The Levitt 2x2 Matrix Problem PhL 4.5.08

The problem is stated and its solution is given below in a box on page 7.

Contents:

A. Review of solving the Schrodinger Equation.

B. Applying the above to the current problem.

C. Details of the Calculation (General Case, answer in a box below)
- C1. Compute the eigenvalues
- C2. Compute the eigenvectors and the matrix X
- C3. Compute X^{-1}.
- C4. Compute $\rho(t)$

D. Special Cases
- D1: Special case #1. **Exchange between A and B species where k = k' :**
- D2 Special case #2. **A and B exchange species k = k', A and B independently relax at rate W**
- D3: Special case #3. **System of two spin-1/2 with d-d interaction so W_0, W_1 and W_2 etc.**
- D4: Special case #4: **Exchange between A and B species where $k \neq k'$:**

Comment: This problem arises in about three places in Levitt, including exchange A B and the Solomon equations Case #3 above. I would like to solve the problem in the most general case and be done with it once and for all. So here I have copied in my notes on Levitt appendix 17.12, and generalized them to a more general 2x2 matrix:

$$L = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix}$$

A. Review of solving the Schrodinger Equation.

Now, let's digress to think about the Schrodinger Equation SE. We have a TI and TD version of this equation, namely

$$H\phi_n = E_n\phi_n \qquad\qquad H\psi = +\, i\, d\psi/dt$$

From the second equation, if H itself is time-independent, we solve to get

$$\psi(t) = e^{-iHt}\,\psi(0)$$

and this gives us a formal solution of the SE for $\psi(t)$. If it happens that H is a 2x2 matrix, then we are faced with the **technical problem of exponentiating a 2x2 matrix**. If the matrix H were diagonal, this exponentiation is trivial, but if it is not diagonal, you have a problem on your hands. In what follows, we learn a "trick" for, in effect, doing this exponentiation of a matrix.

In the case of a Hamiltonian, we know we can find a 2x2 unitary matrix X such that

$X^{-1} H X = H_d$ = a diagonal matrix

We formally know this is possible because H is Hermitian. We also know that one possibility for the matrix X is the matrix whose columns are the eigenvectors of H. That is, $X = \{ \phi_1, \phi_2 \}$ in the N=2 case. If the eigenvalues are distinct, this is especially simple. If they are not, we may have to fiddle with GSO to come up with linearly independent eigenvectors, but we can ignore that in our present example.

Suppose then that we "go off" and we solve the TI SE in our case of interest, and we find the values of E_n and of ϕ_n. Then we will have found an X which brings H to diagonal form. Assume that we have done this in our 2x2 case. We can then conclude without much effort that

$X^{-1} e^{-iHt} X = e^{-iHdt}$ = a diagonal matrix = $\text{diag}(e^{-iE1t}, e^{-iE2t})$

by just sandwiching the X's around each term in the expansion for e^{-iHt}.

Now, this leads us to a closed form solution for $\psi(t)$ which is what we are after in our study of the TI SE. We have

$\psi(t) = e^{-iHt} \psi(0) = X e^{-iHdt} X^{-1} \psi(0)$

Since we have solved the TDSE, we know all three matrices shown on the right and we then just multiply things out and we have our solution $\psi(t)$. This method of course applies for any dimension H we want, not just N=2, and surely also for N=∞ as would arise in continuous spectrum situations.

B. Applying the above to the current problem.

$L\phi_n = d_n\phi_n$ $\quad L\rho = d\rho/dt$ $\quad \rho(t) = e^{Lt} \rho(0)$

Our "TDSE" here lacks the -i we had in the true TDSE, and so this -i is also missing from the exponential formal solution to the problem shown on the right. The TISE looks the same The functions here are all 2D vectors, I have bolded them but Gk letters are hard to see bolded in my font. We know the solution on the right is correct because we can apply d/dt to it, to get the TDSE in the middle, and as before, we assume that L is itself not a function of time. So, our technical problem is "how to compute e^{Lt}" so we can write down our solution $\rho(t)$ in a closed and useful form. I have called the eigenvalues d_n instead of E_n.

We could make this problem look just like the real SE problem by defining -iH = L or H = iL. However, H so defined would not be Hermitian (much less real symmetric), so we expect that our eigenvalues won't be real (they are complex). So in our little SE analogy, we cannot use "matrix theorems" which relate to Hermitian matrices.

Nevertheless, we have some matrix theorems which are useful. In my matrix binder, the first theorem of interest is Theorem 15D in the "2 section" (page 18) which says this: if you have already solved the TI SE problem and know the eigenvectors and eigenvalues, then you can write $LX = XL_d$ which merely groups things and says that $L \{ \phi_1, \phi_2 \} = \{ d_1\phi_1, d_2\phi_2 \}$ which is just a restatement of $L\phi_n = d_n\phi_n$.

Next we have Theorem 15E following which says the obvious: if it happens that $\det X \neq 0$, then we know we can compute X^{-1} and then we have $X^{-1}LX = L_d$. Then we have shown that our matrix of

eigenvectors X is a candidate similarity for bringing L to diagonal form. In our current example this will turn out to be the case, and we can then go on to solve our problem as follows:

$$X^{-1}LX = L_d \qquad \Rightarrow \qquad X^{-1}e^{Lt}\,X = e^{Ldt} = \text{diag}\,(\,e^{d1t}, d^{d2t})$$

$$\rho(t) = e^{Lt}\,\rho(0) = X\,e^{Ldt}\,X^{-1}\,\rho(0)$$

which is what Malcolm says in his equation α on page 631 where he has already assumed the TE value for ρ(0) [just above equation α]. He uses D instead of L_d for the diagonalized matrix, and $V = e^{Lt}$.

