We wish to fix the divergences in the Kramers-Heisenberg formula when $\omega = \omega_{IA}$ ($\omega =$ frequency of incident photon, $\omega_{IA} = \epsilon_I - \epsilon_A =$ energy necessary to raise atom from initial state $A$ to "intermediate" state $I$, where $I \rightarrow A$; we use units where $\hbar = 1$, although we restore the $\hbar$'s when it makes a formula look more familiar). A qualitative analysis indicates that the problem has to do with our failure to take into account the decay of state $I$ into lower energy states + a photon. Such processes were not included in our derivation of the K-H formula because that derivation was based on time-dependent perturbation theory (TDPT), which is only valid for short times.

We put the K-H formula on hold and turn attention to the long time behavior of matter interacting with the EM field, where "long time" means times comparable to or longer than the decay time of excited states. We will study a model problem for this purpose, the decay of an excited atomic state into lower states with the emission of a photon.

We assume the initial state of the system is $|BO\rangle$, in which the atom is in state $|B\rangle$
and the photon field is empty, and we will consider a collection of final state $|\text{A}\lambda\rangle = |\text{A}\rangle a_\lambda^+ |0\rangle$, in which the atom is in state $|\text{A}\rangle$ and a photon of mode $\lambda = (\mathbb{F},k)$ has appeared. There may be several states lower in energy than $|\text{B}\rangle$, as shown in the diagram.

First we analyze the process by first order TDPT. The initial and final states and their energies are

$$|i\rangle = |\text{B}0\rangle, \quad E_i = E_B$$
$$|f\rangle = |\text{A}\lambda\rangle, \quad E_f = E_A + \omega$$

$$\omega_{fi} = E_f - E_i = E_A + \omega - E_B = \omega - \omega_{\text{BA}}.$$ 

By 1st order TDPT, the transition amplitudes in the interaction picture are (case $n\neq i$):

$$C_n(t) = C_{\text{A}\lambda}(t) = -2i e^{-i\omega_{fi}t/2} \frac{\sin \omega_{fi}t/2}{\omega_{fi}} \langle \text{A}\lambda | H_1 | \text{B}0 \rangle,$$

where the Hamiltonian is

$$H_0 = \frac{\mathbf{p}^2}{2} + V(\mathbf{r}) + \sum_\lambda \omega_\lambda a_\lambda^+ a_\lambda \quad (\text{single electron atom for simplicity})$$
$$H_1 = \frac{1}{c} (\mathbf{p} \cdot \mathbf{A}(\mathbf{r}) + \mathbf{E} \cdot \mathbf{B}(\mathbf{r}))$$
$$H_2 = \frac{1}{2c^2} \mathbf{A}(\mathbf{r})^2$$

We ignore $H_2$ in the matrix element because we are only working to 1st order of perturbation theory. Squaring to get the
probabilities, we have

\[ P_{\lambda \alpha}(t) = 2\pi t \Delta_t (\omega - \omega_{BA}) \left| \langle \alpha|H_1|\beta \rangle \right|^2 \]

using notation from earlier notes for the function \( \Delta_t \), or, dividing by \( t \) and summing on \( \lambda \) to get the total transition rate,

\[
\omega_{\text{decay}} = \frac{2\pi}{\lambda} \sum_{\lambda} \delta (\omega - \omega_{BA}) \left| \langle \alpha|H_1|\beta \rangle \right|^2 \approx \frac{\Gamma}{\hbar}
\]

Here we have assumed \( t \) is long enough to replace \( \Delta_t \) by \( \delta \), and we have introduced standard notation for the lifetime of an excited state, which is \( \Gamma \) in energy units or \( \Gamma/\hbar \) in units of time\(^{-1}\).

