# PHY662, Spring 2004, Apr. 13, 2004

13th April 2004

## 1 Miscellaneous

1. Reading: Continue Shankar Ch. 18 for electromagnetism, also Griffiths Ch. 9 (though it is a bit simplified, especially as it sticks to two-level systems at first). Skip higher order perturbation theory in Shankar and read up to "Field Quantization" (p. 506 in the second edition) by Tuesday, April 13. Much of what follows in today's notes is derived from Shankar and Ch. 13 of G. Bayms' *Lectures on Quantum Mechanics*.
2. Office hours are at 4:00 on Wednesday this week. This week's homework is due Tuesday, April 20.

## 2 Electromagnetism

[See Shankar for Maxwell's equation and this discussion.]
The highlights are: rewriting the electromagnetic field using the potentials $\vec{A}$ and $\phi$,

$$\begin{aligned}\vec{B} &= \nabla\times\vec{A}\\ \vec{E} &= -\frac{1}{c}\frac{\partial\vec{A}}{\partial t}-\nabla\phi\,;\end{aligned}$$

Choosing the Coulomb gauge for the "free electromagnetic field", where the sources for the EM field, density $\rho$ and current $\vec{j}$, satisfy $\rho = 0$ and $\vec{j} = 0$, gives

$$\begin{aligned}\nabla\cdot\vec{A} &= 0\\ \phi &= 0\,.\end{aligned}$$

The equations of motion for $\vec{A}$ in the Coulomb gauge are then

$$\nabla^2\vec{A}-\frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2} = 0\,.$$

These equations give that waves in $\vec{A}$ travel at speed $c$ and that plane wave solutions for $\vec{A}$ are of the form

$$\vec{A}=\vec{A}_0\cos(\vec{k}\cdot\vec{r}-\omega t)$$

with $k^2c^2 = \omega^2$ and with the important resulting condition (transverse waves)

$$\vec{k} \cdot \vec{A}_0 = 0\,.$$

The resulting $\vec{E}$ and $\vec{B}$ fields have equal magnitude and the energy density is

$$u = \frac{1}{8\pi}(|\vec{E}|^2 + |\vec{B}|^2)\,.$$

**Note on units**: $\frac{e^2}{r}$ has the units of energy, so $e$ has the units of $\sqrt{\mathrm{E} \cdot \mathrm{L}}$. For $r = \frac{\hbar^2}{me^2} = 0.0529\,\mathrm{nm}$ (the Bohr radius), $\frac{e^2}{r}$ has the value $13.6\,\mathrm{eV}$ as a Rydberg is $13.6\,\mathrm{eV}$ and $\langle V \rangle = -2\langle H \rangle$. So $e^2 = 13.6 \times 0.0529\,\mathrm{eV} \cdot \mathrm{nm} = 0.72\,\mathrm{eV} \cdot \mathrm{nm}$ (mixing up CGS and SI units in a controlled way).

## 2.1 Potentials in quantum theory

Last time we reviewed the homework question that showed how the Schrodinger equation was preserved under a gauge transformation for $\vec{A}$ and $\phi$, $\vec{A} \rightarrow \vec{A} + \nabla\Lambda(\vec{r}, t)$, $\phi \rightarrow \phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t}$, for an arbitrary scalar function $\Lambda(\vec{r}, t)$. if the wave function was changed by $\psi \rightarrow e^{iq\Lambda/\hbar c}$. Note that this changes the phase of $\psi$, of course, but not $\psi^*\psi$, so we still interpret $\psi^*\psi$ as the probability of finding a particle at a particular location.

Shankar works using path integrals. This is important and I suggest you read it, but we are not focusing on path integrals this term. Remember that the Hamiltonian for a charged particle in only an electromagnetic potential is

$$\frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi\,.$$

Let's rederive the conservation of current using this Hamiltonian in the Schrodinger equation and multiplying on the left by $\psi*$:

$$\begin{aligned}
\left[\frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi\right]\psi &= i\hbar\frac{\partial\psi}{\partial t} \\
\psi^*\left[\frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi\right]\psi &= \psi^* i\hbar\frac{\partial\psi}{\partial t} \\
(i\hbar)^{-1}\psi^*\left[\frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + q\phi\right]\psi &= \psi^*\frac{\partial\psi}{\partial t} \\
(i\hbar)^{-1}\psi^*\left[\frac{1}{2m}(p^2 - \frac{q}{c}\vec{p}\cdot\vec{A} - \frac{q}{c}\vec{A}\cdot\vec{p} + \frac{q^2}{c^2}A^2) + q\phi\right]\psi &= \psi^*\frac{\partial\psi}{\partial t} \\
(i\hbar)^{-1}\psi^*\left[\frac{1}{2m}(-\hbar^2\nabla^2 + i\hbar\frac{q}{c}(\vec{\nabla}\cdot\vec{A}) + i\hbar\frac{2q}{c}\vec{A}\cdot\vec{\nabla} + \frac{q^2}{c^2}A^2) + q\phi\right]\psi &= \psi^*\frac{\partial\psi}{\partial t}
\end{aligned}$$