So now at least we know what Malcolm is doing here.

C. Details of the Calculation.

So now we want to solve $L\phi_n = d_n\phi_n$ for the matrix L shown page 630. We can write our TI SE as

$$(L - d_n 1)\phi_n = 0$$

C1. Compute the eigenvalues $L = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix}$

We know that if $\det(L - d_n 1) \neq 0$, we can invert this equation and we get $\phi_n = 0$ meaning there is no non-zero solution to the problem. We are looking for interesting solutions, so we require that $\det(L - d_n 1) = 0$, which is the secular or characteristic equation I suppose. [I am not powering up my ODE module at this time because that will cost several hours of swap time.] Setting $\det(L - d_n 1) = 0$ tells us what the eigenvalues are for our problem. We get

$$\begin{vmatrix} \alpha-d & \beta \\ \delta & \gamma-d \end{vmatrix} = 0$$

Here are some algebra steps following the above:

$$(\alpha-d)(\gamma-d) - \delta\beta = 0$$

$$d^2 - (\alpha+\gamma)d + (\alpha\gamma-\delta\beta) = 0$$

$$A = 1 \qquad B = -(\alpha+\beta) \qquad C = \alpha\gamma-\delta\beta$$

$$B^2-4AC = (\alpha+\gamma)^2 - 4(\alpha\gamma-\delta\beta) = (\alpha-\gamma)^2 + 4\delta\beta = 4 * \{\ [(\alpha-\gamma)/2]^2 + \delta\beta\ \}$$

We then find these solutions for d

$$d_\pm = (\alpha+\gamma)/2 \pm \sqrt{[(\alpha-\gamma)/2]^2 + \delta\beta}$$

So maybe define some new symbols here just to make the algebra easier:

$\sigma = (\alpha+\gamma)/2 \qquad \tau = (\alpha-\gamma)/2 \qquad r = \sqrt{\tau^2 + \delta\beta}$

Then our solution eigenvalues are:

$d_\pm = \sigma \pm r$

C2. Compute the eigenvectors and the matrix X $\qquad L = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix}$

Now, how to we find the eigenvectors? In general, given equation Ax=0, how to you find the eigenvectors which span the 2D nullspace of A? It's easy: Imagine that $\phi = (u, v)$ column vector. Then we have

$$\begin{pmatrix} \alpha-d & \beta \\ \delta & \gamma-d \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = 0 \qquad \Rightarrow (\alpha-d)u + \beta v = 0 \quad \text{and} \quad \delta u + (\gamma-d)v = 0$$

The second equation says $\delta u = (d-\gamma)v$. So set $v = \delta$ arbitrarily and get $u =(d-\gamma)$. So our eigenvectors are therefore

$$\begin{pmatrix} u \\ v \end{pmatrix}_\pm = \begin{pmatrix} d_\pm - \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} \tau \pm r \\ \delta \end{pmatrix}$$

The second form shown above follows because

$d_\pm - \gamma = \sigma \pm r - \gamma = (\alpha+\gamma)/2 \pm r - \gamma = (\alpha-\gamma)/2 \pm r = \tau \pm r \equiv \varepsilon_\pm$

So, assuming my result is correct, I get the matrix X whose columns are eigenvectors

$$X = \begin{pmatrix} \tau+r & \tau-r \\ \delta & \delta \end{pmatrix} = \begin{pmatrix} \varepsilon_+ & \varepsilon_- \\ \delta & \delta \end{pmatrix} = (\psi_+, \psi_-) \qquad \text{where} \quad \varepsilon_\pm = \tau \pm r$$

C3. Compute X^{-1}.

I can look up the inverse of this on my "summary of matrix facts" page

$$X = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad \Rightarrow \qquad X^{-1} = \begin{pmatrix} d & -b \\ -c & a \end{pmatrix} / \det X$$

In our case $\det X = (\tau+r)\delta - (\tau-r)\delta = 2r\delta$. We then get

$$X^{-1} = \begin{pmatrix} \delta & r-\tau \\ -\delta & r+\tau \end{pmatrix} / 2r\delta = \begin{pmatrix} \delta & -\varepsilon_- \\ -\delta & \varepsilon_+ \end{pmatrix} / 2r\delta$$

C4. Compute $\rho(t)$

We know that the solution is this:

$$\rho(t) \;=\; X\, e^{Ldt}\, X^{-1}\, \rho(0) \quad \text{where } e^{Ldt} \begin{pmatrix} \exp(d_+t) & 0 \\ 0 & \exp(d_-t) \end{pmatrix}$$

So do this one piece at a time. First, we abbreviate the vector $\rho(0)$ as (x,y). Then we have:

$$X^{-1}\,\rho(0) \;=\; \begin{pmatrix} \delta & r-\tau \\ -\delta & r+\tau \end{pmatrix} / 2r\delta \begin{pmatrix} x \\ y \end{pmatrix} \;=\; (1/2r\delta) \begin{pmatrix} \delta x + (r-\tau)y \\ -\delta x + (r+\tau)y \end{pmatrix} = (1/2r\delta) \begin{pmatrix} q \\ s \end{pmatrix}$$

where we have defined q and s as shown. We then find that:

$$e^{Ldt}\, X^{-1}\, \rho(0) \;= (1/2r\delta) \begin{pmatrix} q\exp(d_+t) \\ s\exp(d_-t) \end{pmatrix}$$

The final step then is this:

$$\rho(t) \;= X\,(1/2r\delta) \begin{pmatrix} q\exp(d_+t) \\ s\exp(d_-t) \end{pmatrix} = (1/2r\delta) \begin{pmatrix} \tau+r & \tau-r \\ \delta & \delta \end{pmatrix} \begin{pmatrix} q\exp(d_+t) \\ s\exp(d_-t) \end{pmatrix}$$

$$= (1/2r\delta) \begin{pmatrix} (\tau+r)qe^{+} + (\tau-r)se^{-} \\ \delta q\, e^{+} + \delta s e^{-} \end{pmatrix}$$