A \( \delta \)-fn is only meaningful under an integral sign, but in the notation \( \sum_{\lambda} \) we intend that the limit \( N \to \infty \) (\( N \) = volume of box) is taken, so \( \sum_{\lambda} \) really means

\[
\sum_{\lambda} \frac{N}{(2\pi)^3} \int_0^\infty dk \int d\Omega \sum_k \]

\uparrow \text{density of states in } k\text{-space.}

The \( k \)-integral engages the \( \delta \)-fn, since \( \omega = ck \). We sum over all photon states, but only those that conserve energy are picked up by the \( \delta \)-fn.
According to 1st order TDPT, the probability to decay is \( \frac{\Gamma}{\hbar} t \), or, the probability to remain in the initial state is \( P_{\text{00}}(t) = 1 - \frac{\Gamma}{\hbar} t \). This is absurd for times \( t \gg \frac{\hbar}{\Gamma} \) = lifetime of the state, which shows the breakdown of TDPT for long times. Instead, we expect a curve for \( P_{\text{00}}(t) \) as in the figure,

\[
P_{\text{00}}(t) \quad \text{correct answer}
\]

1st order TDPT gives the correct slope at \( t=0 \), but it does not give us the shape of the curve for long times. We might expect an exponential decay law, \( P_{\text{00}}(t) = e^{-\frac{\Gamma}{\hbar} t} \), but this is not proven by 1st order TDPT. We do seem to have the first term in the series expansion of the exponential,

\[
e^{-\frac{\Gamma}{\hbar} t} = 1 - \frac{\Gamma}{\hbar} t + ...
\]

but we haven't proven that the higher order terms are the right ones.

To access the long time behavior it won't help to go to higher-
order in T-DPT. These higher-order terms will generate powers of $t$, which amounts to doing a Taylor series expansion of the probabilities about $t=0$. A Taylor series is a poor way to understand the large $t$ limit.

Instead we will take a different approach. Let us go back to the general formalism of time-dependent systems, using a general notation. We put the specific application of spontaneous emission on hold. As in Notes 29, we let the Hamiltonian be $H=H_0+V$ (it is $t$-independent. $V=V_1$, not necessarily a potential in the ordinary sense), we let $|i\rangle, |n\rangle$ etc. be eigenstates of $H_0$ with energies $E_i, E_n$, etc., we let $U(t)=e^{-itH}$ and $U_0(t)=e^{-itH_0}$. We define the transition amplitudes in the Schrödinger picture $a_n(t)$ and in the interaction picture $c_n(t)$ by

$$
|\Psi^i_S(t)\rangle = \sum_n a_n(t) \langle n|,
$$

$$
|\Psi^i_I(t)\rangle = \sum_n c_n(t) \langle n|.
$$

We let the initial state be $|i\rangle$ (an eigenstate of $H_0$) and so that

$$
|\Psi^i_S(0)\rangle = |\Psi^i_I(0)\rangle = |i\rangle ,
$$

so that

$$
|\Psi^i_S(t)\rangle = U(t) |i\rangle,
$$

$$
|\Psi^i_I(t)\rangle = U_0^+(t) |\Psi^i_S(t)\rangle = U_0^+(t) U(t) |i\rangle .
$$
Then
\[ a_n(t) = \langle n | U(t) | i \rangle \]
\[ c_n(t) = \langle n | U_0(t)^+ U(t) | i \rangle = e^{+iE_n t} a_n(t). \]

In other words,
\[ a_n(t) = e^{-iE_n t} c_n(t). \]

To go from the transition amplitudes in the Schrödinger picture to those in the interaction picture, we just strip off the phase factor \( e^{-iE_n t} \), which is the part of the time evolution due to the unperturbed Hamiltonian. The transition probabilities are the same in both pictures,
\[ P_n(t) = |a_n(t)|^2 = |c_n(t)|^2. \]

In the following we will work mostly in the Schrödinger picture, but we have given the translation to the interaction picture in order to make comparison with earlier results.

It is easy to get equations of evolution for the \( a_n(t) \).

