22.51 Quantum Theory of Radiation Interactions

Final Exam

December 19, 2011 Solution

Problem 1: Rutherford Scattering *35 points*

100 years ago, in 1911, Rutherford explained the observed surprising behavior of alpha particles scattering from a gold foil, leading to the discovery of the nucleus. In this problem we want to derive from quantum-mechanics scattering theory the expression for Rutherford cross-section for electrons.

The system is described by an electron and a nucleus, for convenience enclosed in a cavity of volume $V = L^3$. The interaction between the electron and the nucleus is the Coulomb interaction between the electron and the Z protons in the nucleus.

You can use the following steps to calculate the scattering cross section $d\sigma = \frac{W_{fi}}{\Phi_{inc}}$, with $W_{fi} = \frac{2\pi}{\hbar}|\langle f|T|i\rangle|^2\rho(E_f)$, where T is the transition matrix and $\rho(E_f)$ the final density of states.

a) *Assume the electron energy is very large, so that $v_e \approx c$ and $pc \gg m_e c^2$. What is the flux of incoming electrons and the density of states of the outgoing electrons?*

Solution:

$$\Phi_{inc} = v_e/L^3 \approx c/L^3$$

and setting $E' = \sqrt{p'^2c^2 + m_e^2c^4} \approx p'c$, we have

$$\rho(E') = \left(\frac{L}{2\pi\hbar}\right)^3 p'^2 \frac{d\,p'}{d\,E'}d\Omega = \left(\frac{L}{2\pi\hbar}\right)^3 \frac{E'^2}{c^3}d\Omega$$

b) *The interaction Hamiltonian is given by $V = e\varphi(\vec{r})$, where φ is the scalar potential given by the charge distribution $Ze\rho_e(\vec{r})$ of the nucleus via the equation $\nabla^2\varphi(\vec{r}) = -Ze\rho_e(\vec{r})/\epsilon_0$. The initial and final state of the electron can be described by a plane wave, normalized to the cavity volume.*

What is the transition matrix element $|\langle f|T|i\rangle|^2$ to lowest order?

[Note: here you can assume that the nucleus does not change its state, so we can neglect it altogether in the calculation and consider its effects indirectly, through the potential V acting only on the electron]

Solution:

The electron initial state is $|p\rangle = \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{\sqrt{L^3}}$ and its final state $|p'\rangle = \frac{e^{i\vec{p}'\cdot\vec{r}/\hbar}}{\sqrt{L^3}}$. Thus we have:

$$\langle f|T|i\rangle = \langle p'|e\varphi(\vec{r})|p\rangle = \frac{e}{L^3}\int_V e^{-i\vec{p}'\cdot\vec{r}/\hbar}\varphi(\vec{r})e^{i\vec{p}\cdot\vec{r}/\hbar}d^3r = \frac{e}{L^3}\int_V e^{i\vec{q}\cdot\vec{r}/\hbar}\varphi(\vec{r})d^3r$$

with $\vec{q} = \vec{p} - \vec{p}'$.

d) *Use Green's theorem, $\int d^3r\,(u\nabla^2v - v\nabla^2u) = 0$ (with $u = e^{i\vec{q}\cdot\vec{r}/\hbar}$ and $v = \varphi(\vec{r})$) to give the transition matrix a simple physical interpretation as the Fourier Transform of a physical quantity.*

What information can then be gathered from a Rutherford scattering experiment? How does this relate to the discovery of the nucleus?

Solution:

From the properties of the exponential, we have $\vec{\nabla}e^{i\vec{q}\cdot\vec{r}/\hbar} = i\vec{q}/\hbar e^{i\vec{q}\cdot\vec{r}/\hbar}$ and $\nabla^2e^{i\vec{q}\cdot\vec{r}/\hbar} = -|\vec{q}|^2/\hbar^2e^{i\vec{q}\cdot\vec{r}/\hbar}$.

