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Relativistic Quantum Information

Homework 1: Light-matter interaction & photon absortion

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1. Light-matter interaction

Let me first try to understand this stuff and then I will try to compress it into half a page.

In the radiation gauge we have

$$U(t,\vec{x})=0 \quad \text{and} \quad \vec{\nabla}\cdot\vec{A}(t,\vec{x})=0.$$

To see this is in fact achievable, start from arbitrary smooth potentials U and $\vec{A}$ defined on some open set. We must show that there is a smooth χ in this set s.t.

$$\vec{\nabla}\cdot\left(\vec{A}(t,\vec{x})+\frac{\hbar}{e}\vec{\nabla}\chi(t,\vec{x})\right)=0,$$

$$U(t,\vec{x})-\frac{\hbar}{e}\frac{\partial\chi}{\partial t}(t,\vec{x})=0.$$

Let us focus on the first of these. It can be recasted into the form

$$\Delta \chi(t,\vec{x}) = -\frac{e}{\hbar}\,\vec{\nabla}\cdot\vec{A}\,(t,\vec{x}).$$

One thus recognizes Poisson's eqn. Assuming $\vec{\nabla}\cdot\vec{A}$ is appropriately localized, this can be solved by

$$\chi_0(t,\vec{x}) = \frac{e}{4\pi\hbar}\int d^3\vec{x}'\,\frac{\vec{\nabla}\cdot\vec{A}(t,\vec{x}')}{\|\vec{x}-\vec{x}'\|}.$$

Of course, taking $\chi = \chi_0 + G$ for any harmonic G will also do the job. The second eqn can then be cast into the form

$$\frac{e}{\hbar}\,U(t,\vec{x}) = \frac{\partial\chi}{\partial t}(t,\vec{x}) = \frac{\partial\chi_0}{\partial t}(t,\vec{x}) + \frac{\partial G}{\partial t}(t,\vec{x}).$$

This is solved by

$$G(t,\vec{x}) = \int_{t_0}^{t} d\lambda\left(\frac{e}{\hbar}\,U(\lambda,\vec{x}) - \frac{\partial\chi_0}{\partial\lambda}(\lambda,\vec{x})\right) + F(\vec{x})$$

for any smooth F on the space projecton of this set.

To make sure G is harmonic, we just need to demand that

$$\Delta F(\vec{x}) = -\Delta \int_{t_0}^{t} d\lambda \left(\frac{e}{\hbar} U(\lambda, \vec{x}) - \frac{\partial \chi_0}{\partial \lambda}(\lambda, \vec{x}) \right).$$

Assuming U and $\vec{A}$ decay at the appropriate rates, we can once again solve this Poisson eqn.

In the radiation gauge we have

$$[p_i, A^i(t,\vec{x})]\,\psi(t,\vec{x}) = -i\hbar\, \partial_i (A^i \psi)(t,\vec{x}) + i\hbar A^i(t,\vec{x})\,\partial_i \psi(t,\vec{x})$$

$$= -i\hbar\, \cancel{\vec{\nabla}\cdot\vec{A}(t,\vec{x})}^{\,0}\, \psi(t,\vec{x}) - i\hbar\, \cancel{\vec{A}(t,\vec{x})\cdot\vec{\nabla}\psi(t,\vec{x})} + i\hbar\, \cancel{\vec{A}(t,\vec{x})\cdot\vec{\nabla}\psi(t,\vec{x})}$$

$$= 0.$$

Then, the Hamiltonian is

$$H(t) = \frac{1}{2m}\left(\vec{p} - e\vec{A}(t,\vec{x})\right)^2 + e\,\cancel{U(t,\vec{x})}^{\,0} + V(\vec{x})$$

$$= \frac{\vec{p}^{\,2}}{2m} - \frac{e}{2m}\left(\vec{p}\cdot\vec{A}(t,\vec{x}) + \vec{A}(t,\vec{x})\cdot\vec{p}\right) + \frac{e^2}{2m}\vec{A}(t,\vec{x})^2 + V(\vec{x})$$

$$= \frac{\vec{p}^{\,2}}{2m} - \frac{e}{2m}\left(2\vec{A}(t,\vec{x})\cdot\vec{p} - \cancel{[A^i(t,\vec{x}), p_i]}^{\,0}\right) + \frac{e^2}{2m}\vec{A}(t,\vec{x})^2 + V(\vec{x})$$

$$= \frac{\vec{p}^2}{2m} - \frac{e}{m} \vec{A}(t,\vec{x})\cdot\vec{p} + \frac{e^2}{2m}\vec{A}(t,\vec{x})^2 + V(\vec{x}).$$

