

limit as $\epsilon \rightarrow 0$ of this sum exists and is finite, but it is not purely real. To understand this we make a digression into distribution theory.

A distribution is like a ~~real~~ function but is not a real function, although it can be considered the limit of a real function. Instead, a distribution only has meaning when used under an integral.

The most familiar distribution is the "δ-function", which can be thought of as a limit,

$$\delta(x-x_0) = \lim_{a \rightarrow 0} \frac{1}{\sqrt{2\pi a^2}} e^{-(x-x_0)/2a^2}$$

$$= \lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \frac{\epsilon}{(x-x_0)^2 + \epsilon^2}$$

As shown, there are several different limits of real functions that produce the δ-function. Although we write such "bare" formulas as this, the limits indicated do not really exist ($\delta(x-x_0)$ is not a real function), instead it is understood that the limits should be taken under an integral sign.

(20)

Now consider an integral of the form

$$\lim_{\epsilon \rightarrow 0} \int_a^b dx \frac{f(x)}{x-x_0-i\epsilon},$$

which captures the essence of the k -integral that must be done in the expression for $D(E+i\epsilon)$ as $\epsilon \rightarrow 0$. Here the range of integration $[a, b]$ is assumed to straddle the singularity at $x=x_0$. We ~~can't~~^{break} the function $\frac{1}{x-x_0-i\epsilon}$ into its real and imag. parts,

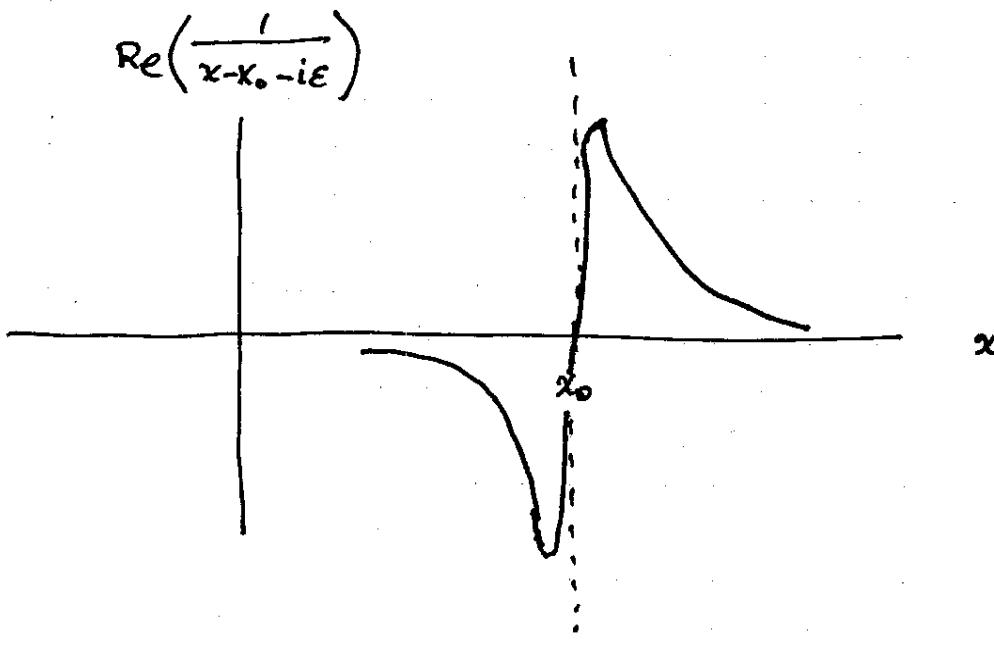
$$\frac{1}{x-x_0-i\epsilon} = \frac{x-x_0}{(x-x_0)^2 + \epsilon^2} + \frac{i\epsilon}{(x-x_0)^2 + \epsilon^2}.$$

On taking the limit $\epsilon \rightarrow 0$, the imaginary part becomes one of the standard representations of the δ -fn,

$$\lim_{\epsilon \rightarrow 0} \frac{1}{x-x_0-i\epsilon} = \begin{pmatrix} \text{real} \\ \text{part} \end{pmatrix} + \overset{i\pi}{\cancel{\delta}}(x-x_0),$$

so the imaginary part of the integral above is nonzero (in fact it is $i\pi f(x_0)$).

