaller than unity, *i.e.* we demand that $P_{\max} \ll 1$. Using this restriction, we must have

$$\frac{\pi e^2 \mathcal{E}_0^2 \hbar^2}{m} \exp(-1) \ll (\hbar\omega)^3,$$

for $P_{\max}$ to be valid.

Problem 2. Scattering theory

In this problem we will consider a three dimensional stationary scattering problem, described by the stationary Schrödinger equation

$$\left(\nabla^2 + k^2\right)\psi(\vec{r}) = U(\vec{r})\psi(\vec{r}), \tag{10}$$

where $k = \sqrt{2mE/\hbar^2}$ and $U(\vec{r}) = 2mV(\vec{r})/\hbar^2$. This equation describes a particle of mass m and energy E that scatters at the potential $V(\vec{r})$, that we take to be at rest at the origin. At large (asymptotic) distances, the wave function of the particle is

$$\psi(\vec{r}) \simeq \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} + f(\vartheta,\varphi)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}, \tag{11}$$

where $f(\vartheta,\varphi)$ is the scattering amplitude.

a) Give a physical definition of the differential and the total scattering cross section, and write down how these quantities are related to the scattering amplitude $f(\vartheta,\varphi)$ (no derivations are required).

Solution: The number of particles scattered into the angular element $\mathrm{d}\Omega$ must be proportional to the incoming particle current density j_{inc} as well as the size of $\mathrm{d}\Omega$ itself. The differential scattering cross section is defined as the constant of proportionality:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\text{number of particles scattered into } \mathrm{d}\Omega \text{ per unit time}}{\mathrm{d}\Omega j_{\mathrm{inc}}}.$$

The number of particles scattered *out* in $\mathrm{d}\Omega$ per unit time, equals the number of incoming particles passing through the area $\mathrm{d}\sigma$ per unit time. The total cross section is obtained if we integrate the differential cross section over all scattering angles:

$$\sigma = \int \mathrm{d}\Omega \, \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}.$$

The total number of particles scattered by the potential (in any direction), equals the number of incoming particles passing through the cross section σ of the incoming particle beam. The relation between the scattering amplitude and the cross section is

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\vartheta, \varphi)|^2 .$$

In the first Born approximation, the scattering amplitude is

$$f^B(\vartheta, \varphi) = -\frac{1}{4\pi} \int \mathrm{d}\vec{r}\,' \, \mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}\,'} U(\vec{r}\,'), \tag{12}$$

where $\vec{q} = \vec{k}' - \vec{k} = k\vec{r}/r - \vec{k}$.

b) Consider the spherically symmetric potential described by

$$V_{\mathrm{S}}(r) = \frac{V_0 \mathrm{e}^{-\lambda r}}{\lambda r}, \tag{13}$$

where λ^{-1} characterizes the range of the potential. Use the first Born approximation to find an expression for the scattering amplitude, and show that the differential scattering cross section for this potential can be written

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{2mV_0}{\lambda\hbar^2}\right)^2 \frac{1}{\left(\lambda^2 + q^2\right)^2}, \tag{14}$$

where $q = 2k \sin\theta/2$.

Solution: V_{S} is the Yukawa potential, a screened Coulomb potential. We let $\vec{q}$ point along the z-direction, so that $\vec{q}\cdot\vec{r}' = qr'\cos\theta$. We get

$$f^B(\vartheta) = -\frac{mV_0}{2\pi\lambda\hbar^2}\int \mathrm{d}\vec{r}'\,\mathrm{e}^{-\mathrm{i}\vec{q}\cdot\vec{r}'}\frac{\mathrm{e}^{-\lambda r'}}{r'} = -\frac{mV_0}{\lambda\hbar^2}\int_0^{\pi}\mathrm{d}\theta\,\sin\theta\int_0^{\infty}\mathrm{d}r'\,r'\mathrm{e}^{-\mathrm{i}qr'\cos\theta}\mathrm{e}^{-\lambda r'}.$$