Inserting this in the integral $\int_V e^{i\vec{q}\cdot\vec{r}/\hbar}\varphi(\vec{r})d^3r$, we have

$$\langle f|\, T\,|i\rangle = -\frac{e\hbar^2}{L^3|\vec{q}|^2}\int_V \varphi(\vec{r})\nabla^2 e^{i\vec{q}\cdot\vec{r}/\hbar} = \frac{e\hbar^2}{L^3|\vec{q}|^2}\int_V e^{i\vec{q}\cdot\vec{r}/\hbar}\nabla^2\varphi(\vec{r})$$

Using then the definition of the potential, we have

$$\langle f|\, T\,|i\rangle = -\frac{Ze^2\hbar^2}{\epsilon_0 L^3|\vec{q}|^2}\int_V e^{i\vec{q}\cdot\vec{r}/\hbar}\rho_e(\vec{r}) = -\frac{Ze\hbar^2}{\epsilon_0 L^3|\vec{q}|^2}F(\vec{q})$$

Thus we found that the transition matrix is proportional to the Fourier Transform of the charge distribution. $F(\vec{q})$ is called the *form factor* of the charge distribution.

Performing a scattering experiment varying $\vec{q}$ (varying the electron energy and as we will see below, the scattering angle) one can thus recover the nuclear charge distribution. This means that one can map the *shape* of the nucleus. In particular, the observed angular dependence of the cross-section indicates that the atom presents a point-like target to the electrons, thus supporting the idea of a small nucleus inside the atomic electron cloud.

e) *Assume a point distribution for the charge density, $\rho_e(\vec{r}) = \delta(\vec{r})$. What is the scattering cross-section?*

Solution:

For a point distribution,

$$F(\vec{q}) = \int_V e^{i\vec{q}\cdot\vec{r}/\hbar}\rho_e(\vec{r}) = \int_V e^{i\vec{q}\cdot\vec{r}/\hbar}\delta(\vec{r}) = 1$$

Bringing together the various terms calculated, we have

$$\frac{d\,\sigma}{d\,\Omega} = \Phi_{inc}^{-1}\frac{2\pi}{\hbar}|\,\langle f|\,T\,|i\rangle\,|^2\rho(E_f) = \frac{L^3}{c}\frac{2\pi}{\hbar}\frac{Z^2e^4\hbar^4}{\epsilon_0^2L^6|\vec{q}|^4}\quad {\frac{L}{2\pi\hbar}}^{3}\frac{E'^2}{c^3} = \frac{e^4Z^2E'^2}{4\pi^2\epsilon_0^2|\vec{q}|^4c^4}$$

or, using the fine structure constant, $\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c}$,

$$\frac{d\,\sigma}{d\,\Omega} = \frac{4\alpha^2Z^2\hbar^2E'^2}{|\vec{q}|^4c^2}$$

f) *Since we neglected the nucleus recoil, the scattering is elastic, and the only change is the electron momentum direction, which is deflected at an angle ϑ with respect to the initial direction. Use this consideration to find the famous angular dependence of Rutherford scattering.*

Solution:

For elastic scattering, $|\vec{p}| = |\vec{p}\,'|$ and we assumed $\vec{p}\cdot\vec{p}\,' = p^2\cos\vartheta$. Then, $|\vec{q}| = 2p\sin\left(\frac{\vartheta}{2}\right) = 2E'/c\sin\left(\frac{\vartheta}{2}\right)$. Thus we have,

$$\frac{d\,\sigma}{d\,\Omega} = \frac{4\alpha^2Z^2\hbar^2E'^2}{|2E'/c\sin\left(\frac{\vartheta}{2}\right)|^4c^2} = \frac{\alpha^2Z^2\hbar^2c^2}{4E'^2\sin^4\left(\frac{\vartheta}{2}\right)}$$

Problem 2: Short Questions *15 points*

a) *We classified various types of e.m. field scattering with atomic electrons. What were the criteria for the classification? What are examples of different types of scattering?*

Solution:

Energy of the incoming radiation wrt ionization energy. Elastic or inelastic scattering.

