22.51 Quantum Theory of Radiation Interactions

Final Exam

December 17, 2012 Name: ....

Problem 1: Quantized LC circuit *30 points*

A) *The energy of an LC circuit is given by $E = \frac{1}{2}\left(\frac{Q^2}{C} + \frac{\Phi^2}{L}\right)$, where Q is the charge stored in the capacitor C and Φ the magnetic flux stored in the inductance L.*
1. Propose a quantum mechanical model for the LC circuit and show that its (quantum) energy eigenvalues can be written in terms of the frequency $\omega = 1/\sqrt{LC}$.
2. What is the meaning of the quantum eigenstates?
[Hint: if you are not satisfied to find the quantum model by simple similarity with a very well-known model, consider that we have: $\frac{\partial E}{\partial Q} = -\dot{\Phi}$ and $\frac{\partial E}{\partial \Phi} = \dot{Q}$, thus Φ and Q are generalized canonical variables]

Solution:

Given the form of the classical hamiltonian, we expect the system to have the form of an harmonic oscillator, with Q and Φ playing the role of effective position an momentum. Since we usually have $\omega = \sqrt{k/m}$ we can identify e.g. $L \to 1/k$ and Φ with the position, while $C \to m$ and Q with the momentum. The Hamiltonian is diagonalized as usual in terms of creation and annihilation operators, in this case, of (microwave) photons:

$$\mathcal{H} = \frac{1}{2}\left(\frac{\hat{Q}^2}{C} + \frac{\hat{\Phi}^2}{L}\right) = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right),$$

with

$$\hat{\Phi} = \sqrt{\frac{\hbar}{2C\omega}}(a^\dagger + a) = \sqrt{\frac{\hbar Z}{2}}\left(a^\dagger + a\right) \qquad \hat{Q} = i\sqrt{\frac{C\omega\hbar}{2}}(a^\dagger - a) = i\sqrt{\frac{\hbar}{2Z}}\left(a^\dagger - a\right),$$

where Z is the circuit impedance $Z = \sqrt{L/C}$. The eigenvalues are then $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$ and the eigenvectors $|n\rangle$ represents the number of microwave photons in the circuit.
Note that an equivalent good solution would have been to identify Φ with the momentum. Then we would have had:

$$\hat{\Phi} = i\sqrt{\frac{\omega C\hbar}{2}}(a^\dagger - a) = i\sqrt{\frac{\hbar}{2Z}}\left(a^\dagger - a\right) \qquad \hat{Q} = \sqrt{\frac{\hbar}{2\omega C}}(a^\dagger + a) = \sqrt{\frac{\hbar Z}{2}}\left(a^\dagger + a\right)$$

B) *Consider the current in the circuit, $I = \dot{Q}$.*
1. What is the quantum operator $\hat{I} = \frac{d\hat{Q}}{dt}$?
2. Is this consistent with the usual expression of the current in terms of the flux, $I = \Phi/L$?

Solution:

We want to calculate $\dot{Q}$. To do so, we use the expression for Q and use the Heisenberg equation to find its time derivative:

$$\hat{I} = \dot{Q} = \frac{i}{\hbar}[\mathcal{H}, \hat{Q}] = -\sqrt{\frac{\hbar}{2Z}}\omega[a^\dagger a, (a^\dagger - a)] = \sqrt{\frac{\hbar}{2Z}}\omega(a^\dagger + a) = \frac{1}{L}\sqrt{\frac{\hbar Z}{2}}\left(a^\dagger + a\right) = \frac{1}{L}\hat{\Phi}$$

We thus found that $\hat{I}$ can be indeed expressed also as $\hat{\Phi}/L$.

C) *If the current $\hat{I}$ is a quantum operator, we expect its behavior to be different than the corresponding classical variable. However, if the LC circuit (quantum) system is in a particular state, most of the classical behavior is recovered.*

1. What is this particular state?

2. What would be instead the expectation value of the current $\langle\hat{I}\rangle$ if the state was an eigenstate of the Hamiltonian?