Writing this out in detail gives

$$\text{top} = \;\{\; \delta\,[\,(\tau+r)e^{+} - (\tau-r)e^{-}\,]\,x \;+\; (\tau+r)(r-\tau)\,[\,e^{+} - e^{-}\,]\,y \;\}\; / 2r\delta$$

$$\text{bot} = \;\{\; \delta\,[\,e^{+} - e^{-}\,]\;x \;+\; [\,(r-\tau)\,e^{+} + (r+\tau)\,e^{-}\,]\,y \;\}\; / 2r$$

where of course $e^{\pm}$ stands for $\exp(d_\pm t)$ where $d_\pm = \tau \pm r$. Suppose we rewrite everything putting τ first:

$$\text{top} = \;\{\; \delta\,[\,(\tau+r)e^{+} - (\tau-r)e^{-}\,]\,x \;-\; (\tau+r)(\tau-r)\,[\,e^{+} - e^{-}\,]\,y \;\}\; / 2r\delta$$

$$\text{bot} = \;\{\; \delta\,[\,e^{+} - e^{-}\,]\;x \;-\; [\,(\tau-r)\;e^{+} - (\tau+r)\,e^{-}\,]\,y \;\}\; / 2r$$

Then let's define (well, I added this above, but OK)

$$\varepsilon_\pm = \tau \pm r$$

so get

$$\text{top} = \;\{\; \delta\,[\,\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}\,]\,x \;-\; \varepsilon_+\varepsilon_-\,[\,e^{d+t} - e^{d-t}\,]\,y \;\}\; / 2r\delta$$

$$\text{bot} = \;\{\; \delta\,[\,e^{d+t} - e^{d-t}\,]\;x \;-\; [\,\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}\,]\,y \;\}\; / 2r$$

where $e^{\varepsilon_\pm t}$ stands for $\exp(d_\pm t)$. Maybe more symmetrical to then write this as

$$\text{top} = \{ + [\varepsilon_+ e^{d_+ t} - \varepsilon_- e^{d_- t}] x - (\varepsilon_+ \varepsilon_- / \delta)[e^{d_+ t} - e^{d_- t}] y \} / 2r$$

$$\text{bot} = \{ - [\varepsilon_- e^{d_+ t} - \varepsilon_+ e^{d_- t}] y + \delta [e^{d_+ t} - e^{d_- t}] x \} / 2r$$

So here is our answer to this problem:

Summary of The General Problem and its Solution. Our equation of interest is:

$$d/dt \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = L \begin{pmatrix} x(t) \\ y(t) \end{pmatrix}$$

We know that a formal solution may be written as

$$\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \exp\left(\begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} t \right) \begin{pmatrix} x(0) \\ y(0) \end{pmatrix}$$

because if we differentiate we get

$$d/dt \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} \exp\left(\begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} t \right) \begin{pmatrix} x(0) \\ y(0) \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} \begin{pmatrix} x(t) \\ y(t) \end{pmatrix}$$

The explicit solution to the problem is this:

$$\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = (1/2r) \begin{pmatrix} [\varepsilon_+ e^{d_+ t} - \varepsilon_- e^{d_- t}] & -(\varepsilon_+ \varepsilon_- / \delta)[e^{d_+ t} - e^{d_- t}] \\ \delta [e^{d_+ t} - e^{d_- t}] & -[\varepsilon_- e^{d_+ t} - \varepsilon_+ e^{d_- t}] \end{pmatrix} \begin{pmatrix} x(0) \\ y(0) \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} x(0) \\ y(0) \end{pmatrix}$$

where

$\varepsilon_\pm = \tau \pm r$
$d_\pm = \sigma \pm r$
$\sigma = (\alpha+\gamma)/2$
$\tau = (\alpha-\gamma)/2$
$r = \sqrt{\tau^2 + \delta\beta}$

Here then is a summary of the problem and its solution:

Given the 2x2 matrix problem,

$d\boldsymbol{\rho}(t)/dt = L\,\boldsymbol{\rho}(t)$ where $L = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix}$

the solution to the problem is,

$\boldsymbol{\rho}(t) = M\,\rho(0)$ where $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ // formal solution: $\boldsymbol{\rho}(t) = e^{\mathbf{Lt}}\,\rho(0)$

where

$A = (1/2r)\,[\,\varepsilon_+ e^{\mathbf{d+t}} - \varepsilon_- e^{\mathbf{d-t}}]$
$B = -(1/2r)\,(\varepsilon_+\varepsilon_-/\delta)\,[e^{\mathbf{d+t}} - e^{\mathbf{d-t}}]$
$C = (1/2r)\,\delta\,[e^{\mathbf{d+t}} - e^{\mathbf{d-t}}]$
$D = -(1/2r)\,[\varepsilon_- e^{\mathbf{d+t}} - \varepsilon_+ e^{\mathbf{d-t}}]$

with // eigenvector matrix $= X = \begin{pmatrix} \varepsilon_+ & \varepsilon_- \\ \delta & \delta \end{pmatrix} = (\psi_+, \psi_-)$

$\varepsilon_\pm = \tau \pm r$
$d_\pm = \sigma \pm r$ // $d_\pm$ are eigenvalues of $L\psi_\pm = d_\pm\psi_\pm$

and where

$\sigma = (\alpha+\gamma)/2$
$\tau = (\alpha-\gamma)/2$
$r = \sqrt{\tau^2 + \delta\beta}$ // solution singular if $r = 0$, $(\alpha-\gamma)^2 + 4\delta\beta = 0$