Note that
\[ i\dot{a}_n(t) = \langle n | i \frac{\partial U(t)}{\partial t} | i \rangle = \langle n | H U(t) | i \rangle \]
\[ = \sum_k \langle n | H_0 + V | k \rangle \langle k | U(t) | i \rangle \rightarrow a_k(t) \]
\[ \rightarrow E_n \delta_{nk} + \langle n | V | k \rangle \]
or,

\[ i \dot{a}_n(t) = E_n a_n(t) + \sum_k \langle n | V | k \rangle a_k(t) \]

This is essentially a version of the Schrödinger equ, and it is exact.

We will solve these equations by the method of Laplace transforms.

A Laplace transform is a kind of one-sided Fourier transform, i.e., the \( t \)-integral only goes from 0 to \( \infty \) instead of \( -\infty \) to \( \infty \). This is necessary in our applications since we are interested in decay processes that damp as \( t \to \infty \) and diverge as \( t \to -\infty \). The variable conjugate to \( t \) is an energy-like variable, so we want to consider something like

\[ \int_0^\infty dt \, e^{iEt} a_n(t) = \int_0^\infty dt \, e^{iEt} \langle n | U(t) | i \rangle. \]

The essence of the integral is

\[ \int_0^\infty dt \, e^{iEt} U(t). \]

But as shown in Sec. 31.9, this integral does not converge at the upper limit. To fix that we push the parameter \( E \) into the upper \( 1/2 \) plane, \( E \to E + i\epsilon = z \), where \( z \) is a complex energy.

Then the integral gives the Green's operator, to within constant factors. To get these right, define the "Laplace transform" for our purposes as the integral operator.
\[ \kappa(t=1) \]

\[ -i \int_{0}^{\infty} dt \ e^{-i z t} \]

for \( \text{Im} z > 0 \). Then we have

\[ -i \int_{0}^{\infty} dt \ e^{-i z t} a_n(t) = -i \int_{0}^{\infty} dt \ e^{-i z t} \langle n | U(t) | i \rangle \]

\[ = \langle n | G(z) | i \rangle. \]

The Laplace transform of the transition amplitudes in the Schrödinger picture are the corresponding matrix elements of the Green’s operator or resolvent for the system.

The advantage of Laplace transforms is that they convert differential equations into algebraic equations, which are easier to solve, and they also deal nicely with initial conditions and transients. This is like the method of complex impedances when analyzing an electrical circuit: much easier than solving the coupled differential equations for the currents and charges in the various circuit elements.

For example, applying the Laplace transform to the LHS of the eqns for \( a_n \), we have

\[ -i \int_{0}^{\infty} dt \ e^{-i z t} \dot{a}_n(t) = e^{-i z t} a_n(t) \bigg|_{0}^{\infty} - \int_{0}^{\infty} dt \ iz \ e^{-i z t} a_n(t) \]

\[ = -a_n(0) + \zeta \langle n | G(z) | i \rangle. \]
Note that \( a_n(t) = \delta_{ni} \). Taking the Laplace transform also of the RHS of the boxed eqn on p. 7, we get

\[
(z - E_n) \langle n | G(z) | i \rangle = \delta_{ni} + \sum_k \langle n | V | k \rangle \langle k | G(z) | i \rangle
\]

(\( \text{Im} z > 0 \) understood)

These are a set of algebraic equations for the unknowns \( \langle n | G(z) | i \rangle \).

When we solve for these, we must use the inverse Laplace transform to get back to the amplitudes \( a_n(t) \).

Here is how we do the inverse Laplace transform. Consider the integral

\[
\frac{-1}{2\pi i} \int_{C^+} dz \ e^{-izt} G(z)
\]

where the contour \( C^+ \) runs just above the real energy axis,

\[
\text{Im } E
\]

\[
\rightarrow C^+
\]

\[
R \rightarrow E
\]

Actually \( C^+ \) can be located at any distance above the real axis (the integral is independent of where we put it) but often we will want to push it down close to the real axis. \( G(z) = \frac{1}{z - H} \) is an analytic fn. of \( z \) for \( \text{Im } z > 0 \).