Let us now assume that $\vec{A}$ can be written as a sum of plane waves

$$\vec{A}(t,\vec{x}) = \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{x}} \mathfrak{F}(\vec{A})(t,\vec{k}).$$

Note that, for an electron localized in an atom we expect its wave function to be neglible outside of a ball of some radius δ around the atom $\vec{x}_0$. As far as the Schrödinger eqn is concerned, we are then only interested in the values of $\vec{A}$ in this ball. The dipole approximation consist of assuming that the modes $\mathfrak{F}(\vec{A})(t,\vec{k})$, with wavelengths which are not much larger than the radius of our ball $\frac{1}{\|\vec{k}\|} \gg \delta$, are neglible. Thus, for all $\vec{x}$ within this ball we have that

$$|\vec{k}\cdot(\vec{x}-\vec{x}_0)| \leq \|\vec{k}\|\|\vec{x}-\vec{x}_0\| < \|\vec{k}\|\delta \ll 1$$

is neglible, and

$$\vec{A}(t,\vec{x}) = \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{x}_0} \mathcal{F}(\vec{A})(t,\vec{k}) \left(1 + i\vec{k}\cdot(\vec{x}-\vec{x}_0) + \cdots \right)$$

$$\simeq \int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot\vec{x}_0} \mathcal{F}(\vec{A})(t,\vec{k}) = \vec{A}(t,\vec{x}_0).$$

In this approximation, we have the Hamiltonian

$$H(t) = \frac{\vec{p}^{\,2}}{2m} - \frac{e}{m}\vec{A}(t,\vec{x}_0)\cdot\vec{p} + \frac{e^2}{2m}\vec{A}(t,\vec{x}_0)^2 + V(\vec{x}).$$

The $\vec{A}\cdot\vec{p}$ model is obtained when the electromagnetic field is weak enough so that the $\vec{A}(t,\vec{x}_0)$ term is neglible

$$H(t) = \frac{\vec{p}^{\,2}}{2m} - \frac{e}{m}\vec{A}(t,\vec{x}_0)\cdot\vec{p} + V(\vec{x}).$$

Now, without the last approximation, consider the gauge transformation given by

$$\chi(t,\vec{x}) = -\frac{e}{\hbar}\vec{A}(t,\vec{x}_0)\cdot\vec{x}$$

Then the Hamiltonian transforms by taking the new vector potential

$$\vec{A}_\chi(t,\vec{x}) = \vec{A}(t,\vec{x}) - \vec{\nabla}\Big(\vec{A}(t,\vec{x}_0)\cdot\vec{x}\Big)$$

$$= \vec{A}(t,\vec{x}) - \vec{A}(t,\vec{x}_0) \approx \vec{A}(t,\vec{x}_0) - \vec{A}(t,\vec{x}_0) = 0.$$

and the new scalar potential

$$U_\chi(t,\vec{x}) = \cancelto{0}{U(t,\vec{x})} + \frac{\partial\vec{A}(t,\vec{x}_0)}{\partial t}\cdot\vec{x} = -\vec{E}(t,\vec{x}_0)\cdot\vec{x}\,.$$

Thus our new Hamiltonian is

$$H_\chi = \frac{\vec{p}^{\,2}}{2m} + V(\vec{x}) - e\vec{E}(t,\vec{x}_0)\cdot\vec{x}\,,$$

which has the $\vec{x}\cdot\vec{E}$ coupling. Mind you, to obtain H_χ $(\vec{A}\cdot\vec{p})$ from H $(\vec{E}\cdot\vec{x})$ we need to do a gauge transformation. Thus, in our observables we must simultaneously perform the transformation

$$\psi \longmapsto \psi_\chi := e^{i\chi}\psi.$$

In order to see this, note that

$$i\hbar \frac{\partial \psi_\chi}{\partial t} = i\hbar e^{i\chi}\left(i\frac{\partial \chi}{\partial t}\psi + \frac{\partial \psi}{\partial t}\right) = -\hbar e^{i\chi}\frac{\partial \chi}{\partial t}\psi + e^{i\chi} i\hbar \frac{\partial \psi}{\partial t}$$

while, for general potentials,

$$H_\chi(t)\psi_\chi(t,\vec{x}) = \left(\frac{1}{2m}\left(\vec{p} - e\vec{A}(t,\vec{x}) - \hbar\vec{\nabla}\chi(t,\vec{x})\right)^2 + eU(t,\vec{x}) - \hbar\frac{\partial \chi}{\partial t}(t,\vec{x}) + V(\vec{x})\right)\left(e^{i\chi(t,\vec{x})}\psi(t,\vec{x})\right).$$