D. SPECIAL CASES

D1: Special case #1. **Exchange between A and B species where k = k' :**

Suppose $L = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} = \begin{pmatrix} -k-\lambda+i\Omega^0_{\mathbf{A}} & k \\ k & -k-\lambda+i\Omega^0_{\mathbf{B}} \end{pmatrix}$ as on Levitt page 629. Then

$\alpha = -k-\lambda+i\Omega^0_{\mathbf{A}}$ $\beta = k$ $\delta = k$ $\gamma = -k-\lambda+i\Omega^0_{\mathbf{B}}$

$\sigma = (\alpha+\gamma)/2 = -k-\lambda+i\,\Omega_{\mathbf{av}}$ where $\Omega_{\mathbf{av}} = (\Omega^0_{\mathbf{A}} + \Omega^0_{\mathbf{B}})/2$

$\tau = (\alpha-\gamma)/2 = i\,(\Omega^0_{\mathbf{A}} - \Omega^0_{\mathbf{B}})/2 = i\,\Omega_\Delta/2$ where $\Omega_\Delta = (\Omega^0_{\mathbf{A}} - \Omega^0_{\mathbf{B}})$

$r = \sqrt{-(\Omega_\Delta/2)^2 + k^2} = i\sqrt{(\Omega_\Delta/2)^2 - k^2} = iR$

$\varepsilon_\pm = \tau \pm r = i\,\Omega_\Delta/2 \pm iR$
$d_\pm = \sigma \pm r = -k-\lambda+i\,\Omega_{\mathbf{av}} \pm iR$ // agrees with Levitt when $i\Omega_{\mathbf{av}}$ added

Then we get

$$\text{top} = \{ + [\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}] x - (\varepsilon_+\varepsilon_- /k)[e^{d+t} - e^{d-t}] y \} / 2iR$$

$$\text{bot} = \{ - [\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}] y + k [e^{d+t} - e^{d-t}] x \} / 2iR$$

We can do algebra to show that

$$\varepsilon_+\varepsilon_- = [R^2 - (\Omega_\Delta/2)^2] = -k^2$$

so rewrite the above as

$$\text{top} = \{ + [\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}] x + k [e^{d+t} - e^{d-t}] y \} / 2iR$$

$$\text{bot} = \{ - [\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}] y + k [e^{d+t} - e^{d-t}] x \} / 2iR$$

Now suppose we set x = y = (1/4i) as Levitt does on page 631, which assumes a TE start. We can then replace (1/4i)(1/2iR) = - (1/8R) and then

$$\text{top} = -\{ + [\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}] + k [e^{d+t} - e^{d-t}] \} / 8R$$

$$\text{bot} = -\{ - [\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}] + k [e^{d+t} - e^{d-t}] \} / 8R$$

Our next instruction from Levitt is to multiply each of these by 2i and then add them together, in which case we get

$$(2i)(\text{top} + \text{bot}) = - 2i /8R *$$

$$\{ [\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}] + k [e^{d+t} - e^{d-t}] - [\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}] + k [e^{d+t} - e^{d-t}] \}$$

The bracket becomes

$$\{ (\varepsilon_+ - \varepsilon_-) e^{d+t} + (\varepsilon_+ - \varepsilon_-) e^{d-t} + 2k (e^{d+t} - e^{d-t}) \}$$

$$= \{ (\varepsilon_+ - \varepsilon_-) (e^{d+t} + e^{d-t}) + 2k (e^{d+t} - e^{d-t}) \}$$

But now

$$(\varepsilon_+ - \varepsilon_-) = [i \Omega_\Delta/2 + iR] - [i \Omega_\Delta/2 - iR] = 2iR$$

so we have above

$$(2i)(\text{top} + \text{bot}) = - i/4R * \{ 2iR (e^{d+t} + e^{d-t}) + 2k (e^{d+t} - e^{d-t}) \}$$

$$= -i/2R \{ iR\ (e^{d+t} + e^{d-t}) + k\,(e^{d+t} - e^{d-t}) \}$$

Now group by expo powers to get

$$= -i/2R \{\ (iR+k)\, e^{d+t} + (iR-k)\, e\, e^{d-t} \}$$

Now put the R inside and the 2 out front to get

$$= (-i/2) \{ (i + k/R)\, e^{d+t} + (i - k/R)\, e^{d-t} \}$$

Now consider that

$$d_{\pm} = \sigma \pm r = -k - \lambda + i\,\Omega_{av} \pm iR$$

If we use Levitt definitions on page 630 bottom we have

$$d_{+} = d_2 \qquad d_{-} = d_1$$

Our result is then:

$$(-i/2) \{ (i + k/R)\, e^{d2t} + (i - k/R)\, e^{d1t} \}$$

But now push the -i inside to get

$$= (1/2) \{(1 - ik/R)\, e^{d2t} + (1 + ik/R)\, e^{d1t}\}$$

and finally reorder the two terms

$$= (1/2) \{+ (1 + ik/R)\, e^{d1t} + (1 - ik/R)\, e^{d2t} \}$$

and we have **exactly replicated Levitt bottom of 631**, so this acts as at least a partial check on our algebra.

Also in this application we have

$X = \begin{pmatrix} \varepsilon_+ & \varepsilon_- \\ \delta & \delta \end{pmatrix}$ with $\varepsilon_{\pm} = i\,\Omega_{\Delta}/2 \pm iR$ and $\delta = k$ so the X matrix is given by:

$$X = \begin{pmatrix} i\,\Omega_{\Delta}/2 + iR & i\,\Omega_{\Delta}/2 - iR \\ k & k \end{pmatrix} = \begin{pmatrix} i\,(\Omega_{\Delta}/2 + R) & i\,(\Omega_{\Delta}/2 - R) \\ k & k \end{pmatrix} = (1/2) \begin{pmatrix} i\,(\Omega_{\Delta} + 2R) & i\,(\Omega_{\Delta} - 2R) \\ 2k & 2k \end{pmatrix}$$

so I stick by my guns that Levitt has a sign error on Ω_{Δ} here, but it does not matter in the end results.