b) *In class we saw two different types of Hamiltonians describing the interaction of the e.m. field with matter, the dipole interaction, $-\vec{d}\cdot\vec{E}$ and the vector potential $-\frac{e}{mc}\vec{p}\cdot\vec{A} + \frac{e^2}{2mc}A^2$. When is it more appropriate to use one interaction or the other? Which interaction should we generally use to describe scattering and why?*

Solution:

The two Hamiltonians arise from quantizations of the e.m. fields in different gauges, in particular the dipole Hamiltonian is derived in the Lorentz gauge, which assumes no sources. Thus, the dipole Hamiltonian can be used for optical wavelength, which are much larger than the atom's dimension (so that the approximation of having no sources is justified).

For scattering, we should generally use the vector potential Hamiltonian, since it allows two-photon transitions even to first order approximation, although for optical light scattering, the dipole Hamiltonian does give the same result.

c) *What state best describes a classical e.m. field? Why?*

Solution:

A coherent state, since the expectation value of the electric and magnetic fields have the same time evolution as the classical fields.

d) *What differential equation describes the evolution of an open quantum system (a system interacting with the environment)? Is this equation always valid?*

Solution:

The Lindblad master equation, which is valid only for a Markovian environment (i.e. a memory-less environment).

e) *What type of information can you gather from a scattering experiment of X-rays or neutrons from a crystal? What extra information can a neutron scattering experiment provide you?*

Solution:

From scattering experiment we can derive the structure factor, which gives information on the crystal planes via Bragg's Law (thus we get information on crystal structure). Neutron scattering also depends on spins, hence we can get isotope information and magnetic structure (the main difference between the two scatterings is that neutrons interact with nuclei, while x-rays with electrons).

Problem 3: Radiation Pressure on a Cantilever *30 points*

Consider a cantilever of frequency ω_c and mass m_c. A beam of (single-mode) light of frequency ν is directed perpendicular to the surface of the cantilever. Radiation pressure can be represented by an interaction Hamiltonian $V = \hbar g(a^\dagger a)\hat{x}$, where $a,\ a^\dagger$ represent the light (e.m. field) operators, and $\hat{x}$ is the quantum mechanical position operator of the cantilever (a quantum harmonic oscillator).

a) *What is the total Hamiltonian $\mathcal{H} = \mathcal{H}_0 + V$ representing the e.m. field, the cantilever and their interaction? What are the eigenstates and eigenvalues of the uncoupled Hamiltonian $\mathcal{H}_0$?*

Solution:

The Hamiltonian is represented by two harmonic oscillators, one for the field and one for the cantilever, coupled by V:

$$\mathcal{H} = \mathcal{H}_0 + V = \hbar\nu(a^\dagger a + \frac{1}{2}) + \hbar\omega_c(b^\dagger b + \frac{1}{2}) + \hbar g a^\dagger a\sqrt{\frac{\hbar}{2m_c\omega_c}}(b^\dagger + b)$$

where I defined $b,\ b^\dagger$ the cantilever operators.

The eigenstates of the uncoupled system are simply the number states of both oscillators, $|n_\gamma, n_c\rangle$, where I called n_γ the photon number, and the corresponding eigenvalues are $E_{n_\gamma,n_c} = \hbar\nu(n_\gamma + \frac{1}{2}) + \hbar\omega_c(n_c + \frac{1}{2})$.

b) *Consider now the radiation pressure as a perturbation coupling the two systems. What is the energy shift Δ_{n_γ,n_c} to the lowest non-zero order?*

Solution:

We can use time-independent perturbation theory to calculate the energy shift. Since $\hat{x}$ does not have diagonal terms in the number-state basis, the first order is zero. The second order is given by:

$$\Delta^{(2)}_{n_\gamma,n_c} = \sum_{n'_\gamma,n'_c} \frac{|\langle n_\gamma, n_c| V |n'_\gamma, n'_c\rangle|^2}{E^{(0)}_{n_\gamma,n_c} - E^{(0)}_{n'_\gamma,n'_c}}$$

