April 3, 2007

LECTURE #20

Quantum Generalization of
The Lorentz Model
Rigorous deduction of the oscillator strength
The Lorentz and Drude Models and Their Extension to Quantum Mechanical Two Level Systems.

Basic model - Lorentz

charge \( q \), field \( \vec{E} \), mass \( m \) constrained by a spring with viscous forces included

\[
\frac{m d^2 \vec{x}}{dt^2} + \gamma m \frac{d \vec{x}}{dt} + m \omega_0^2 \vec{x} = q \vec{E}
\]

inertial viscous potential energy

\[
\omega_0 = \frac{k}{\sqrt{m}} ; \quad k = \text{spring constant.}
\]

Extension to 2 level quantum system

\[
H |\psi_2\rangle = E_2 |\psi_2\rangle ; \quad E_2 > 2 |\psi_2\rangle
\]

\[
H |\psi_1\rangle = E_1 |\psi_1\rangle ; \quad E_1 < 1 |\psi_1\rangle
\]

- Dipole moment /Vol = \( N q \Delta \vec{r} \); \( N = \frac{N_0}{m^3} \)

- For quantum system \( N \rightarrow (N_2(t) - N_1(t)) \)

\( N_2(t) \) = upper level population density

\( N_1(t) \) = lower "

- Equation for \( N_2(t) - N_1(t) \)

\[
\frac{d}{dt} (N_2(t) - N_1(t)) = \left| \frac{\vec{E}}{T_1} \right|^2 \sum_{\text{m}} (N_2(t) - N_1(t)) \left[ (N_2(t) - N_1(t)) - (N_{20} - N_{10}) \right]
\]

when system leaves \( \psi_1 \), it necessarily goes into \( \psi_2 \) (closed)

Simple relaxation to an equilibrium population difference with characteristic time \( T_1 \) (Markov Approx)
Oscillator strength - rigorous derivation (2)

A quantum system does not necessarily correspond to 1 full electron making the transition. Introduce the oscillator strength \( f \) by writing (1) as

\[
\frac{d^2 \tilde{E}}{dt^2} + \kappa \frac{d \tilde{E}}{dt} + \omega_0^2 \tilde{E} = f \frac{q^2}{m} (N_1 - N_2) \quad \text{(1)}
\]

Form of \( f \)

1) Involves dipole perturbation

\[
\nu_{21} = \int \psi_2^* \mathbf{E} \psi_1 \, dV
\]

Dipole coupling between states 2 and 1. This enters through the Schrödinger Equation

\[
H = H_0 - \mathbf{\hat{p}} \cdot \mathbf{E}
\]

\[
H |\psi\rangle = \frac{\partial}{\partial t} |\psi\rangle
\]

Let \( |\psi\rangle = |\psi\rangle \ e^{-iH_0 \frac{\Delta t}{\hbar}} \) so

Now consider the expectation of the dipole moment. Letting \( |\psi\rangle \) be a linear superposition of \( |\psi_1\rangle \) and \( |\psi_2\rangle \)

\[
|\psi\rangle = A_1 |\psi_1\rangle + B_1 |\psi_2\rangle e^{\frac{-iE_1 t}{\hbar}} + B_2 |\psi_2\rangle e^{\frac{-iE_2 t}{\hbar}}
\quad \text{(2)}
\]

where \( H_0 |\psi_1\rangle = E_1 |\psi_1\rangle \) and \( H_0 |\psi_2\rangle = E_2 |\psi_2\rangle \)

Consider \( \langle \psi_1|\rho|\psi_1\rangle \) and generally \( \langle \psi_1|\rho|\psi_2\rangle \) and \( \langle \psi_2|\rho|\psi_2\rangle \) are taken as zero (why?).

So

\[
\langle \psi_1|\rho|\psi_1\rangle = A_1^* A_1 \langle \psi_1|\rho|\psi_1\rangle e^{\frac{i(E_1 - E_2) t}{\hbar}} + \text{c.c.} \quad \text{(3)}
\]

\( |\psi_1\rangle \) and \( |\psi_2\rangle \) are "stationary" eigenstates and thus are independent of time. \( \langle \psi_1|\rho|\psi_1\rangle = \langle \psi_2|\rho|\psi_2\rangle = 1 \)
Take the time derivative of \( \langle \psi_1 | \psi_2 \rangle \)
\[
\frac{d}{dt} \langle \psi_1 | \psi_2 \rangle = \left( \frac{\partial A}{\partial t} + A \frac{\partial B}{\partial t} \right) e^{i(E_1 - E_2) t} \langle \psi_1 | \psi_2 \rangle + \text{complex conjugate}
\]

Now apply perturbation:

1) Start out in lower state \( |\psi_1\rangle \) and assume the change in this is small. \( |\psi_2\rangle \) is initially unoccupied. Thus at \( t=0 \)
\[
\langle \psi_1 | \psi_1 \rangle = 1 \quad \langle \psi_2 | \psi_2 \rangle = 0
\]
we must always have \( \langle \psi_1 | \psi_1 \rangle + \langle \psi_2 | \psi_2 \rangle = 1 \)

As an example a 10% change in \( |\psi_1\rangle \) is small but the change in \( |\psi_2\rangle \) is significant since it was unoccupied initially.