Solution:

1. This would be a coherent state of the field, $|\alpha\rangle$, which is an eigenstate of the annihilation operator.

2. If the system is in one eigenstate of the Hamiltonian, that is, a number state $|n\rangle$, then the expectation value is always zero.

d) *What is the expectation value of the current, $\langle\hat{I}(t)\rangle$, as a function of time, if the initial state of the LC circuit is as you found in question C.1?*

Solution:

We now have the expectation value with respect to the coherent state $|\alpha\rangle$. Now we know that $a^\dagger(t) = a^\dagger(0)e^{i\omega t}$ and $a(t) = a(0)e^{-i\omega t}$, thus we have

$$\langle\hat{I}(t)\rangle = \sqrt{\frac{\hbar}{2Z}}\omega(e^{i\omega t}\left\langle a^\dagger(0)\right\rangle + e^{-i\omega t}\left\langle a(0)\right\rangle) == \sqrt{\frac{\hbar}{2Z}}\omega[e^{i\omega t}\alpha^*(0) + e^{-i\omega t}\alpha(0)] = \langle I(0)\rangle\cos(\omega t+\varphi)$$

which is the classical result. More explicitly:

$$\left\langle a^\dagger(0)\right\rangle = \frac{1}{\sqrt{2\hbar Z}}(\Phi_0 + iZQ_0), \qquad \langle a(0)\rangle = \frac{1}{\sqrt{2\hbar Z}}(\Phi_0 - iZQ_0)$$

where $Q_0 = \langle Q(0)\rangle$ and $\Phi_0 = \langle\Phi(0)\rangle$. Then we have:

$$\langle\hat{I}(t)\rangle = \sqrt{\frac{2\hbar}{Z}}\omega\frac{1}{\sqrt{2\hbar Z}}[\cos(\omega t)\Phi_0 + Z\sin(\omega t)Q_0] = \frac{1}{L}\Phi_0\cos(\omega t) + \omega Q_0\sin(\omega t)$$

Problem 2: Quantized RLC circuit *30 points*

A) *Real circuits always contain dissipative elements, which can be modeled by a resistance R (an RLC circuit).*

We can model the resistance by introducing a Lindblad operator $\hat{\mathcal{L}} = \sqrt{\frac{L}{R}}\frac{1}{2\hbar}\left(\frac{\hat{Q}^2}{C} + \frac{\hat{\Phi}^2}{L}\right)$.

Write the equation of motion for the current $\hat{I}$, simplifying the expression of $\hat{\mathcal{L}}$ based on your answer to Problem 1.A

Solution:

In the Heisenberg picture, the evolution is given by the master equation in the Lindblad form:

$$\dot{I} = \frac{i}{\hbar}[\mathcal{H}, I] - \left[\mathcal{L}^\dagger I\mathcal{L} - \frac{1}{2}(\mathcal{L}^\dagger\mathcal{L}I + I\mathcal{L}^\dagger\mathcal{L})\right]$$

Note that $\mathcal{L}$ is proportional to the Hamiltonian, thus we have $\mathcal{L} = \sqrt{\frac{L}{R}}\omega\left(a^\dagger a + \frac{1}{2}\right) = \frac{1}{\sqrt{RC}}\left(a^\dagger a + \frac{1}{2}\right)$.

B) *Consider the operator $\hat{A} = \frac{1}{\sqrt{2\hbar Z}}(\hat{\Phi} + iZ\hat{Q})$, where $Z = \sqrt{L/C}$ is the (classical) circuit impedance. Find an explicit expression for the equation of motion for $\hat{A}$ (under the action of the Hamiltonian and the Lindblad operator).*

[Note: depending on how you solved Problem 1, it might be easier to calculate the evolution of $\hat{A}' = \sqrt{\frac{1}{2\hbar Z}}(\hat{Q} + iZ\hat{\Phi})$]

Solution:

The operator $\hat{A}$ is nothing else than the annihilation operator a. Writing $\mathcal{L} = \sqrt{\gamma}(N + 1/2) = \frac{\sqrt{\gamma}}{\hbar\omega}\mathcal{H}$ we have the equation of motion:

$$\dot{a} = -i\omega a - \gamma \left[\left(N + \frac{1}{2}\right) a \left(N + \frac{1}{2}\right) - \frac{1}{2}\left(N + \frac{1}{2}\right)^2 a - \frac{1}{2} a \left(N + \frac{1}{2}\right)^2 \right]$$

$$\dot{a} = -i\omega a - \gamma \left[NaN - \frac{1}{2}(N^2 a + aN^2) + a/4 - a/4 + (Na + aN)/2 - (Na + aN)/2 \right]$$

$$= -i\omega a - \frac{\gamma}{2}[N(aN - Na) + (aN - Na)N]$$

we finally obtain:

$$\dot{a} = -i\omega a - \frac{\gamma}{2} a$$

thus the evolution of $A = a$ is now: $a(t) = a(0)e^{-i\omega t - \gamma t/2}$.

c) *Given your result above, what is the time evolution of the expectation value of the current? How does it compare to the classical result?*

Solution:

We have to add an exponential decay to the time evolution found above:

$$\langle \hat{I}(t) \rangle = e^{-\gamma t/2} \left[\frac{1}{L} \Phi_0 \cos(\omega t) + \omega Q_0 \sin(\omega t) \right]$$

a result similar to what found classically.

Problem 3: Electron scattering from an harmonic potential *40 points*

We consider the scattering of an electron from a nucleus. The nucleus-electron potential is given by $V(\vec{r}, t) = V_0(\vec{r}) \cos(\omega t)$, where $V_0(\vec{r})$ represents the potential at the nucleus rest position.

A) *Write a formal expression for the scattering cross section and explain how this is related to perturbation theory.*

Solution:

The scattering cross-section can be written in terms of the scattering matrix, which gives the transition probability from the initial and final state,

$$P_{i \to f} = |\langle f| S |i\rangle|^2 = |\langle f| U_I(t) |i\rangle|^2$$

The cross-section is then given by the rate of scattering, $W_s = \frac{dP}{dt}$ divided by the incoming electron flux, Φ_e:

$$\frac{d\sigma}{d\Omega} = \frac{W_s}{\Phi_e}$$

B) *Calculate the probability of scattering to first order approximation and derive from it the scattering rate.*
[Hint: here you can express your result in terms of $V_{fi} = \langle f| V_0(\vec{r}) |i\rangle L^3$ (where L is the side of the usual cubic cavity) and the initial and final electron energies $E_i = \hbar\omega_i$ and $E_f = \hbar\omega_f$]

Solution:

The scattering probability is given to first order by the propagator in the interaction picture. We want to calculate:

$$\langle f| U_I(t) |i\rangle = \delta_{if} - i \int_{-\infty}^{\infty} V_{fi}/L^3 \cos(\omega t) e^{-it(\omega_f - \omega_i)}$$

Defining $\omega_{fi} = \omega_f - \omega_i$, this is nothing else than the Fourier Transform of the cosine:

$$\langle f| U_I(t) |i\rangle = 2\pi V_{fi}/L^3 [\delta(\omega - \omega_{fi}) + \delta(\omega + \omega_{fi})]$$

Taking the modulus square and using the formula given for the delta function we have:

$$P_{i\to f} = \frac{2\pi}{\hbar} t|V_{fi}/L^3|^2[\delta(E - E_{fi}) + \delta(E + E_{fi})]$$

(where I switched to energies instead of frequencies). Thus the scattering rate can also be calculated very easily.

C) *Assume that the initial and final states of the electron are given by plane waves and calculate*
1. the final density of state (assume no recoil of the nucleus),
2. the electron flux.

Solution:

The density of state can be calculated from the usual considerations. We consider a cubic cavity that imposes constraints on the acceptable values of the wavenumber $k_\alpha = n_\alpha 2\pi/L$, so that

$$dN = \rho(E)dE = n^2 dn d\Omega = \left(\frac{L}{2\pi}\right)^3 k^2 dk d\Omega, \qquad E = \frac{\hbar^2 k^2}{2m_e}$$

Calculating $\frac{dE}{dk} = \frac{\hbar^2 k}{m_e}$, we find:

$$\rho(E) = 2\left(\frac{L}{2\pi}\right)^3 \frac{k m_e}{\hbar^2} = 2\left(\frac{L}{2\pi}\right)^3 \frac{\sqrt{2m_e E}}{\hbar^3}$$

(where I consider a factor 2 for the two spin states of the electron, although this might not be necessary if the interaction conserves the spin). Note that we need to evaluate $\rho(E)$ at $\rho(E_f = E_i + \hbar\omega)$ and $\rho(E_f = E_i - \hbar\omega)$.