Note that $\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p} = 2\vec{A}\cdot\vec{p} - i\hbar(\nabla\cdot\vec{A})$. Taking the complex conjugate of the above equation gives

$$(-i\hbar)^{-1}\psi\left[\frac{1}{2m}(-\hbar^2\nabla^2 - i\hbar\frac{q}{c}(\vec{\nabla}\cdot\vec{A}) - i\hbar\frac{2q}{c}\vec{A}\cdot\vec{\nabla} + \frac{q^2}{c^2}A^2) + q\phi\right]\psi^* \;=\; \psi\frac{\partial\psi^*}{\partial t}\,.$$

Adding these two equations gives

$$\begin{aligned}\frac{\hbar}{2mi}\left[-\psi^*\nabla^2\psi+\psi\nabla^2\psi^*\right]+\frac{q}{mc}\left[\psi^*\vec{A}\cdot\vec{\nabla}\psi+\psi\vec{A}\cdot\vec{\nabla}\psi^*+(\vec{\nabla}\cdot\vec{A})\psi^*\psi\right] &= \frac{\partial}{\partial t}(\psi^*\psi)\\ \vec{\nabla}\cdot\left[\frac{\hbar}{2mi}(\psi\nabla\psi^*-\psi^*\nabla\psi)+\frac{q}{mc}\psi^*\psi\vec{A}\right] &= \frac{\partial}{\partial t}(\psi^*\psi)\,,\end{aligned}$$

giving the current

$$\vec{j}=\frac{\hbar}{2mi}(\psi^*\nabla\psi-\psi\nabla\psi^*)-\frac{q}{mc}\psi^*\psi\vec{A}$$

that satisfies the continuity equation

$$\vec{\nabla}\cdot\vec{j}+\frac{\partial\rho}{\partial t}=0\,.$$

## 2.2 Aharonov-Bohm effect

Classically, charged particles respond to electric and magnetic fields via the classical force

$$\vec{F}=q(\vec{E}+\frac{\vec{v}}{c}\times\vec{B})\,.$$

This is a local effect; the path of charged particles does not depend on distant $\vec{E}$ and $\vec{B}$ fields.

The phase of $\psi$ does depend on $\vec{A}$, not $\vec{B}$. For example, one can set $\vec{A}=0$ along a *single* given path from $\vec{r}_0$ to $\vec{r}_1$ parametrized by distance $s$ by carrying out a gauge transformation with $\frac{d\Lambda}{ds}=\vec{\nabla}\Lambda\cdot d\vec{s}=-\vec{A}\cdot d\vec{s}$. This gauge change modifies the wave function at $\vec{r}_1$ by a phase change,

$$\psi(\vec{r}_1)\to e^{-i(q/\hbar c)\int_{\vec{r}_0}^{\vec{r}_1}\vec{A}\cdot d\vec{s}}\psi(\vec{r}_1)\,.$$

So $\vec{A}$ along a path gives a change in the phase of the wave function. This time-independent change in phase along a *single* path leads to no observable effects.

But relative changes in phases along two paths can lead to changes in interference: a quantum particle can explore more than one path simultaneously, so changes in $\vec{A}$ can lead to observable effects!

If we compare the phase change due to $\vec{A}$ for two paths of a particle about a solenoid, we can see this interference effect, whenever the flux is *not* a multiple of the flux quantum $\frac{hc}{q}$.

This interference effect has applications in imaging. Tonomura's group at Hitachi lab has imaged vortices of magnetic flux in superconductors using this effect. [INSERT PICTURE].

This sensitivity to magnetic fields is used in SQUID (Superconducting Quantum Inteference Detector) [CHECK ACRONYM] or even for electrons in mesoscopic devices.

### 2.3 Electromagnetic modes

We can simply express solutions to the wave equation for $\vec{A}$ using plane waves in a box of volume $V$ as

$$\vec{A}(\vec{r},t) = \sum_{k\vec{\lambda}} \frac{1}{\sqrt{V}} \left[ A_{k\vec{\lambda}} \vec{\lambda}(\vec{k}) e^{i(\vec{k}\cdot\vec{r}-\omega t)} + A^*_{\vec{k}\lambda} \vec{\lambda}^*(\vec{k}) e^{-i(\vec{k}\cdot\vec{r}-\omega t)} \right] ,$$

where the second term is the c.c. of the first to ensure that $\vec{A}$ is real (which it must be, in order for particle conservation to hold and for $\vec{B}$ to be real) and the $V^{-1/2}$ factor is a convenient normalization. The Coulomb gauge condition $\vec{\nabla}\cdot\vec{A} = 0$ is satisfied iff $\vec{k}\cdot\vec{\lambda} = 0$. The polarization vectors $\vec{\lambda}$ can be complex, but one often chooses two plane polarizations, with $\vec{\lambda_{1,2}} \perp \vec{k}$, $\vec{\lambda}_1 \perp \vec{\lambda}_2$. The scalar $A_{\vec{k}\lambda}$ gives the amplitude and phase of the wave.