Note that the term $a^\dagger a$ only connects states with the same number of photons. The term $\hat{x}$ instead has non-zero matrix elements between states differing by one vibration excitation of the cantilever:

$$\Delta^{(2)}_{n_\gamma,n_c} = \hbar^2 g^2 \frac{\hbar}{2m_c\omega_c} |\langle n_\gamma| a^\dagger a |n_\gamma\rangle|^2 \sum_{n_c'} \frac{|\langle n_c| (b^\dagger + b) |n_c'\rangle|^2}{\hbar\omega_c(n_c - n_c')}$$

$$\Delta^{(2)}_{n_\gamma,n_c} = \frac{\hbar^2 g^2}{2m_c\omega_c^2} n_\gamma^2 \left[\frac{|\langle n_c| b |n_c+1\rangle|^2}{n_c - (n_c+1)} + \frac{|\langle n_c| b^\dagger |n_c-1\rangle|^2}{n_c - (n_c-1)} \right] = \frac{\hbar^2 g^2}{2m_c\omega_c^2} n_\gamma^2 \left[-(n_c+1) + n_c\right] = -\frac{\hbar^2 g^2}{2m_c\omega_c^2} n_\gamma^2$$

c) *What is the expectation value of the cantilever displacement (the displacement from the position it had in the absence of light, $\delta x = \langle \hat{x}' \rangle - \langle \hat{x}_0 \rangle$)?*
[Hint: calculate the perturbed eigenstate of the system to the lowest non-zero order and use it to calculate $\langle \hat{x}' \rangle$]

Solution:

The system perturbed eigenstates are $|\psi\rangle = |n_\gamma, n_c\rangle + \left|\psi^{(1)}\right\rangle$, with the first order eigenstate,

$$\left|\psi^{(1)}\right\rangle = \sum_{n_\gamma', n_c'} \frac{\langle n_\gamma', n_c' \; V |n_\gamma, n_c\rangle}{E^{(0)}_{n_\gamma,n_c} - E^{(0)}_{n_\gamma',n_c'}} \; n_\gamma', n_c'$$

Note that here we neglected the normalization of the eigenstate, since it is a second order effect.
Using the results found in the previous question, we have

$$\left|\; \psi^{(1)}\right\rangle = \hbar g \sqrt{\frac{\hbar}{2m_c\omega_c}} n_\gamma \left[\frac{\langle n_c - 1| b |n_c\rangle |n_\gamma, n_c - 1\rangle}{\hbar\omega[n_c - (n_c-1)]} + \frac{\langle n_c + 1| b^\dagger |n_c\rangle |n_\gamma, n_c + 1\rangle}{\hbar\omega[n_c - (n_c+1)]} \right]$$

$$\left|\; \psi^{(1)}\right\rangle = \frac{g}{\omega} \sqrt{\frac{\hbar}{2m_c\omega_c}} n_\gamma \left[\sqrt{n_c} |n_\gamma, n_c - 1\rangle - \sqrt{n_c + 1} |n_\gamma, n_c + 1\rangle \right]$$

In the absence of the interaction, the expectation value of the position is zero, since $\langle n_c| \hat{x} |n_c\rangle = 0$. With the perturbation, the state is now $|\psi\rangle = |n_\gamma, n_c\rangle + |\psi^{(1)}$ and the expectation value of the position is $\langle \psi|\hat{x}|\psi\rangle = \langle n_\gamma, n_c|\hat{x}|\psi^{(1)} + \langle \psi^{(1)}| \hat{x} |n_\gamma, n_c\rangle$ (other terms are zero, since $\hat{x}$ only links states that differ by one excitation). Then, the displacement is