What about the real part? Let's plot the real part for small but nonzero ϵ :



For $\epsilon \neq 0$, the real part of the integral (of this fn times the smooth fn $f(x)$) is defined, and moreover the limit is ($\epsilon \rightarrow 0$) well defined, too, if $f(x)$ is smooth at x_0 . In effect we have a prescription for resolving the $\infty-\infty$ in the integral $\int dx \frac{f(x)}{x-x_0}$; it is interpreted as

$$\lim_{\epsilon \rightarrow 0} \int dx f(x) \frac{x-x_0}{(x-x_0)^2 + \epsilon^2}.$$

This gives us another distribution, called the "principal part of $\frac{1}{x-x_0}$ ". Notations for this distribution include

$$\frac{\mathcal{P}}{x-x_0} = \mathcal{P}\left(\frac{1}{x-x_0}\right) = \lim_{\epsilon \rightarrow 0} \frac{x-x_0}{(x-x_0)^2 + \epsilon^2}.$$

This limit, as in the case of the δ -fn, is not meaningful in this "bare" formula, but instead must be used under an integral.

(22)

Like the δ -fn, there is more than one representation for the principal value. Two of them are:

$$\begin{aligned} \int_a^b dx f(x) P\left(\frac{1}{x-x_0}\right) &= \lim_{\epsilon \rightarrow 0} \int_a^b dx f(x) \frac{x-x_0}{(x-x_0)^2 + \epsilon^2} \\ &= \lim_{\epsilon \rightarrow 0} \left[\int_a^{x_0-\epsilon} + \int_{x_0+\epsilon}^b \right] \frac{f(x)}{x-x_0}. \end{aligned}$$

Now using the distribution notation, we can write

$$\begin{aligned} D(E) &\equiv \lim_{\epsilon \rightarrow 0} D(E+i\epsilon) \\ &= E - E_B - P \sum_{A\lambda} \frac{|\langle A\lambda | H_1 | B_0 \rangle|^2}{E - E_A - \omega} + i\pi \sum_{A\lambda} \delta(E - E_A - \omega) \times \\ &\quad |\langle A\lambda | H_1 | B_0 \rangle|^2. \end{aligned}$$

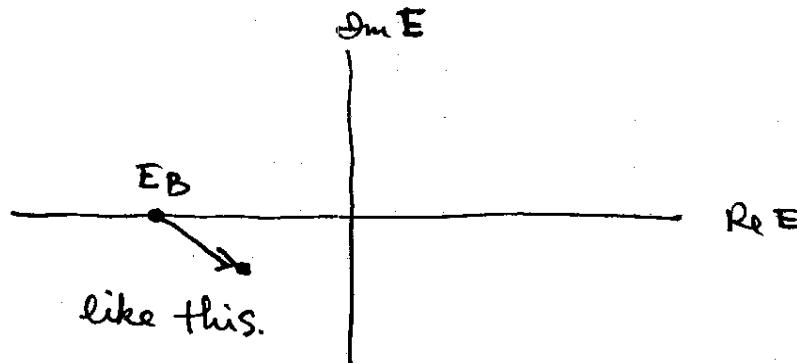
The imaginary part of $D(E)$ is nonzero (positive in fact), so $D(E)$ has no zero on the real axis. Therefore $\langle B_0 | G(z) | B_0 \rangle = 1/D(z)$ has no pole on the real axis, either, and the discrete state $|B_0\rangle$ of the unperturbed system ceases to exist as a discrete state when we turn on the perturbation. In the perturbed system, there are only continuum states near $E=E_B$; the discrete state of the unperturbed system has "dissolved into the continuum." This is a way of saying

(23)

that it has become a resonance.

The discrete state $|B_0\rangle$ of the unperturbed system is an example of a discrete state imbedded in the continuum. We saw such states previously in the doubly excited states of helium. In the present case, $|B_0\rangle$ (speaking of the unperturbed system) lies in a continuum of states $|A\lambda\rangle$, assuming $E_A < E_B$, where the frequency ω of the photon can vary continuously in an interval around $\omega = E_B - E_A = \omega_{BA}$. These of course are the photon states to which our initial state $|B_0\rangle$ makes transitions when the perturbation is turned on.