Let's **do this again using our general formula**: from above we had all these evaluations:

$\alpha = -k-\lambda+i\Omega^0_A \qquad \beta = k \quad \delta = k \quad \gamma = -k-\lambda+i\Omega^0_B$

$\sigma = (\alpha+\gamma)/2 = -k - \lambda + i\,\Omega_{av}$ where $\Omega_{av} = (\Omega^0_A + \Omega^0_B)/2$

$\tau = (\alpha-\gamma)/2 = i\,(\Omega^0_A - \Omega^0_B)/2 = i\,\Omega_\Delta/2$ where $\Omega_\Delta = (\Omega^0_A - \Omega^0_B)$

$r = \sqrt{-(\Omega_\Delta/2)^2 + k^2} = i\sqrt{(\Omega_\Delta/2)^2 - k^2} = iR \qquad R = \sqrt{(\Omega_\Delta/2)^2 - k^2}$

$\varepsilon_\pm = \tau \pm r = i\,\Omega_\Delta/2 \pm iR$

$d_\pm = \sigma \pm r = -k - \lambda + i\,\Omega_{av} \pm iR$ // agrees with Levitt when $i\Omega_{av}$ added

$\varepsilon_+\varepsilon_- = [\,R^2 - (\Omega_\Delta/2)^2] = -k^2 \qquad \delta = k$

The general formulas are these,

$$A = (1/2r)\,[\,\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}]$$
$$B = -(1/2r)\,(\varepsilon_+\varepsilon_-/\delta)\,[e^{d+t} - e^{d-t}]$$
$$C = (1/2r)\,\delta\,[e^{d+t} - e^{d-t}]$$
$$D = -(1/2r)\,[\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}]$$

hence we get

$$A = (1/2iR)\,[(i\,\Omega_\Delta/2 + iR)\,e^{d+t} - (i\,\Omega_\Delta/2 - iR)\,e^{d-t}]$$
$$B = (k/2iR)\,[e^{d+t} - e^{d-t}]$$
$$C = (k/2iR)\,[e^{d+t} - e^{d-t}]$$
$$D = -(1/2iR)\,[(i\,\Omega_\Delta/2 - iR)\,e^{d+t} - (i\,\Omega_\Delta/2 + iR)\,e^{d-t}]$$

where $R = \sqrt{(\Omega_\Delta/2)^2 - k^2}$ and $d_\pm = -k - \lambda + i\,\Omega_{av} \pm iR$. Notice that B = C.

D2 Special case #2. **A and B exchange species k = k', A and B independently relax at rate W.**

Suppose $L = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} = \begin{pmatrix} -k-2W & k \\ k & -k-2W \end{pmatrix}$ as on Levitt page 632. We get

$\sigma = (\alpha+\gamma)/2 = -k - 2W$

$\tau = (\alpha-\gamma)/2 = 0$

$r = \sqrt{\tau^2 + \delta\beta} = \sqrt{0 + k^2} = k$

$\varepsilon_\pm = \tau \pm r = \pm k$

$d_\pm = \sigma \pm r = -k - 2W \pm k$ // agreeing bottom page 632.

Our general solution is this

$$\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = (1/2r) \begin{pmatrix} [\,\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}] & -(\varepsilon_+\varepsilon_-/\delta)\,[e^{d+t} - e^{d-t}] \\ \delta\,[e^{d+t} - e^{d-t}] & -[\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}] \end{pmatrix} \begin{pmatrix} x(0) \\ y(0) \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} x(0) \\ y(0) \end{pmatrix}$$

and we then have

$$A = (1/2r)\,[\,\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}] = (1/2k)\,[\,k\,e^{d+t} + k\,e^{d-t}] = (1/2)\,[e^{d+t} + e^{d-t}\,]$$

$$B = (1/2r)\,(-\varepsilon_+\varepsilon_-/\delta)\,[e^{d+t} - e^{d-t}] = (1/2k)(\,k^2/k)\,[e^{d+t} - e^{d-t}] = (1/2)\,[e^{d+t} - e^{d-t}]$$

$$C = (1/2r)\,\delta\,[e^{d+t} - e^{d-t}] = (1/2k)k[e^{d+t} - e^{d-t}] = (1/2)\,[e^{d+t} - e^{d-t}]$$

$$D = -(1/2r)\,[\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}\,] = -(1/2k)[\,-k\,e^{d+t} - k\,e^{d-t}] = (1/2)\,[e^{d+t} + e^{d-t}\,]$$

Now consider $e^{d+t} = e^{-2Wt}$ and $e^{d-t} = e^{-2Wt}\,e^{-2kt}$

$$(1/2)\,[e^{d+t} + e^{d-t}\,] = e^{-2Wt}(\,1 + e^{-2kt})/2 = e^{-2Wt}e^{-kt}\,(\,e^{kt} + e^{-kt})/2 = e^{-(k+2W)t}\cosh(kt)$$

$$(1/2)\,[e^{d+t} - e^{d-t}] = e^{-(k+2W)t}\sinh(kt)$$

So we get

$$A = D = e^{-(k+2W)t}\cosh(kt) = a_{diag} = a_{A\to A} = a_{B\to B}$$

$$B = C = e^{-(k+2W)t}\sinh(kt) = a_{cross} = a_{A\to B} = a_{B\to A}$$

and our solution is then

$$\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}\begin{pmatrix} x(0) \\ y(0) \end{pmatrix} = \begin{pmatrix} a_{diag} & a_{cross} \\ a_{cross} & a_{diag} \end{pmatrix}\begin{pmatrix} x(0) \\ y(0) \end{pmatrix}$$