D) *Using the results from the previous questions, write an explicit expression for the scattering cross-section.*

Solution:

The scattering rate is given by

$$W_s = \frac{2\pi}{\hbar} L^6 |V_{fi}|^2 [\rho(E_f = E_i + \hbar\omega) + \rho(E_f = E_i - \hbar\omega)]$$

The flux of incoming electron is $\Phi_e = \hbar k_i/(mL^3) = \sqrt{2E_i/m}/L^3$. Thus we finally have:

$$\frac{d\sigma}{d\Omega} = \frac{W_s}{\Phi_e} = \frac{2\pi}{L^6\hbar}(|V_{fi}^+|^2\sqrt{E_i + \hbar\omega} + |V_{fi}^-|^2\sqrt{E_i - \hbar\omega})L^3\sqrt{\frac{m_e}{2E_i}}2\left(\frac{L}{2\pi}\right)^3 \frac{\sqrt{2m_e}}{\hbar^3}$$

where I have taken into account that if the final state of the electron has a different energy, the matrix element might also be different.

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{L^6\hbar}\frac{2m_e}{(2\pi\hbar)^3\sqrt{E_i}}(|V_{fi}^+|^2\sqrt{E_i + \hbar\omega} + |V_{fi}^-|^2\sqrt{E_i - \hbar\omega})$$

e) *Assuming that the potential (at rest)* $V_0(\vec{r})$ *is given by the Coulomb interaction of the electron with the protons,* $V_0(\vec{r}) = -\frac{Ze^2}{|\vec{r}|}$,
*1. find a (**formal**) expression for the matrix element* $V_{fi} = L^3 \langle f|V_0(\vec{r})|i\rangle$.
2. What information can one extract from the scattering cross-section?

Solution:

We want to calculate

$$\langle f|V_0(\vec{r})|i\rangle = \int_{L^3} \psi_i(\vec{r})^* V_0(\vec{r})\psi_f(\vec{r})d^3r = -\frac{Ze^2}{L^3}\int_{L^3} e^{-i\vec{k}_i\cdot\vec{r}}e^{i\vec{k}_f\cdot\vec{r}}\frac{1}{|\vec{r}|}d^3r$$

Thus the matrix element is the Fourier transform of the potential,

$$F(\vec{q}) = \langle f|V_0(\vec{r})|i\rangle = \int_{L^3} e^{i\vec{q}\cdot\vec{r}}V(\vec{r})$$

From the nuclear form factor $F(q)$ we can extract information about the charge distribution.

f) *We now want to analyze higher order terms in the scattering cross-section.*

*1. In order to do so, calculate the scattering probability to second order perturbation theory and use this result to **propose** (with no further complex calculations) a modified scattering cross-section.*

2. Describe what this second order term represents physically and which terms in it give the largest contributions.

3. Can you relate the results you obtained to the neutron scattering by crystal lattices?

Solution:

We go back the the scattering probability and expand to second order:

$$\langle f| U_I(t) |i\rangle = \delta_{if} - i\int_{-\infty}^{\infty} V_{fi}/L^3 \cos(\omega t) e^{-it(\omega_f-\omega_i)}$$

$$-\int_{-\infty}^{\infty}\int_{-\infty}^{t}\sum_m \langle f| V_0 |m\rangle \langle m| V_0 |i\rangle \cos(\omega t)\cos(\omega t') e^{-it(\omega_f-\omega_m)} e^{-it'(\omega_m-\omega_i)} dt' dt$$