The pole of the Green's fn at $z=E_B$ in the unperturbed system does not disappear, however, when we turn the perturbation on, instead it moves into the lower γ_2 plane:



Let us ~~denote~~ denote the shift in the pole of $\langle B_0 | G(z) | B_0 \rangle$ (the shift in the zero of $D(z)$) by Δz , which we assume is

(24)

small, since the correction term (the sum \sum_{λ} etc) is $\Theta(H^2)$. To find Δz we set $E = E_B + \Delta z$ in the formula for $D(E)$,

$$D(E_B + \Delta z) = 0 = E_B + \Delta z - E_B - \wp \sum_{A\lambda} \frac{|\langle A\lambda | H_1 | B0 \rangle|^2}{E_B - E_A - \omega} + i\pi \sum_{A\lambda} \delta(E_B - E_A - \omega) |\langle A\lambda | H_1 | B0 \rangle|^2,$$

where we have just replaced E by E_B (ignoring Δz) in the correction terms, which are already small. This gives

$$\Delta z = \wp \sum_{A\lambda} \frac{|\langle A\lambda | H_1 | B0 \rangle|^2}{\omega_{BA} - \omega} - i\pi \sum_{A\lambda} \delta(\omega_{BA} - \omega) |\langle A\lambda | H_1 | B0 \rangle|^2.$$

Notice that $\text{Im } \Delta z < 0$. Notice also that the imaginary part of the shift is ~~$-i\Gamma/2$~~ $-i\Gamma/2$, where Γ is the decay rate of state B according to 1st order TDPT (see p. 3).

The real part can also be put into a more familiar looking form. Recall from bound state perturbation theory (see Eq. 19.23) that the second order energy shift of a state due to a perturbation is a sum over intermediate states of a square of a matrix element divided by an energy denominator. It is not valid to use bound state perturbation theory on the state $|B0\rangle$ because it is embedded in the continuum (it is not separated in energy from other states of the system), but if

(25)

if we used the formula 19.23 anyway for $|B_0\rangle$ with perturbation H_1 , we would get

$$\Delta E_{B_0}^{(2)} = \sum_{k \neq B_0} \frac{|\langle k | H_1 | B_0 \rangle|^2}{E_B - E_k}$$

means, 2nd order pertn. theory

Restricting the sum over $|k\rangle$ to only one-photon states $|A\lambda\rangle$, since only these can be reached from $|B_0\rangle$ by applying H_1 , we get

$$\Delta E_{B_0}^{(2)} = \sum_{A\lambda} \frac{|\langle A\lambda | H_1 | B_0 \rangle|^2}{E_B - E_A - \omega},$$

which is precisely the real part of Δz , except for the principal value. In fact, without the principal value, this expression for $\Delta E_{B_0}^{(2)}$ is not defined. So let's just define

$$\Delta E_{B_0}^{(2)} = P \sum_{A\lambda} \frac{|\langle A\lambda | H_1 | B_0 \rangle|^2}{E_B - E_A - \omega},$$

so that

$$\Delta z = \Delta E_{B_0}^{(2)} - i \frac{\Gamma_B}{2}$$

where we now put a B subscript on Γ because it is the decay rate of state B.

We seem to be dealing with the energy shifts in the atomic state $|B\rangle$ due to the interactions with the field. What happened to the first order energy shift?

(26)

By Eq. 19.23, this should be.

$$\Delta E_{B0}^{(1)} = \langle B_0 | H_1 | B_0 \rangle = 0,$$

since H_1 changes the number of photons. Therefore to make the formula look nicer, we can write

$$\Delta z = \Delta E_{B0}^{(1)} + \Delta E_{B0}^{(2)} - i\Gamma_B/2,$$

i.e., $D(z)$ has a ~~zero~~^{zero} at

$$\begin{aligned} z &= E_B + \Delta E_{B0}^{(1)} + \Delta E_{B0}^{(2)} - i\Gamma_B/2 \\ &= \tilde{E}_B - i\Gamma_B/2, \end{aligned}$$