So this is the solution of the problem on page 632-633 Levitt, but the confusion is that Levitt never states that it is the conclusion! He then uses this in Chapter 15. In my meta meta notes I quote this as

$$\begin{pmatrix} \langle I_z\rangle^A(t) \\ \langle I_z\rangle^B(t) \end{pmatrix} = \begin{pmatrix} a_{A\to A}(t) & a_{B\to A}(t) \\ a_{A\to B}(t) & a_{B\to B}(t) \end{pmatrix}\begin{pmatrix} \langle I_z\rangle^A(0) \\ \langle I_z\rangle^B(0) \end{pmatrix} \qquad \text{// "longitudinal mag exchange"}$$

where I was just guessing that this was the result, but now I know it is.

Note on this case: It is clear that the results for x(t) and y(t) $\to 0$ as $t \to \infty$. So we might want our *starting* equation to look like this:

$$d\rho(t)/dt = L\,[\rho(t) - \rho(\infty)] \qquad \text{where } L = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix}$$

so that when things stop changing at $t = \infty$, both sides will be zero. We can cast this into our formalism by defining

$\rho'(t) = \rho(t) - \rho(\infty)$

to get

$d\rho'(t)/dt = L\,\rho'(t)$

then our solution will be

$$\rho'(t) = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \rho'(0)$$

from which we then get the solution to this slightly altered problem,

$$\rho(t) = \begin{pmatrix} A & B \\ C & D \end{pmatrix} [\,\rho(0) - \rho(\infty)] \quad + p(\infty)$$

D3: Special case #3. **System of two spin-1/2 with W_0, W_1 and W_2 etc.**

In case #2 we had $L = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} = \begin{pmatrix} -k-2W & k \\ k & -k-2W \end{pmatrix}$. In this new case we are on page 635 and we have

$$L = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} = \begin{pmatrix} -R_{auto} & R_{cross} \\ R_{cross} & -R_{auto} \end{pmatrix}$$

The solution is the same as before where we make these replacements:

$k+2W \rightarrow R_{auto}$ $\qquad$ $k \rightarrow R_{cross}$

This, the solution of this case #3 problem is the following

$$\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} x(0) \\ y(0) \end{pmatrix} \text{ where}$$

$A = D = e^{-tR_{auto}} \cosh(R_{cross}t) = a_{diag} = a_{1\rightarrow1} = a_{2\rightarrow2}$

$B = C = e^{-tR_{auto}} \sinh(R_{cross}t) = a_{cross} = a_{1\rightarrow2} = a_{2\rightarrow1}$

and this result is used on page 544 in the NOESY theory section.

Attempt at computing "the Knight shift" :

D4: Special case #4: **Exchange between A and B species where $k \neq k'$:**

According to my scribble on page 629, we have

$$L = \begin{pmatrix} \alpha & \beta \\ \delta & \gamma \end{pmatrix} = \begin{pmatrix} -k-\lambda+i\Omega^0_A & k' \\ k & -k'-\lambda+i\Omega^0_B \end{pmatrix}$$

$\alpha = -k-\lambda+i\Omega^0_A$ $\beta = k'$ $\delta = k$ $\gamma = -k'-\lambda+i\Omega^0_B$ let $(k'+k)/2 = k_{av}$ and $(k'-k) = k_\Delta$

$\sigma = (\alpha+\gamma)/2 = -k_{av} - \lambda + i\,\Omega_{av}$ where $\Omega_{av} = (\Omega^0_A + \Omega^0_B)/2$

$\tau = (\alpha-\gamma)/2 = i\,(\Omega^0_A - \Omega^0_B)/2 - (k-k')/2 = (i\,\Omega_\Delta/2 + k_\Delta/2) = (i\,\Omega_\Delta + k_\Delta)/2, \quad \Omega_\Delta = (\Omega^0_A - \Omega^0_B)$

Define an altered difference frequency $i\,\Omega_\Delta' = i\,\Omega_\Delta + k_\Delta$ or $\Omega_\Delta' = \Omega_\Delta - ik_\Delta$. Then we have

$\tau = i\,\Omega_\Delta'/2$

Then

$r = \sqrt{\tau^2 + \delta\beta} = \sqrt{\tau^2 + \delta\beta}$

$r = \sqrt{\tau^2 + \delta\beta} = \sqrt{-(\Omega_\Delta'/2)^2 + k'k} = i\sqrt{(\Omega_\Delta'/2)^2 - k'k} = iR$ $R = \sqrt{(\Omega_\Delta'/2)^2 - k'k}$

$\varepsilon_\pm = \tau \pm r = i\,\Omega_\Delta'/2 \pm iR$

$d_\pm = \sigma \pm r = -k_{av} - \lambda + i\,\Omega_{av} \pm iR$

The solution matrix M to our problem has these matrix elements:

$A = (1/2r)\,[\,\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}]$
$B = -(1/2r)\,(\varepsilon_+\varepsilon_-/\delta)\,[e^{d+t} - e^{d-t}]$
$C = (1/2r)\,\delta\,[e^{d+t} - e^{d-t}]$
$D = -(1/2r)\,[\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}]$

In this case we have $\varepsilon_+\varepsilon_- = -kk'$ and $r - iR$ and $\delta = k$ and $r = iR$ so rewrite as

$A = [\,\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}]/2iR$
$B = k'\,[e^{d+t} - e^{d-t}]/2iR$
$C = k\,[e^{d+t} - e^{d-t}]/2iR$
$D = -\,[\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}]/2iR$

where

$d_\pm = -k_{av} - \lambda + i\,\Omega_{av} \pm iR$
$\varepsilon_\pm = \tau \pm r = i\,\Omega_\Delta'/2 \pm iR$
$R = \sqrt{(\Omega_\Delta'/2)^2 - k'k}$

Notice that B and C differ only in the prime on k.