Noting that

$$\left(\vec{p} - e\vec{A}(t,\vec{x}) - \hbar\vec{\nabla}\chi(t,\vec{x})\right) e^{i\chi(t,\vec{x})}\psi(t,\vec{x})$$

$$= e^{i\chi(t,\vec{x})}\left(\cancel{-ii\hbar\vec{\nabla}\chi(t,\vec{x})} + \vec{p} - e\vec{A}(t,\vec{x}) - \cancel{\hbar\vec{\nabla}\chi(t,\vec{x})}\right)\psi(t,\vec{x}),$$

we obtain

$$H_\chi(t)\psi_\chi(t,\vec{x}) = e^{i\chi}\left(\frac{1}{2m}\left(\vec{p} - e\vec{A}(t,\vec{x})\right)^2 + eU(t,\vec{x})\right)\psi(t,\vec{x}) - \hbar e^{i\chi}\frac{\partial \chi}{\partial t}\psi.$$

We conclude ψ satisfies the Schrödinger eqn for

H if and only if ψ_X does for H_X. Now we are ready to solve the problem.

a) Both can be related into each other if the dipole approximation is valid. This means that the electromagnetic field is composed of wavelengths that are much larger than the size of the atom.

b) The two Hamiltonians do not share the same set of solutions of the Schrödinger eqn. and in particular, don't have the same eigenfunctions. Thus, the transition amplitudes might change. However, fortunately the mechanical Hamiltonian $H(t) = \frac{1}{2m}(\vec{p} - e\vec{A}(t,\vec{x}))^2 + eV(\vec{x})$ gets transformed under gauge transformations unitarily $H \mapsto e^{iX} H(t) e^{-iX}$. Thus, all inner products, including transition amplitudes, remain invariant as long as we simultaneously transform our wavefunctions by $\psi \longmapsto e^{iX}\psi$.

2. Photon Absortion

a) We have

$$1 = \langle \psi' | \psi' \rangle = |C|^2 \langle \psi | \hat{a}^+_{k,\varepsilon} a_{k,\varepsilon} | \psi \rangle = |C|^2 \langle \psi | \hat{N}_{k,\varepsilon} | \psi \rangle$$

$$= |C|^2 \langle \hat{N}_{k,\varepsilon} \rangle_\psi = |C|^2 n ,$$

that is, we can take

$$C = \frac{1}{\sqrt{n}}$$

Now, note that

$$\langle \hat{N}^2_{k,\varepsilon} \rangle_\psi = \langle \psi | \hat{a}^+_{k,\varepsilon} \hat{a}_{k,\varepsilon} \hat{a}^+_{k,\varepsilon} \hat{a}_{k,\varepsilon} | \psi \rangle$$

$$= \frac{1}{|C|^2} \langle \psi' | \hat{a}_{k,\varepsilon} \hat{a}^+_{k,\varepsilon} | \psi' \rangle$$

$$= n \left(\langle \psi' | [\hat{a}_{k,\varepsilon}, \hat{a}^+_{k,\varepsilon}] | \psi' \rangle + \langle \psi' | \hat{a}^+_{k,\varepsilon} \hat{a}_{k,\varepsilon} | \psi' \rangle \right).$$

Since quantization procedures are normally divergent, let us take $T_{\psi'} := \langle \psi' | [\hat{a}_{k,\varepsilon}, \hat{a}^+_{k,\varepsilon}] | \psi' \rangle$. Then

$$\langle \hat{N}^2_{k,\varepsilon} \rangle_\psi = n \left(T_{\psi'} + \langle \psi' | \hat{N}_{k,\varepsilon} | \psi' \rangle \right) = n \left(T_{\psi'} + \langle \hat{N}_{k,\varepsilon} \rangle_{\psi'} \right).$$

We conclude

$$(\Delta N_{\kappa,\varepsilon})_\psi = \sqrt{n\left(T_{\psi'} + \langle \hat{N}_{\kappa,\varepsilon}\rangle_{\psi'}\right) - \langle \hat{N}_{\kappa,\varepsilon}\rangle^2_\psi}$$

$$= \sqrt{n\left(T_{\psi'} + \langle \hat{N}_{\kappa,\varepsilon}\rangle_{\psi'}\right) - n^2}\,.$$

We conclude

$$\frac{1}{n}(\Delta N_{\kappa,\varepsilon})^2_\psi + n - T_{\psi'} = \langle \hat{N}_{\kappa,\varepsilon}\rangle_{\psi'}$$