where

$$\tilde{E}_B = E_B + \Delta E_B^{(1)} + \Delta E_B^{(2)}$$

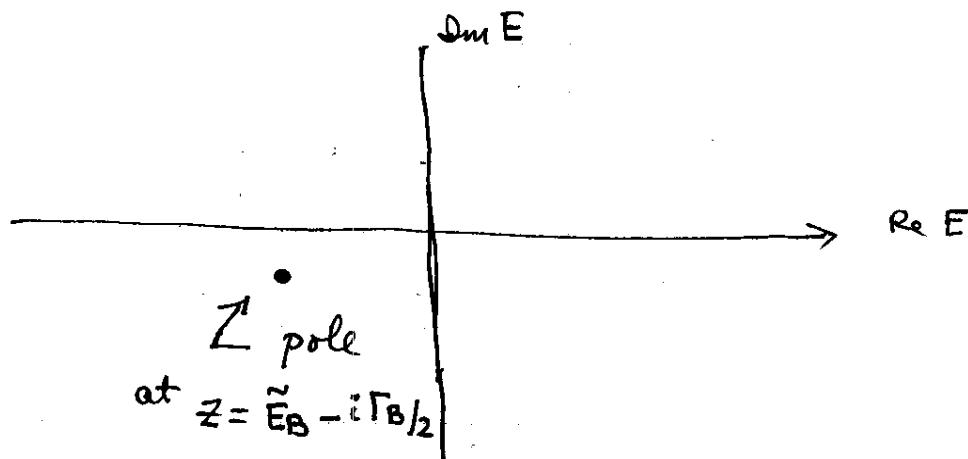
is the real part of the energy, corrected for the interaction with the field. *

It is as if the total energy of the excited state of the atom-plus-field is complex. The Hamiltonian for the system is Hermitian so all energy eigenvalues are real, but the state $|B_0\rangle$ evolves in time approximately as if it had a complex energy. The imaginary part of the energy is responsible for the decay of the state, as is strongly suggested by its relation to Γ . We will see this decay

more explicitly in a moment.

Now we can write out the inverse Laplace transform for the amplitude $a_{B0}(t)$ for the system to remain in the initial state. We can push the contour down onto the real axis since $D(E) \neq 0$ there. This gives

$$a_{B0}(t) = -\frac{1}{2\pi i} \int_{C+}^{+\infty} dE \frac{e^{-iEt}}{D(E)}$$



The denominator $D(E)$ is smallest for real E when E is closest to the pole, i.e. when $E \approx \tilde{E}_B$. The integral is dominated by the contributions from this region. Let us write $E = \tilde{E}_B + \Delta E$ ($\Delta E = \text{real}$), so that

$$D(E) = D(\tilde{E}_B + \Delta E) = \tilde{E}_B + \Delta E - E_B - \Delta E_B^{(2)} + i\Gamma_B/2,$$

where we have just replaced E in the 2nd order terms by E_B . Thus,

$$D(E) \approx \Delta E + i\Gamma_B/2 = (E - \tilde{E}_B) + i\Gamma_B/2$$

in the region of the energy axis where the integrand is largest.

Thus

$$Q_{B0}(t) = \frac{-1}{2\pi i} \int_{-\infty}^{+\infty} dE \frac{e^{-iEt}}{E - \tilde{E}_B + i\Gamma_B/2}$$

By closing the contours in the lower $\frac{1}{2}$ plane this integral can be done, giving

$$Q_{B0}(t) = e^{-i\tilde{E}_B t - \Gamma_B t/2}$$

The real part of the phase has been corrected by the real energy shift $\Delta E_B^{(2)}$, and there has appeared a damping term.

Taking the square, we have

$$P_{B0}(t) = e^{-\Gamma_B t}$$

showing the exponential decay law.

This derivation has been based on a model of an atom, but applies in its essence to the decay of any excited state of a system, including radioactive decays of nuclei and decays of unstable particles. The derivation looks complicated, but that is because the exponential law is

not exact. The usual "simple" derivations of the exponential decay law rely on a type of statistical assumption of the Markov type, which means that the transition probability for a system depends only on the present state and not the previous history. This is what we usually assume about radioactive decay. For example, if a nucleus has not decayed after 10 times its average lifetime, the probability that it will decay in the next second is the same as it always was. The nucleus does not try to "hurry up and decay" because it has failed to decay for so long. At least this is what we assume. But if we study the decay by solving the Schrödinger equation, we find that the exponential decay law is only approximate. See the Appendix in the first volume of Sakurai.

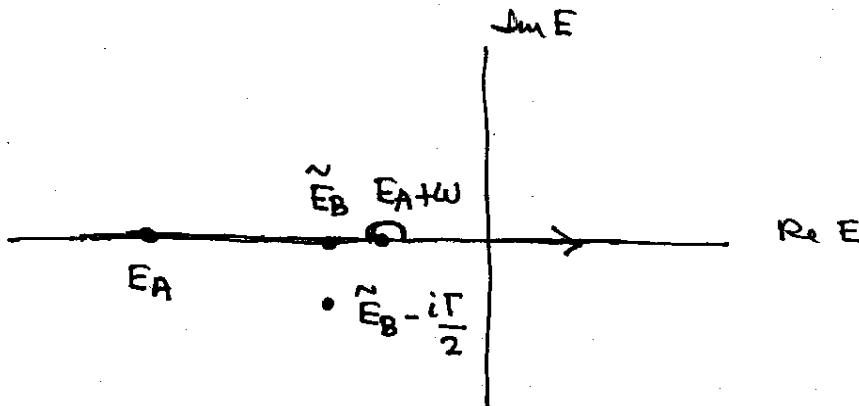
We can also compute the amplitudes to make transitions to various final states $|A\lambda\rangle$. By the inverse Laplace transform we have