First take the case that \( t < 0 \). Then \( e^{-izt} \) is
exponentially damping as we move up into the upper ½ plane, so contour C_+ can be closed with a semicircle at \( \infty \),

\[ \text{Im} E \quad \rightarrow \quad \text{Re} E \]

without changing the value of the integral. But the integrand is analytic inside the contour, so the integral vanishes. Thus:

\[ -\frac{1}{2\pi i} \int_{C_+} dz \ e^{-izt} G(z) = 0 \quad , \quad t < 0. \]

Now for \( t > 0 \), we cannot close the contour in the upper ½ plane because \( e^{-izt} \) blows up there. Nor can we close it in the lower ½ plane because the contour would have to cross the real axis where \( G(z) \) is singular.

So consider the integral

\[ -\frac{1}{2\pi i} \int_{C_-} dz \ e^{-izt} G(z) \]

where contour \( C_- \) runs just below the real axis:

\[ \text{Im} E \quad \rightarrow \quad \text{Re} E \]
For \( t > 0 \) we can close this contour in the lower half plane, and, since it encloses no singularities, the answer is zero:

\[
-\frac{1}{2\pi i} \int_{C_{-}} dz \ e^{-izt} G(z) = 0, \quad t > 0.
\]

Subtracting 0 from our former integral, we have (for \( t > 0 \)),

\[
-\frac{1}{2\pi i} \int_{C_{+}} dz \ e^{-izt} G(z) = -\frac{1}{2\pi i} \int_{C_{+}-C_{-}} dz \ e^{-izt} G(z)
\]

The total contour runs back and forth above and below the real axis. Pushing both contours very close to the real axis, the integral involves the difference between \( G(E+i\epsilon) \) and \( G(E-i\epsilon) \),

\[
\lim_{\epsilon \to 0} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE \ e^{-iEt} \left[ G(E+i\epsilon) - G(E-i\epsilon) \right]
\]

\[
= -\frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE \ e^{-iEt} (-2\pi i) \delta(E-H) \quad \text{(see Eq. 31.58)}
\]

\[
= e^{-iHt} = U(t) \quad \text{for} \quad t > 0.
\]
altogether, we have

\[-\frac{1}{2\pi i} \int_{C_{+}} dz \ e^{-izt} G(z) = \begin{cases} 0, & t < 0 \\ \rho(t), & t > 0 \end{cases} = K_{+}(t).\]

Taking matrix elements in the case \( t > 0 \), we find

\[-\frac{1}{2\pi i} \int_{C_{+}} dz \ e^{-izt} \langle n | G(z) | i \rangle = a_{n}(t). \quad (t > 0)\]

This is the inverse of the Laplace transform.

Let us now apply these results to solve the long-time behavior of a decay process. Let the atomic states be

\[ |i\rangle \rightarrow |B0\rangle \quad E_{i} \rightarrow E_{B} \]

\[(n+i) \rightarrow |\Lambda\rangle \quad E_{n} \rightarrow E_{\Lambda} + \omega \quad (\kappa = i)\]
\[ \omega_{ni} \rightarrow E_n - E_i \rightarrow E_A + \omega - E_B = \omega - \omega_{BA} \]

Now we transpose the boxed eqn on p. 9 into the notation appropriate for this problem, so we can solve algebraically for the matrix elements of \( G(z) \). We will make 2 approximations while doing this:

1) Ignore \( H_2 \) (because \( H_2 \ll H_1 \)).

2) Ignore all states of the matter-field system except \( |BO\rangle \) (the initial state) and \( |A\lambda\rangle \) (any single photon state times any atomic state).

Thus,
\[
\sum_k |k'\rangle\langle k| \rightarrow |BO\rangle\langle BO| + \sum_{A\lambda} |A\lambda\rangle\langle A\lambda| .
\]

In particular, we ignore any states with 2 or more photons. The 2nd approximation is equivalent to working on a subspace of the full space, that spanned by \( |BO\rangle \) and \( |A\lambda\rangle \) (for all \( A, \lambda \)).