The total electromagnetic energy in the volume $V$ is

$$E = \sum_{\vec{k}\vec{\lambda}} \frac{\omega^2}{2\pi c^2} |A_{\vec{k}\lambda}|^2 .$$

# 3 Calculating electromagnetic transition rates

So let's imagine a single-electron atom in its ground state and bathed in incoherent radiation, such as from a typical black body or vapor lamp. How long does the atom spend in the ground state $|0\rangle$ before it is excited to a given state $|n\rangle$ of higher energy?

Applying Fermi's golden rule gives

$$\Gamma_{0\to n} \quad = \quad \frac{2\pi}{\hbar} |\langle n| \left(\frac{-e}{mc}\right) \vec{A}\cdot\vec{p}|0\rangle|^2 \delta(E_n - E_0 - \hbar\omega) ,$$

where the interaction term that is proportional to $A^2$ in the interaction Hamiltonian has been dropped, taking the intensity of the incident radiation small compared to the electric field due to the nucleus of the atom and we are working in the Coulumb gauge, $\vec{A}\cdot\vec{p} = \vec{p}\cdot\vec{A}$.

For light atoms, transitions involve photons with wavelengths of the order of 100's of nm, much larger than the atomic size of order $0.1\,\mathrm{nm}$, so it is fair to write $A_{\vec{k}\vec{\lambda}} e^{-i\vec{k}\cdot\vec{r}}$ just as $A_{\vec{k}\vec{\lambda}}$ (in a moment we will see why this is referred to as the electric dipole approximation).

Writing this as a sum over incoherent positive-frequency modes (since absorption) gives

$$\Gamma_{0\to n} \quad = \quad \frac{2\pi}{\hbar} \sum_{\vec{k},\vec{\lambda}} V^{-1} |A_{\vec{k}\vec{\lambda}}|^2 |\langle n| \left(\frac{-e}{mc}\right) \vec{\lambda}\cdot\vec{p}|0\rangle|^2 \delta(E_n - E_0 - \hbar\omega) .$$

Now consider the matrix element $\langle n|\vec{p}|0\rangle$. Using $\vec{p}/m = (i\hbar)^{-1}[\vec{r}, H_0]$,

$$\begin{aligned}\langle n|\vec{p}|0\rangle &= \frac{m}{i\hbar}\langle n|(\vec{R}H_0 - H_0\vec{R})|0\rangle \\ &= \frac{m}{i\hbar}(E_0 - E_n)\langle n|\vec{R}|0\rangle\,.\end{aligned}$$

Using $(E_n - E_0) = \hbar\omega$, we can now write

$$\Gamma_{0\to n} = \frac{2\pi e^2}{\hbar c^2}\sum_{\vec{k},\vec{\lambda}}\omega^2 V^{-1}|A_{\vec{k}\vec{\lambda}}|^2|\lambda\cdot\langle n|\vec{R}|0\rangle|^2\delta(E_n - E_0 - \hbar\omega)\,.$$

To carry out the calculation further, we need to work with the sum $\sum_{\vec{k},\vec{\lambda}}$, to convert it into an integral over energy. As the dispersion relation for light is rather simple, $\omega = ck$,

$$\sum_{\vec{k}} \to \left(\frac{L}{2\pi}\right)^3\int d^3k = V\int\frac{k^2 dk d\Omega}{(2\pi)^3} = V\int\frac{\omega^2 d\omega d\Omega}{(2\pi c)^3}\,,$$

we get

$$\begin{aligned}\Gamma_{0\to n} &= \frac{2\pi e^2}{\hbar c^2(2\pi c)^3}\int d\omega d\Omega\omega^4|A_{\vec{k}\vec{\lambda}}|^2|\lambda\cdot\langle n|\vec{R}|0\rangle|^2\delta(E_n - E_0 - \hbar\omega) \\ &= \frac{2\pi e^2\omega^4}{\hbar^2 c^2(2\pi c)^3}\int d\Omega|A_{|\vec{k}|=\omega/c,\vec{\lambda}}|^2|\lambda\cdot\langle n|\vec{R}|0\rangle|^2\,.\end{aligned}$$

Consider radiation incident upon the atom from an incoherent polarized source with an intensity measured in energy per unit solid angle per frequency interval, $I(\omega)$. It turns out that

$$I(\omega) = \frac{d\Omega\omega^4|A_{k\lambda}|^2}{(2\pi c)^4}\,.$$

Substituting this in gives

$$\Gamma_{0\to n} = \frac{2\pi e^2\omega^4}{\hbar c^2(2\pi c)^3}(2\pi c)^4\omega^{-4}I(\omega)|\lambda\cdot\langle n|\vec{R}|0\rangle|^2\,.$$