$$a_{A\lambda}(t) = -\frac{1}{2\pi i} \int_{C+} dz \frac{e^{-izt}}{(z-E_A-\omega) D(z)} \langle A\lambda | H_1 | B\rangle .$$

The matrix element is independent of z and can be taken out of the integral. The integrand has poles at $z = E_A + \omega$

(on the real axis) and at $z = \tilde{E}_B - i\Gamma_B/2$.

This amplitude can be computed for any final state $A\lambda$, including those whose energy is not close to that of the initial state E_B . But the amplitude will be small unless energy is approximately conserved. Therefore let us assume that $E_A + \omega \approx E_B \approx \tilde{E}_B$. Moving the contour C_+ down onto the real axis but avoiding the pole at $z = E_A + \omega$, we get a picture like this:



We assume $E_A < E_B$, so $E_A + \omega$ can be placed near E_B or \tilde{E}_B for some $\omega > 0$. Then the 2 poles of the integrand are near one another, in a region where

$$\mathcal{D}(E) \approx E - \tilde{E}_B + i\Gamma_B/2.$$

This region dominates the integral, so

$$a_{A\lambda}(t) \approx \frac{-1}{2\pi i} \int_{C_+} dz \frac{e^{-izt}}{(z - E_A - \omega)(z - \tilde{E}_B + i\Gamma_B/2)} \quad \langle A\lambda | H_1 | B_0 \rangle$$

$$= \left[\frac{e^{-i(E_A+\omega)t}}{E_A + \omega - \tilde{E}_B + i\Gamma_B/2} + \frac{e^{-i(\tilde{E}_B t - \Gamma_B/2)}}{\tilde{E}_B - i\frac{\Gamma_B}{2} - E_A - \omega} \right] \langle A\lambda | H_1 | B_0 \rangle$$

where we evaluate the integral by the residue theorem.

This can be written

$$a_{A\lambda}(t) = \frac{\langle A\lambda | H_1 | B_0 \rangle}{\omega - \omega_{BA} + i\Gamma_B/2} e^{-i(E_A+\omega)t} \left[1 - e^{i(\omega - \omega_{BA})t - \Gamma_B t/2} \right]$$

where we have slightly redefined ω_{BA} as $\tilde{E}_B - E_A$ (not $E_B - E_A$).
The phase factor $e^{-i(E_A+\omega)t}$ gets removed if we go to the interaction picture.

If we drop the terms involving Γ_B and ignore the difference between E_B and \tilde{E}_B (these are all 2nd order corrections), then we get the usual result from TDPT,

$$a_{A\lambda}(t) = \langle A\lambda | H_1 | B_0 \rangle \left[\frac{1 - e^{i(\omega - \omega_{BA})t}}{\omega - \omega_{BA}} \right]$$

$$\hookrightarrow -2i e^{i(\omega - \omega_{BA})t/2} \frac{\sin((\omega - \omega_{BA})t/2)}{\omega - \omega_{BA}}$$

But the result above is valid for long times, $t \gtrsim \frac{\hbar}{\Gamma}$.

In the limit $t \gg \frac{\hbar}{\Gamma}$, the factor $e^{-\Gamma t/2} \rightarrow 0$, and

we have

$$a_{A\lambda}(t) = \frac{\langle A\lambda | H_1 | B0 \rangle}{\omega - \omega_{BA} + i\Gamma_B/2} e^{-i(E_A+\omega)t},$$

or, in the interaction picture,

$$C_{A\lambda}(t) = \frac{\langle A\lambda | H_1 | B0 \rangle}{\omega - \omega_{BA} + i\Gamma_B/2}.$$

The amplitudes in the interaction picture are independent of time, indicating that the system is evolving according to the unperturbed Hamiltonian only. H_1 has no effect. This is because when $t \gg \Gamma/\hbar$, the atom has dropped into the lower state and the photon has long since departed, travelling away at the speed of light.