Now apply this as was done in Levitt to x = y = (1/4i) and we find that

top = (A + B)/4i
bot = (C + D)/4i

So compute

$$A+B = [\ \varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}]/2iR + k'\ [e^{d+t} - e^{d-t}]\ /2iR$$

$$= \{\ \ (\varepsilon_+ + k')\ e^{d+t}\ -\ \ (\varepsilon_- + k')\ e^{d-t}\ \}/2iR$$

$$D+C = -[\ \varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}]/2iR + k\ [e^{d+t} - e^{d-t}]\ /2iR$$

$$= \{\ \ (-\varepsilon_- + k)\ e^{d+t}\ -\ \ (-\varepsilon_+ + k)\ e^{d-t}\ \}/2iR$$

Now we want to add these two items and multiply by 2i/4i = (1/2), as done on page 631

$$result = 2i\ [A+B+ D +C\ ]/4i\ = [A+B+ D +C\ ]/2$$

$$= \{(\varepsilon_+ + k')\ e^{d+t}\ -\ \ (\varepsilon_- + k')\ e^{d-t}\ +\ (-\varepsilon_- + k)\ e^{d+t}\ -\ \ (-\varepsilon_+ + k)\ e^{d-t}\ \}/4iR$$

$$= \{\ (\varepsilon_+ + k') + (-\varepsilon_- + k)\}\ e^{d+t}/R\ \ -\ \ \{\ \ (\varepsilon_- + k') + (-\varepsilon_+ + k)\ \}\ e^{d-t}/4iR$$

We can evaluate the brackets using $\varepsilon_+ - \varepsilon_- = 2iR$ to find

$$=\ 2[iR+k_{av}]\ e^{d+t}/4iR - 2[-iR+k_{av}]\ e^{d-t}/4iR$$

$$= [iR+k_{av}]\ e^{d+t}/2iR + [+iR-k_{av}]\ e^{d-t}/2iR$$

$$= [1 + k_{av}/iR]\ e^{d+t}/2\ + [\ 1 - k_{av}/iR]\ e^{d-t}/2$$

$$= (1/2)\ (1 - ik_{av}/R)\ e^{d+t}\ + (1/2)\ (1 + ik_{av}/R)\ e^{d-t}$$ // agrees with bottom page 631

So here is the result for our $k \neq k'$ case for the final NMR signal:

$$s(t) = (1/2)\ (1 + ik_{av}/R)\ e^{d-t}\ + (1/2)\ (1 - ik_{av}/R)\ e^{d+t}$$

where

$$d_{\pm}\ =\ - k_{av} - \lambda + i\ \Omega_{av} \pm iR \qquad k_{av}\ = (k'+k)/2$$

$$R = \sqrt{(\Omega_\Delta'/2)^2 - k'k} \qquad \Omega_\Delta' = \Omega_\Delta - ik_\Delta \qquad (k'-k) = k_\Delta$$

This correctly reduces to the k=k' result. The spectrum, however, is fairly complicated because not R is complex all the time. We might look at some limits.

Comment: What happens here in **large k limit**? As shown below we get $R \approx ik_{av}$ so the above formula then becomes:

$$s(t) = (1/2)\,(1+1)\,e^{d-t} + (1/2)\,(1-1)\,e^{d+t} = e^{d-t}$$

and only the d_- peak survives (in this limit). The frequency will be shifted by an amount relating to the real part of R which we compute in more detail below. So this says that even if we start at time 0 with equal amounts of both species (ie, we start not in equilibrium), we get our Knight shift effect at large k.

Let's back up now and apply this to a **different ρ(0) vector**, namely

$$(x_0, y_0) = (\rho_A(0), \rho_B(0)) = ([A]_{eq}, [B]_{eq}) = [A]_{eq}(1, K) \qquad K = k/k' \qquad k = Kk'$$

Let's forget the normalization and just call it (1,K). Then we are interested in this solution to our problem:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}\begin{pmatrix} 1 \\ K \end{pmatrix} = \begin{pmatrix} A+BK \\ C+DK \end{pmatrix}$$

and we then want to add the coherences from each, so the final result is

$$s(t) = A + BK + C + DK \qquad \text{// ignore constants overall}$$

So modify results above to get

$$A+BK = [\,\varepsilon_+ e^{d+t} - \varepsilon_- e^{d-t}]/2iR + K\,k'\,[e^{d+t} - e^{d-t}]/2iR$$

$$= \{\ (\varepsilon_+ + K\,k')\,e^{d+t} - (\varepsilon_- + K\,k')\,e^{d-t}\ \}/2iR$$

$$DK+C = -K[\,\varepsilon_- e^{d+t} - \varepsilon_+ e^{d-t}]/2iR + k\,[e^{d+t} - e^{d-t}]/2iR$$

$$= \{\ (-K\varepsilon_- + k)\,e^{d+t} - (-K\varepsilon_+ + k)\,e^{d-t}\ \}/2iR$$

Then add these signals to get

$$s(t) = \{\,[(\varepsilon_+ + K\,k') + (-K\varepsilon_- + k)]\,e^{d+t} - [(\varepsilon_- + K\,k') + (-K\varepsilon_+ + k)]\,e^{d-t}\}/2iR$$