We use that

$$\int_0^{\pi}\mathrm{d}\theta\,\sin\theta\mathrm{e}^{-\mathrm{i}qr'\cos\theta} = \frac{2\sin(qr')}{qr'},$$

and

$$\int_0^{\infty}\mathrm{d}r'\,\sin(qr')\mathrm{e}^{-\lambda r'} = \frac{q}{\lambda^2+q^2},$$

and obtain

$$f^B(\vartheta) = -\frac{2mV_0}{\lambda\hbar^2\left(\lambda^2+q^2\right)},$$

with $q = 2k\sin\frac{\vartheta}{2}$. The differential cross section reads

$$\left(\frac{\mathrm{d}\sigma^B}{\mathrm{d}\Omega}\right)_{\mathrm{S}} = \left(\frac{2mV_0}{\lambda\hbar^2}\right)^2\frac{1}{\left(\lambda^2+q^2\right)^2}.$$

c) The Coulomb potential is

$$V_{\mathrm{C}}(r) = \frac{ZZ'e^2}{4\pi\epsilon_0 r}. \tag{15}$$

Use the result from **b)** to find the differential scattering cross section for the potential V_{C}.

Solution: We let $\lambda\to 0$, while we take $V_0/\lambda \to ZZ'e^2/(4\pi\epsilon_0)$, and find

$$\left(\frac{\mathrm{d}\sigma^B}{\mathrm{d}\Omega}\right)_{\mathrm{C}} = \left(\frac{ZZ'e^2}{16\pi\epsilon_0 E}\right)^2\frac{1}{\sin^4\frac{\vartheta}{2}},$$

which is the (hopefully) well-known differential scattering cross section for the Coulomb potential.

d) The Born approximation is valid if the following inequality holds:

$$\int_0^{\infty}\mathrm{d}r'\,r'|U(r')| \ll 1. \tag{16}$$

The potential V_{S} is strong enough to form a bound state if

$$\frac{2m|V_0|}{\lambda^2\hbar^2} \geq 2.7\,. \tag{17}$$

Discuss the validity of the Born approximation for the potential V_{S} based on the requirement in Eq. (16) and the condition in Eq. (17)! Is the first Born approximation valid for the potential V_{C}?

Solution: From the requirement in Eq. (16), we find for V_S the following condition:

$$\frac{2m|V_0|}{\lambda^2\hbar^2} \ll 1.$$

This agrees with the observation made during the lectures, that the first Born approximation may be used if the potential is not strong enough to form bound states. The situation is different for the Coulomb potential, however, because the integral in Eq. (16) diverges when V_C is used. Thus, the condition for validity of the first Born approximation is not fulfilled. However, the first Born approximation gives the correct result for the differential scattering cross section, a fact that must be considered a lucky coincidence (f^B differs from the exact scattering amplitude by a complex phase factor; a factor that is important for scattering of identical particles, but not for potential scattering that is considered in this problem).

Problem 3. Quantization of the Electromagnetic Fields

The Hamiltonian for the electromagnetic field in vacuum is

$$H = \frac{1}{2}\int d^3r\,(\mathbf{E}\cdot\mathbf{D} + \mathbf{B}\cdot\mathbf{H})\,. \tag{18}$$

We choose the Coulomb gauge, $\boldsymbol{\nabla}\cdot\mathbf{A} = 0$, where $\mathbf{A}$ is the electromagnetic vector potential. The electromagnetic fields can be expressed in terms of the electromagnetic vector potential as

$$\begin{aligned}
\mathbf{B} &= \boldsymbol{\nabla}\times\mathbf{A},\\
\mathbf{H} &= \mathbf{B}/\mu_0,\\
\mathbf{E} &= -\frac{\partial\mathbf{A}}{\partial t},\\
\mathbf{D} &= \varepsilon_0\mathbf{E},
\end{aligned}$$

where ε_0 is the dielectricity constant and μ_0 is the magnetic permeability that are related by the velocity of light $c^2 = (\mu_0\varepsilon_0)^{-1}$. The Hamiltonian for the electromagnetic field can then be expressed in terms of the electromagnetic vector potential as

$$H = \frac{\varepsilon_0 c^2}{2}\int d^3r\left[\left(\frac{\partial\mathbf{A}}{\partial ct}\right)^2 + (\boldsymbol{\nabla}\times\mathbf{A})^2\right].$$