Evaluating the second order term we have:

$$-\frac{1}{L^6}\sum_m V_{fm}V_{mi}\int_{-\infty}^{\infty} dt \cos(\omega t) e^{-it(\omega_f-\omega_m)}\int_0^t dt' \cos(\omega t') e^{-it'(\omega_m-\omega_i)}$$

We can evaluate the first integral by adding an exponential term, which will keep it finite at $t' \to -\infty$:

$$\lim_{\epsilon\to 0}\int_0^t dt' \cos(\omega t') e^{-it'\omega_{mi}+\epsilon t'} = \frac{e^{-it(\omega_{mi}+\omega)}}{2i(\omega_{mi}+\omega)} + \frac{e^{-it(\omega_{mi}-\omega)}}{2i(\omega_{mi}-\omega)} = e^{-it\omega_{mi}}\frac{\omega\sin(\omega t) - i\omega_{mi}\cos(\omega t)}{\omega^2-\omega_{mi}^2}$$

Inserting this result in the integral above, we have:

$$-\frac{1}{L^6}\sum_m V_{fm}V_{mi}\int_{-\infty}^{\infty} dt \cos(\omega t) e^{-it(\omega_f-\omega_i)}\left[\frac{e^{-i\omega t}}{2i(\omega_{mi}+\omega)} + \frac{e^{it\omega}}{2i(\omega_{mi}-\omega)}\right]$$

This gives rise to several delta functions:

$$= -\frac{2\pi}{L^6}\sum_m V_{fm}V_{mi}\left[\frac{\delta(\omega_{fi})+\delta(\omega_{fi}-2\omega)}{4i(\omega_{mi}+\omega)} + \frac{\delta(\omega_{fi})+\delta(\omega_{fi}+2\omega)}{4i(\omega_{mi}-\omega)}\right]$$

The second order term contribution to the scattering cross section is then:

$$\frac{d\sigma^{(2)}}{d\Omega} \propto \left|\sum_m \frac{V_{fm}V_{mi}}{4(\omega_{mi}+\omega)}\right|^2 [\rho(E_f\approx E_i)+\rho(E_f\approx E_i-2\omega)] + \left|\sum_m \frac{V_{fm}V_{mi}}{4(\omega_{mi}-\omega)}\right|^2 [\rho(E_f\approx E_i)+\rho(E_f\approx E_i+2\omega)]$$

These terms describe virtual transitions to intermediate states $|m\rangle$. The states $|m\rangle$ s.t. $\omega_{mi}\approx\pm\omega$ are the ones that will contribute most (in particular we could have resonant scattering).

We note that the scattering cross-section contains terms where the electron acquires one quantum of energy $\hbar\omega$ from the oscillating nucleus (to first order) and either zero or two quanta of energy to second order. We expect to find that at higher orders, the electron will acquire n quanta of energy. This is similar to what we found in the scattering of neutron from a crystal, where however we considered a quantized harmonic oscillator, instead of a classical one.

Formulas (not all of them might be useful)

- You can take $\delta(\omega)^2 = t\delta(\omega)/2$ in time-dependent perturbation theory calculations.
- Quantized position and momentum:

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a) \qquad p = i\sqrt{\frac{m\omega\hbar}{2}}(a^\dagger - a)$$

- Lindbladian in the Heisenberg picture for an operator A:

$$\mathcal{L}(A) = -\sum_k\left[L_k^\dagger A L_k - \frac{1}{2}\left(L_k^\dagger L_k A + A L_k^\dagger L_k\right)\right]$$

• Quantized electric field:

$$\mathbf{E}(x,t) = \sum_n \sqrt{\frac{2\hbar\pi\omega_n}{L^3}}[a_n^\dagger(t) + a_n(t)]\mathbf{u}_n(x).$$

• Time-independent perturbation theory:

First-order energy eigenstate: $|\varphi_k^{(1)}\rangle = R_k V\,|k\rangle = \sum_{h\neq k} \frac{\langle h|V|k\rangle}{E_k^0 - E_h^0}\,|h\rangle$

Second-order energy: $E_k^{(2)} = \sum_{h\neq k} \frac{|\,\langle h|\,V\,|k\rangle\,|^2}{E_k^0 - E_h^0}$