$$\delta x = \langle x' \rangle = 2\mathrm{Re}\left[\left\langle \mathrm{n}_\gamma, \mathrm{n_c}|\hat{\mathrm{x}}|\psi^{(1)}\right\rangle\right] = \frac{\hbar \mathrm{g}}{2\mathrm{m_c}\omega_\mathrm{c}^2} \mathrm{n}_\gamma \mathrm{Re}\left\{ \langle \mathrm{n}_\gamma, \mathrm{n_c}| (\mathrm{b}^\dagger + \mathrm{b}) \left[\sqrt{\mathrm{n_c}} |\mathrm{n}_\gamma, \mathrm{n_c} - 1\rangle - \sqrt{\mathrm{n_c} + 1} |\mathrm{n}_\gamma, \mathrm{n_c} + 1\rangle \right] \right\}$$

$$\delta x = \langle x' \rangle = \frac{\hbar g}{m_c\omega_c^2} n_\gamma \mathrm{Re}\left\{ \sqrt{\mathrm{n_c}} \langle \mathrm{n_c}| \mathrm{b}^\dagger |\mathrm{n_c} - 1\rangle - \sqrt{\mathrm{n_c}+1} \langle \mathrm{n_c}| \mathrm{b} |\mathrm{n_c}+1\rangle \right\} = -\frac{\hbar \mathrm{g}}{\mathrm{m_c}\omega_\mathrm{c}^2} \mathrm{n}_\gamma$$

d) *Assume now that the light (the e.m. field) was given by an incandescent bulb, thus it is given by thermal radiation at a temperature T. What is the cantilever displacement?*

Solution:

We need to calculate $\langle x' \rangle$ but averaging over the number of photons, with the usual thermal distribution. We have

$$\langle n_\gamma \rangle = \mathrm{Tr}\{\rho \hat{n}\} = (1 - e^{-\beta\hbar\nu}) \sum_n n e^{-\beta n \hbar\nu}.$$

Now $ne^{-\beta n\hbar\nu} = -\frac{1}{\hbar\nu}\frac{\partial e^{-\beta n\hbar\nu}}{\partial\beta}$, thus

$$\langle n_\gamma \rangle = -\frac{1}{\hbar\nu\,\tilde{Z}} \frac{\partial \sum_n e^{-\beta n\hbar\nu}}{\partial\beta} = -\frac{1}{\hbar\nu\,\tilde{Z}} \frac{\partial\tilde{Z}}{\partial\beta} = -\frac{1}{\hbar\nu}\frac{\partial \ln\tilde{Z}}{\partial\beta} = (e^{\beta\nu\hbar} - 1)^{-1} = \frac{e^{-\beta\nu\hbar}}{1 - e^{-\beta\nu\hbar}}$$

The average displacement is then

$$\langle \delta x \rangle = -\frac{\hbar g}{m_c\omega_c^2} \langle n_\gamma \rangle = -\frac{\hbar g}{m_c\omega_c^2} \frac{e^{-\beta\nu\hbar}}{1 - e^{-\beta\nu\hbar}}$$

Problem 4: Radiation Pressure from a Laser *20 points*

a) *Consider laser light (represented by a coherent state $|\alpha\rangle$ of the e.m. field) hitting a cantilever, which is initially in a number state $|n_c\rangle$. What is the transition rate, $W = \frac{2\pi}{\hbar}|\langle f|T|i\rangle|^2\delta(E_f - E_i)$, to a state $|f\rangle = |\beta\rangle|n_c - 1\rangle$? [Here $|\beta\rangle$ is another coherent state of the e.m. field and the interaction between e.m. field and cantilever is the same as considered above, $V = \hbar g(a^\dagger a)\hat{x}$]*

Solution:

The transition rate is

$$W_- = \frac{2\pi}{\hbar}|\langle f|V|i\rangle|^2\delta(E_f - E_i) = \frac{2\pi}{\hbar}|\langle \beta, n_c - 1|V|\alpha, n_c\rangle|^2\delta(E_f - E_i)$$

The matrix element is

$$\langle \beta, n_c - 1|V|\alpha, n_c\rangle = \hbar g\sqrt{\frac{\hbar}{2m\omega_c}}\langle\beta|a^\dagger a|\alpha\rangle\langle n_c - 1|b|n_c\rangle = \hbar g\sqrt{\frac{\hbar}{2m\omega_c}}\beta^*\alpha\langle\beta|\alpha\rangle\sqrt{n_c}$$

Taking the absolute value, we have

$$W_- = \frac{2\pi\hbar g^2}{2m\omega_c}n_c|\alpha|^2|\beta|^2 e^{-|\alpha-\beta|^2}\delta(E_f - E_i)$$

b) *Is it more probable for the system to make a transition to a state $|n_c - 1\rangle$ or $|n_c + 1\rangle$? In other words: is it more probable that the laser is cooling down or heating up the cantilever?*
What is the most probable final state for the e.m. field?