2) \( |\psi\rangle \) satisfies the Schrödinger Equation \( H |\psi\rangle = \text{im} |\psi\rangle \)
with \( H = H_0 + \vec{P} \cdot \vec{E} \)

3) Taking \( \langle \psi_1 | \) and \( \langle \psi_2 | \), respectively,
\[
\langle \psi_1 | H_0 - \vec{p} \cdot \vec{E} | \psi_2 \rangle = (\text{im} \frac{\partial A}{\partial t} + E_1 A) e^{-iE_1 t} \]
\[
E_1 A = \langle \psi_1 | \psi_1 \rangle B e^{iE_1 t} = (\frac{\partial A}{\partial t} + E_1 A) e^{iE_1 t}
\]
and
\[
- \text{im} E_1 \langle \psi_2 | \psi_2 \rangle A = \text{im} \frac{\partial A}{\partial t} e^{iE_1 t}
\]

4) Because of 1) the second of these is the important one \( (A \equiv \text{const} \approx 1) \)

5) Thus from the top of the page \( (A = 1) \)
(sub for \( \delta B/\delta t \))
\[
\frac{d}{dt} \langle \psi_1 | \psi_2 \rangle = - \frac{A A}{\frac{1}{\hbar}} E \cdot \langle \psi_2 | \psi_1 \rangle \langle \psi_1 | \psi_2 \rangle
\]
\[
+ \text{c.c.} \quad + \frac{i}{\hbar} E (E_1 - E_2) \langle \psi_1 | \psi_2 \rangle
\]
6) Assuming \( E(t, r) = E_0 e^{i(wt - kr)} + \text{c.c.} \) (4)
and we are at \( r = 0 \) (and \( k << \text{size of atom} \))
use phasors to solve. Pick \( e^{-i\omega t} \) term
(its resonant)

\[
\frac{\partial}{\partial t} \langle \psi_1 \vert \rho \vert \psi_2 \rangle - i \hbar \left( E_1 - E_2 \right) \langle \psi_1 \vert \rho \vert \psi_2 \rangle e^{-i\omega t} \\
= -\frac{i}{\hbar} E_0 \cdot \langle \psi_2' \vert \rho \vert \psi_1' \rangle \langle \psi_1' \vert \rho \vert \psi_2' \rangle e^{-i\omega t}
\]

The L.H.S phasor terms are (from Eq. (3))

\[
\frac{\partial}{\partial t} (A^* \cdot B \cdot \langle \psi_1 \vert \rho \vert \psi_2 \rangle e^{i(0 - E_2)/\hbar t})
\]

and thus the two L.H.S terms just become

\[
\frac{\partial}{\partial t} \left( \frac{\partial A^*(t) \cdot B(t)}{\partial t} \right) \cdot e^{i(0 - E_2)/\hbar t} \text{ (which equals from above)}
\]

\[
= -\frac{i}{\hbar} E_0 \cdot \langle \psi_2' \vert \rho \vert \psi_1' \rangle^2 \cdot e^{i(0 - E_2)/\hbar t}
\]

where for short-hand write \( \langle \psi_2' \vert \rho \vert \psi_1' \rangle^2 = \\
\langle \psi_2' \vert \rho \vert \psi_1' \rangle \langle \psi_1' \vert \rho \vert \psi_2' \rangle \text{ (and } E_2 = E_2 - E_1 \text{)}
\]

Thus

\[
\frac{\partial A^* B}{\partial t} = \frac{i}{\hbar} E_0 \cdot \langle \psi_2' \vert \rho \vert \psi_1' \rangle^2 \cdot e^{-i(0 - E_2)/\hbar t}
\]

And \( A^* B = 0 \text{ at } t = 0 \)

\[
A^* B = \frac{1}{\hbar} \frac{1}{i} E_0 \cdot \langle \psi_2' \vert \rho \vert \psi_1' \rangle^2 \cdot e^{-i(0 - E_2)/\hbar t}
\]

And thus the phasor \( \langle \psi_1 \vert \rho \vert \psi_2 \rangle \) is

\[
\langle \psi_1 \vert \rho \vert \psi_2 \rangle = -\frac{1}{i} \frac{\langle \psi_2' \vert \rho \vert \psi_1' \rangle^2}{\hbar} \cdot E_0 \text{ at } t = 0
\]

The total \( \langle \psi_1 \vert \rho \vert \psi_2 \rangle \) is this + c.c. (resonant terms)
This is to be compared with the classical expression for the phasor solution \( \mathbf{E} = E_0 \, e^{-i \omega t} \)

\[
\begin{align*}
\mathbf{\dot{E}} &= \frac{-\omega^2 + i \omega \left( \omega_0 + \omega_0 \right) + \omega_0^2}{m M} \mathbf{E} \\
\mathbf{\ddot{E}} &= \frac{-\omega^2 + i \omega \left( \omega_0 + \omega_0 \right) + \omega_0^2}{m M} \mathbf{E} \\
\mathbf{\dddot{E}} &= \frac{-\omega^2 + i \omega \left( \omega_0 + \omega_0 \right) + \omega_0^2}{m M} \mathbf{E}
\end{align*}
\]

near resonance. With \( \omega_0 = \frac{1}{2} (\omega_2 - \omega_1) / \hbar \)

neglecting \( \Gamma \) (damping), we see that to obtain the quantum result \( \hbar \mathbf{p}^2 \) should

be \( \frac{1}{\hbar} \mathbf{\dot{p}}^2 \) (where \( \mathbf{\dot{p}} = \langle \psi_2 | \mathbf{\dot{p}} | \psi_1 \rangle \)). This one can do by introducing \( f = \frac{2m \omega_0 \mathbf{\dot{p}}^2}{\hbar} \) into the classical oscillator equation.