The electromagnetic field can be quantized and expressed as

$$\hat{\mathbf{A}}(r,t) = \sum_{\mathbf{k}\lambda}\mathbf{e}_{\mathbf{k}\lambda}\sqrt{\frac{\hbar}{2\varepsilon_0 Vck}}\left[a_{\mathbf{k}\lambda}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)} + a^\dagger_{\mathbf{k}\lambda}e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}\right], \tag{19}$$

where λ denotes the two polarization directions ($\lambda = 1$ or $\lambda = 2$) , $\mathbf{e}_{\mathbf{k},\lambda}$ is the polarization vector, and $\mathbf{k}$ is the wavevector. The operator $a_{\mathbf{k},\lambda}$ satisfies

$$\left[a_{\mathbf{k}\lambda}, a^\dagger_{\mathbf{k}'\lambda'}\right] = \delta_{\mathbf{k}\lambda,\mathbf{k}'\lambda'}.$$

The polarization vectors satisfy

$$\begin{aligned}
\mathbf{e}_{\mathbf{k}\lambda} \cdot \mathbf{e}_{\mathbf{k}\lambda'} &= \delta_{\lambda\lambda'}, \\
\mathbf{e}_{\mathbf{k}\lambda} \cdot \mathbf{k} &= 0, \\
\mathbf{e}_{\mathbf{k}1} \cdot \mathbf{e}_{\mathbf{k}1} &= 1, \\
\mathbf{e}_{\mathbf{k}2} \cdot \mathbf{e}_{\mathbf{k}2} &= -1.
\end{aligned}$$

a) Using the expression for the electromagnetic vector potential (19), the Hamiltonian can be written as

$$H = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}} \left(a^{\dagger}_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} + \frac{1}{2} \right),$$

where $\omega_{\mathbf{k}} = ck$. What are the physical interpretations of the quantitites $\hbar\omega_{\mathbf{k}}$, $a_{\mathbf{k}\lambda}$, $a^{\dagger}_{\mathbf{k}\lambda}$, and $a^{\dagger}_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda}$?

Solution: $a_{\mathbf{k}\lambda}$ ($a^{\dagger}_{\mathbf{k}\lambda}$) annihilates (creates) a photon with wave vector $\mathbf{k}$ and polarization λ, $a^{\dagger}_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda}$ is the number of photons with wave vector $\mathbf{k}$ and polarization λ and $\hbar\omega_{\mathbf{k}}$ is the energy of these photons.

b) Explicitly demonstrate that the Hamiltonian (18) can be written as

$$H = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}\lambda} \left(a^{\dagger}_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} + \frac{1}{2} \right).$$

Solution:
We first compute

$$(\boldsymbol{\nabla}\times\mathbf{A}) = i\sum_{\mathbf{k}\lambda}(\mathbf{e}_{\mathbf{k}\lambda}\times\mathbf{k})\sqrt{\frac{\hbar}{2\varepsilon_0 Vck}}\left[a_{\mathbf{k}\lambda}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)} - a^\dagger_{\mathbf{k}\lambda}e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}\right]$$

and

$$\left(\frac{\partial\mathbf{A}}{\partial ct}\right) = -i\sum_{\mathbf{k}\lambda}\mathbf{e}_{\mathbf{k}\lambda}\frac{\omega_k}{c}\sqrt{\frac{\hbar}{2\varepsilon_0 Vck}}\left[a_{\mathbf{k}\lambda}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)} - a^\dagger_{\mathbf{k}\lambda}e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}\right]$$