Solution:

The transition rate to the state $|n_c + 1\rangle$ is calculated in the same way as above, except we need to take the matrix element, $\langle n_c + 1|b|n_c\rangle = \sqrt{n_c + 1}$. Thus the rate is

$$W_+ = 2\pi\hbar g^2(n_c + 1)|\alpha|^2|\beta|^2 e^{-|\alpha-\beta|^2}\delta(E_f - E_i)$$

Thus the rate $W_+ > W_-$. On average, we will have more transition that increase the excitation number of the cantilever. Since the temperature of the cantilever is related to its occupation number by $\langle n\rangle = \frac{e^{-\beta\omega_c\hbar}}{1-e^{-\beta\omega_c\hbar}} \approx \frac{k_b T}{\hbar\omega_c}$, the cantilever is heated up.

The transition probability is also proportional to $|\alpha|^2|\beta|^2 e^{-|\alpha-\beta|^2}$ which can be maximized to find the optimal β. Note that since β is a complex number, caution must be taken to find the maximum.

c) *What is the transition rate to a final state $|\alpha, n_c - 2\rangle$?*

Solution:

Note that in this case there is not transition *to first order*, but we can expect a transition to second order:

$$W_2 = \frac{2\pi}{\hbar}\sum_h \frac{\langle f|V|h\rangle\langle h|V|i\rangle}{E_h - E_i}^2 \delta(E_f - E_i)$$

Since the final state is $|n_c - 2\rangle$, the intermediate state of the cantilever is $|n_c - 1\rangle$. The intermediate state of the e.m. field can be taken to be the coherent state $|\beta\rangle$, thus we need to transform the sum into an integral:

$$W_2 = \frac{2\pi}{\hbar}\left|\int d^2\beta \frac{\langle\alpha|a^\dagger a|\beta\rangle\langle\beta|a^\dagger a|\alpha\rangle}{E_\beta - E_\alpha + \hbar\omega_c[(n_c - 1) - n_c]}\right.^2 n_c(n_c - 1)\delta(E_f - E_i)$$

The energy of the e.m. field is $E_\beta = \langle\beta|(a^\dagger a + \frac{1}{2})|\beta\rangle = |\beta|^2 + \frac{1}{2}$. Thus we have

$$W_2 = \frac{2\pi}{\hbar}\left|\int d^2\beta \frac{e^{-|\alpha-\beta|^2}}{\hbar\nu(|\beta|^2 - |\alpha|^2) - \hbar\omega_c}\right|^2 n_c(n_c - 1)\delta(E_f - E_i)$$

Alternatively, we could have calculated W_2 taking as intermediate states the number states $|n\rangle$:

$$W_2 = \frac{2\pi}{\hbar} \left| \sum_n \frac{\langle\alpha|\, a^\dagger a \,|n\rangle \,\langle n|\, a^\dagger a \,|\alpha\rangle}{E_n - E_\alpha + \hbar\omega_c[(n_c-1)-n_c]} \right|^2 n_c(n_c-1)\delta(E_f - E_i)$$

The sum is

$$\sum_n \frac{n^2 |\,\langle\alpha|\, a^\dagger a \,|n\rangle\,|^2}{\hbar\nu(n-|\alpha|^2) - \hbar\omega_c} = \sum_n \frac{n^2 e^{-|\alpha|^2} |\alpha|^{2n}}{n![\hbar\nu(n-|\alpha|^2) - \hbar\omega_c]}$$

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