The asymptotic ($t \rightarrow \infty$) probability to find ourselves in state $A\lambda$ is

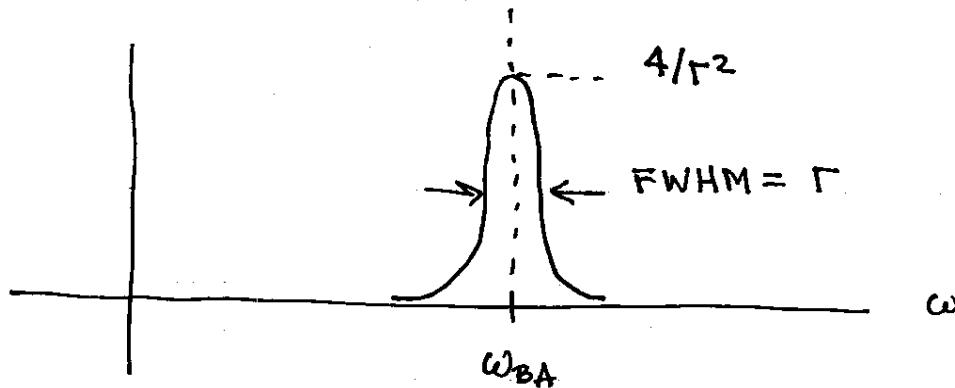
$$P_{A\lambda} = |C_{A\lambda}|^2 = \frac{|\langle A\lambda | H_1 | B0 \rangle|^2}{(\omega - \omega_{BA})^2 + \Gamma_B^2/4}.$$

This probability is largest when $\omega - \omega_{BA} = 0$ and falls off rapidly when $|\omega - \omega_{BA}| \gg \Gamma_B$. Recall that in E1 transitions Γ is of order $\alpha^3 \sim 10^{-6}$ in atomic units, and Γ is even smaller for M1 and higher transitions. Thus the range of

final photon energies over which the probability is appreciable is quite small. This energy is conserved to a good approximation.

It is not exactly conserved, however. Experimentally this is manifested by the fact that there is some spread in photon energies ~~emitted~~ by an atom in an excited state. This spread is called the natural line width of a spectral line. Since it is small, it is easily masked by other sources of line broadening (Doppler shift, pressure broadening), but it can be seen if these other effects are minimized.

The intensity of the emitted radiation as a fn. of frequency is proportional to ~~the square of~~ P_{A2} . But the matrix element is nearly constant over the small range of frequencies near $\omega = \omega_{BA}$ of width Γ_B , so the dependence of the intensity on ω is dominated by the denominator. This is the Lorenzian function, $\frac{1}{(\omega - \omega_{BA})^2 + \Gamma^2/4}$:



The total probability to make a transition when $t \rightarrow \infty$ is

$$P_{\text{decay}} = \sum_{A\lambda} \frac{|\langle A\lambda | H_1 | B0 \rangle|^2}{(\omega - \omega_{BA})^2 + \Gamma^2/4}$$

But since the matrix element varies slowly over the energy difference Γ , we can approximate

$$\frac{1}{(\omega - \omega_{BA})^2 + \Gamma^2/4} = \frac{2\pi}{\Gamma} \delta(\omega - \omega_{BA}).$$

Then

$$P_{\text{decay}} = \frac{2\pi}{\Gamma} \sum_{A\lambda} \delta(\omega - \omega_{BA}) |\langle A\lambda | H_1 | B0 \rangle|^2 = 1$$

by the definition of Γ . Of course this is the answer we must get.

You may wonder why we correct E_B but not E_A for the interaction with the field in

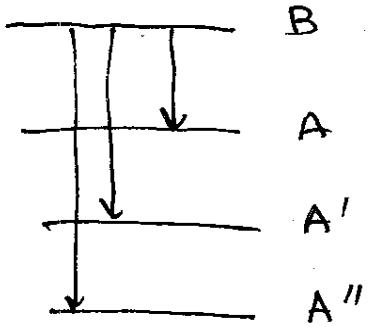
$$\omega_{BA} = \tilde{E}_B - E_A.$$

~~Off/On~~ The answer is that we should make this correction, it just has not appeared in our analysis because we have truncated the Hilbert space at single photon states.

Nor for that matter do we see the decay of state A (there is no Γ_A appearing). If $|A\rangle$ is the ground state

(35)

then $\Gamma_A = 0$, but when there are several states below B in energy, then some of them must have their own decay



rates and we should expect a cascade of decays. Again we do not see that because we have restricted the ket space to single photon states.