First take the case \( n = i = BO \). Then we have
\[
(z - E_B) \langle BO| G(z)|BO\rangle = 1 + \langle BO| H_1 |BO\rangle \langle BO| G(z)|BO\rangle \\
+ \sum_{A\lambda} \langle BO| H_1 |A\lambda\rangle \langle A\lambda| G(z)|BO\rangle .
\]

Next the case \( n \neq i, i \rightarrow BO, n \rightarrow A\lambda \):
\[
(z - E_A - \omega) \langle A\lambda| G(z)|BO\rangle = \sum_{A'\lambda'} \langle A\lambda| H_1 |BO\rangle \langle BO| G(z)|BO\rangle \\
+ \sum_{A'\lambda'} \langle A\lambda| H_1 |A'\lambda'\rangle \langle A'\lambda'| G(z)|BO\rangle .
\]
We simplify by noting that $H_1$ is an operator that changes the number of photons by ±1, so

$$\langle B_0 | H_1 | B_0 \rangle = 0$$

and $$\langle A\lambda | H_1 | A\lambda' \rangle = 0.$$ 

Now writing

$$\chi_{B_0} = \frac{\langle B_0 | G(z) | B_0 \rangle}{\chi_{B_0}}$$

and $$\chi_{A\lambda} = \frac{\langle A\lambda | G(z) | B_0 \rangle}{\chi_{B_0}}$$

we have

$$(z - E_B) \chi_{B_0} = 1 + \sum_{A\lambda} \langle B_0 | H_1 | A\lambda \rangle \chi_{A\lambda}$$

and

$$(z - E_A - \omega) \chi_{A\lambda} = \langle A\lambda | H_1 | B_0 \rangle \chi_{B_0}.$$ 

We must solve these for $\chi_{B_0}$ and $\chi_{A\lambda}$. This is easy. First solve the 2nd eqn. for $\chi_{A\lambda}$,

$$\chi_{A\lambda} = \frac{\langle A\lambda | H_1 | B_0 \rangle}{z - E_A - \omega} \chi_{B_0},$$

and plug into the 1st eqn,

$$(z - E_B) \chi_{B_0} = 1 + \sum_{A\lambda} \frac{|\langle A\lambda | H_1 | B_0 \rangle|^2}{z - E_A - \omega} \chi_{B_0},$$

or

$$\chi_{B_0} = \frac{\langle B_0 | G(z) | B_0 \rangle}{D(z)} = \frac{1}{D(z)}$$

where

$$D(z) = (z - E_B) - \sum_{A\lambda} \frac{|\langle A\lambda | H_1 | B_0 \rangle|^2}{z - E_A - \omega}.$$
Here $D$ just stands for "denominator". Now use this to get $\chi_{\alpha\alpha}$,

$$
\chi_{\alpha\alpha} = \frac{\langle A\lambda | G(z) | B_0 \rangle}{(z - E_A - \omega) D(z)}
$$

Now we must apply the inverse Laplace transform to get the transition amplitudes. Start with the state $B_0$. We have

$$
a_{B_0}(t) = \frac{-1}{2\pi i} \int_{C_+} dz \frac{e^{-izt}}{D(z)}.
$$

To orient ourselves, let us first neglect the sum in the expression for $D(z)$, since this is second order in $H_1$ and presumably small. Then $D(z) \approx z - E_B$, and

$$
a_{B_0}(t) \approx \frac{-1}{2\pi i} \int_{C_+} dz \frac{e^{-izt}}{z - E_B}.
$$

The integrand is analytic except at the pole $z = E_B$.