Observation: In the usual application of quantization of QED we have infinities in $(\Delta N_{\kappa,\varepsilon})_\psi$ because of squaring operator valued distributions of unbounded operators and $T_{\psi'}$, which for a closely related reason to the one before, would also be infinite

$$\langle \psi' | [\hat{a}_{\kappa,\varepsilon}, \hat{a}^+_{\kappa,\varepsilon}] | \psi' \rangle = \delta(\kappa-\kappa)\langle \psi' | \psi' \rangle = \delta(\kappa-\kappa) = \delta(0).$$

Since I doubt the problem has to do with functional analytic subtleties, I will assume that we have quantized in a way as to avoid this infinities. For example, by taking the system to be on a torus we can make

$$[\hat{a}_{k,\varepsilon}, \hat{a}^{+}_{k,\varepsilon}] = \delta_{k,k} = 1, \quad \text{i.e.} \quad T_{\psi'} = 1.$$

Thus

$$\langle \hat{N}_{k,\varepsilon} \rangle_{\psi'} = \frac{1}{n} (\Delta N_{k,\varepsilon})^2_{\psi} + n - 1.$$

b) No, if $(\Delta N_{k,\varepsilon})_{\psi} > \sqrt{n}$, we have

$$\langle \hat{N}_{k,\varepsilon} \rangle_{\psi'} > \frac{n}{n} + n - 1 = n$$

Bonus: A coherent state $|\psi\rangle$ is an eigenstat of $\hat{a}_{k,\varepsilon}$, i.e. $\hat{a}_{k,\varepsilon} |\psi\rangle = \alpha |\psi\rangle$ for some $\alpha \in \mathbb{C}$. In fact $n = \langle \hat{N}_{k,\varepsilon} \rangle_{\psi} = \langle \psi | \hat{a}^{+}_{k,\varepsilon} \hat{a}_{k,\varepsilon} | \psi \rangle = |\alpha|^2$. On the other hand

$$\langle \hat{N}^2_{k,\varepsilon} \rangle_{\psi} = \langle \psi | \hat{a}^{+}_{k,\varepsilon} \hat{a}_{k,\varepsilon} \hat{a}^{+}_{k,\varepsilon} \hat{a}_{k,\varepsilon} | \psi \rangle = |\alpha|^2 \langle \psi | \hat{a}_{k,\varepsilon} \hat{a}^{+}_{k,\varepsilon} | \psi \rangle$$

$$= |\alpha|^2 (1 + |\alpha|^2).$$

We conclude

$$(\Delta N_{k,\varepsilon})_{\psi} = \sqrt{|\alpha|^2 (1 + \cancel{|\alpha|^2}) - \cancel{|\alpha|^4}} = |\alpha| = \sqrt{n}.$$

Thus, it is precisely for coherent states that application of annihilation operators neither increase nor decrease the expected number of excitations of the state.

c) Our quantum theory of electromagnetic fields allows for vectors $|\vec{k},\varepsilon\rangle$ of definite momentum $\vec{k}$ and polarization ε. This however has an infinite norm. Its proper understanding requires rigged Hilbert spaces. In particular, one obtains a proper element of the one particle Hilbert space

$$|\psi\rangle = \sum_{\varepsilon=1}^{2} \int \frac{d^3\vec{k}}{\sqrt{(2\pi)^3 2|\vec{k}|}} \psi_\varepsilon(\vec{k})|\vec{k},\varepsilon\rangle .$$

This would correspond to a photon. However, for us to assign a reality to such a state, its preparation must be possible. Such a preparation would correspond to the rank 1 projection $|\psi\rangle\langle\psi|$. However, if we believe that quantum field theories are described by nets of type III von Neumann algebras, the theorem shown in class guarantees that $|\phi\rangle\langle\phi|$ is not observable.

One could argue that the projector onto the one particle Hilbert space has infinite rank and thus the previous theorem would not prohibit it from being observable. Then, although it would be impossible to prepare $|\psi\rangle$ with certainty, the preparation of a state with a single photon could be implemented, this projection would however be of the form $\sum_n |\psi_n\rangle\langle\psi_n|$ where $(\psi_{n,\varepsilon})_n$ is a basis of $L^2(\mathbb{R}^3)$. Thus, it would be completely delocalized. Thus, by Sorkin's argument, such a preparation would violate causality.

In conclusion, this is a difficult problem. The detector approach gives us an operational out, namely by defining photons as whatever it is photon detectors, such as the one modelled in problem 1, detect. In any case, problem 2 shows us that to distinguish between $|\psi\rangle$ and $a|\psi\rangle$ it is not enough to measure $\langle N_\psi \rangle$. One needs the higher moments as well.