Second, we use

$$\int d^3r\left[a_{\mathbf{k}\lambda}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)} - a^\dagger_{\mathbf{k}\lambda}e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}\right]\left[a_{\mathbf{k}'\lambda'}e^{i(\mathbf{k}'\cdot\mathbf{r}-\omega_{k'} t)} - a^\dagger_{\mathbf{k}'\lambda'}e^{-i(\mathbf{k}'\cdot\mathbf{r}-\omega_{k'} t)}\right] = \tag{20}$$

$$-V\delta_{\mathbf{k},\mathbf{k}'}\left[a_{\mathbf{k}\lambda}a^\dagger_{\mathbf{k}\lambda} + a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda}\right] + V\delta_{\mathbf{k},-\mathbf{k}'}\left[a_{\mathbf{k}\lambda}e^{-2i\omega_k t}a_{-\mathbf{k}\lambda'} + a^\dagger_{\mathbf{k}\lambda}a^\dagger_{-\mathbf{k}\lambda'}e^{2i\omega_k t}\right] \tag{21}$$

where V is the volume of the system. Thirdly, we need

$$\begin{aligned}(\mathbf{e}_{\mathbf{k}\lambda}\times\mathbf{k})\cdot\left(\mathbf{e}_{\pm\mathbf{k}\lambda'}\times(\pm\mathbf{k})\right) &= \pm\left(\mathbf{e}_{\mathbf{k}\lambda}\cdot\mathbf{e}_{\pm\mathbf{k}\lambda'}\right)(\mathbf{k}\cdot\mathbf{k}) \mp (\mathbf{e}_{\mathbf{k}\lambda}\cdot\mathbf{k})\left(\mathbf{k}\cdot\mathbf{e}_{\pm\mathbf{k}\lambda'}\right)\\ &= \pm k^2\left(\mathbf{e}_{\mathbf{k}\lambda}\cdot\mathbf{e}_{\pm\mathbf{k}\lambda'}\right)\end{aligned}$$

We then find

$$\begin{aligned}\frac{\varepsilon_0 c^2}{2}\int d^3r\left[\left(\frac{\partial\mathbf{A}}{\partial ct}\right)^2 + (\boldsymbol{\nabla}\times\mathbf{A})^2\right] &= \frac{\varepsilon_0 c^2}{2}\sum_{\mathbf{k}\lambda}\frac{\hbar}{2\varepsilon_0 Vck}2Vk^2\left[a_{\mathbf{k}\lambda}a^\dagger_{\mathbf{k}\lambda} + a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda}\right]\\ &= \sum_{\mathbf{k}\lambda}\hbar ck\left[a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda} + \frac{1}{2}\right]\\ H &= \sum_{\mathbf{k}\lambda}\hbar\omega_k\left[a^\dagger_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda} + \frac{1}{2}\right]\end{aligned}$$

as we should demonstrate.

Some potentially useful relations

Harmonic oscillator

The Hamiltonian of a one dimensional harmonic oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right), \tag{22}$$

where the ladder operators are defined as

$$a = \sqrt{\frac{m\omega}{2\hbar}}q + \frac{\mathrm{i}}{\sqrt{2m\hbar\omega}}p, \quad \text{and} \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}q - \frac{\mathrm{i}}{\sqrt{2m\hbar\omega}}p.$$

This is equivalent to

$$q = \sqrt{\frac{\hbar}{2m\omega}}\left(a^\dagger + a\right), \quad \text{and} \quad p = \mathrm{i}\sqrt{\frac{m\hbar\omega}{2}}\left(a^\dagger - a\right).$$

The ladder operators satisfy

$$\left[a, a^\dagger\right] = 1,$$

and

$$a|n\rangle = \sqrt{n}|n-1\rangle,$$
$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle,$$

where $|n\rangle$ are the orthonormalized eigenstates of H in Eq. (22):

$$H|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle = E_n|n\rangle.$$

Vector algebra

For the vectors $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and $\mathbf{D}$, this holds

$$(\mathbf{A}\times\mathbf{B})\cdot(\mathbf{C}\times\mathbf{D}) = (\mathbf{A}\cdot\mathbf{C})(\mathbf{B}\cdot\mathbf{D}) - (\mathbf{A}\cdot\mathbf{D})(\mathbf{B}\cdot\mathbf{C}).$$