$\text{Im} E$

$\text{Re} E$

$E_B$

$C_+$

$C_+$ lies on the negative real axis (since $B$ is a bound state of the atom). For $t > 0$ (the only case we are interested in) the contour can be closed in the lower 1/2 plane, so
the contour enclosed the pole and

\[ a_{\text{so}}(t) = e^{-iE_{\text{so}} t} \]

by the residue theorem. This is the evolution of the initial state \( |\text{so}\rangle \) according to the unperturbed Hamiltonian \( H_0 \), which is no wonder since we dropped all terms depending on \( H_1 \) when we approximated \( D(z) \). The transition amplitude in the interaction picture is \( C_{\text{so}}(t) = 1 \) (constant) and the probability is \( P_{\text{so}}(t) = 1 \). There is no decay if we neglect \( H_1 \) (no surprise, but at least we see how the formalism works).

Now let's include the \( \sum_{\Lambda} \) term in \( D(z) \) (p. 14). This term is small, so it moves the zero of \( D(z) \) from \( z = E_{\text{so}} \) to a new location. (The zero of \( D(z) \) is a pole of the matrix element \( \langle \text{so} | a(z) | \text{so} \rangle \).) Do the new location in the upper \( 1/2 \) plane?
No, this impossible, because \( G(z) \) is analytic in the upper \( 1/2 \) plane. Do it on the real axis? Recall that poles of \( G(z) \) on the real axis represent bound states of the system. If the correction term \( \frac{\Sigma}{\Delta} \) etc. in \( D(z) \), which is \( \Theta(H_1^2) \), moves the pole to a new location on the real axis, it would mean that the bound state \( \{ \psi \} \) of the atom, or \( \{ \psi_0 \} \) of the atom-field system (unperturbed system only) would shift its energy slightly because of the perturbation \( H_1 \), but would remain a bound state. Is this possible?

\[
\begin{array}{c}
\text{Im} E \\
\bullet \\
E_B \\
\end{array} \quad \quad \quad \quad \\
\cdots \quad \quad \quad \quad \\
\begin{array}{c}
\text{Re} E \\
\end{array}
\]

To answer this let us evaluate \( D(z) \) in the limit that \( \text{Im } z \to 0 \).

That is, let's set \( z = E + iE \) and define

\[
D(E) = \lim_{\epsilon \to 0} D(E+i\epsilon) = E - E_B - \lim_{\epsilon \to 0} \sum_{\alpha, \lambda} \frac{|\langle \alpha, \lambda | H_1 | \psi_0 \rangle|^2}{E + i\epsilon - E_{\alpha, \lambda} - \epsilon}.
\]

Naively, we might think that taking \( \epsilon \to 0 \) in the sum would be equivalent to just setting \( \epsilon = 0 \) in the denominator, which would produce a purely real quantity (since the numerator is real). But this is wrong. To see why, note that \( \sum_{\alpha, \lambda} \) in the limit \( \epsilon \to 0 \).
really means

\[ \sum_{\mathcal{A}x} \rightarrow \sum_{\mathcal{A}} \frac{\nu}{(2\pi)^3} \int k^2 dk \int d\Omega \sum_{\mu} \]

where \( k \) is the photon wave number. Since \( \omega \) in the denominator is \( \omega = c k \) for the photon, the \( k \)-integral has the form of

\[ \int dk \frac{f(k)}{k_0 - k}, \]

where \( k_0 = \frac{1}{c} (E - E_\mathcal{A}) \), and where \( f(k) \) is a function that is smooth at \( k = k_0 \). That is, the functions in the integrand look like

![Diagram](image)

The problem is that the area under either half of \( \frac{1}{k_0 - k} \) (\( k < k_0 \) or \( k > k_0 \)) goes to \( \infty \) as \( k \rightarrow k_0 \), but with opposite signs.

Multiplying by \( f(k) \) doesn't change this, so the integral has the form \( \infty - \infty \), and is not defined unless we specify some prescription for how to deal with the singularity. In other words, just setting \( \varepsilon = 0 \) in the sum \( \sum_{\mathcal{A}x} \) term in \( D(z) \) \( \infty \) is not correct, because it is not even defined. Actually, the