Now replace k = Kk' to get

$$s(t) = \{\,[(\varepsilon_+ + k) + (-K\varepsilon_- + k)]\,e^{d+t} - [(\varepsilon_- + k) + (-K\varepsilon_+ + k)]\,e^{d-t}\}/2iR$$

where, once again, we have

$\varepsilon_{\pm} = i\,\Omega_{\Delta}'/2 \pm iR$

$d_{\pm} = -k_{av} - \lambda + i\,\Omega_{av} \pm iR$

$R = \sqrt{(\Omega_{\Delta}'/2)^2 - k'k}$ $\qquad \Omega_{\Delta}' = \Omega_{\Delta} - ik_{\Delta}$ $\qquad (k'-k) = k_{\Delta}$

Now, the location of the frequencies is controlled by the real part of R, and we are always going to have our two peak frequencies being centered around Ω_{av}. The only way we can "show a Knight shift" is to show that, as k and k' get large with K constant, one of these peaks goes away, and then we have just the other peak, and it is shifted, and that shift is the Knight shift.

The algebra to show this is just unbelievably messy in my notation. We want to compare these tw peak amplitudes:

e^{d+t}peak: $\qquad [(\varepsilon_{+} + k) + (-K\varepsilon_{-} + k)] \qquad amp_{+}$

e^{d-t} peak: $\qquad -[(\varepsilon_{-} + k) + (-K\varepsilon_{+} + k)] \qquad amp_{-}$

It is not obvious to me what happens in the **large k limit** because dependence is so complex. We can write

$$R = \sqrt{(\Omega_{\Delta}/2)^2 - k_{av}^2 - i\Omega_{\Delta}k_{\Delta}/2}$$

and we can take the large k limit of this to get $R = i\,k_{av}$. Then we have

$\varepsilon_{\pm} = i\,\Omega_{\Delta}'/2 \pm iR = i\,[\Omega_{\Delta} - ik_{\Delta}]/2 \pm iR = i\Omega_{\Delta} + k_{\Delta}/2 \pm iR = i\Omega_{\Delta} + k_{\Delta}/2 \pm i[i\,k_{av}]$

$= i\Omega_{\Delta} + k_{\Delta}/2 \mp k_{av}$

Then we can write

$amp_{+} = [(\varepsilon_{+} + k) + (-K\varepsilon_{-} + k)] = \varepsilon_{+} - K\,\varepsilon_{-} + 2k$

$= i\Omega_{\Delta} + k_{\Delta}/2 - k_{av} - K(i\Omega_{\Delta} + k_{\Delta}/2 + k_{av}) + 2k$

$= i\Omega_{\Delta}(1-K) + (k_{\Delta}/2 - k_{av}) - K(k_{\Delta}/2 + k_{av}) + 2k$

Now we go off to show that

$k_{\Delta}/2 - k_{av} = (k'-k)/2 - (k+k')/2 = -k$

$k_{\Delta}/2 + k_{av} = (k'-k)/2 + (k+k')/2 = k'$

So we then have

$amp_+ = i\Omega_\Delta(1-K) - k - Kk' + 2k = i\Omega_\Delta(1-K) - k - k + 2k = i\Omega_\Delta(1-K)$

Interesting, we get exact cancellation of k and k' terms so as k and k' get large, this term stays constant.

Now look at the other term:

$-amp_- = [(\varepsilon_- + k) + (-K\varepsilon_+ + k)] = \varepsilon_- - K\varepsilon_+ + 2k$

$= i\Omega_\Delta + k_\Delta/2 + k_{av} - K(i\Omega_\Delta + k_\Delta/2 - k_{av}) + 2k$

$= i\Omega_\Delta(1-K) + (k_\Delta/2 + k_{av}) - K(k_\Delta/2 - k_{av}) + 2k$

$= i\Omega_\Delta(1-K) + k' - K(-k) + 2k = i\Omega_\Delta(1-K) + k' + Kk + 2k = i\Omega_\Delta(1-K) + k' + Kk + 2k$

$= i\Omega_\Delta(1-K) + k(K+2) + k'$

$= i\Omega_\Delta(1-K) + (K+2 + 1/K)\, k$

Now as $k \to \infty$, this term becomes very large and swamps the first term. Of course we have to divide each of our amplitudes by $2iR = 2i[ik_{av}] = -2k_{av}$ so then we get $K = k/k'$

$amp_+(norm) = i\Omega_\Delta(1-K)/(-2k_{av}) \to 0$

$amp_-(norm) = [i\Omega_\Delta(1-K) + (K+2 + 1/K)\, k]/(+2k_{av}) \to (1/2)(K+2 + 1/K)(k/k_{av})$

But $(k/k_{av}) = 2/(1+K)$ so we get

$amp_-(norm) \to (1/2)(K+2 + 1/K)\, 2/(1+K) = (K+1)/K$

We find for the large k limit that

$amp_+(norm) \to 0$
$amp_-(norm) \to (K+1)/K$

If I add in the 2i/4i factor that I did last time, that will introduce an extra factor 1/2 and we get

$amp_+(norm) \to 0$
$amp_-(norm) \to (K+1)/2K$ // which goes to 1 in the limit $K \to 1$

which says that **only the - peak survives this limit,** as we had hoped. Now finally let's look at the frequency of this peak in the large k limit:

$$d_{\pm} = - k_{av} - \lambda + i\,\Omega_{av} \pm iR$$

But now we need R to have a real part which will determine the "shift", so

$$R = \sqrt{(\Omega_{\Delta}/2)^2 - k_{av}^2 - i\Omega_{\Delta}k_{\Delta}/2}$$

$$R = i\sqrt{(k_{av}^2 + i\Omega_{\Delta}k_{\Delta}/2)} = i\,k_{av}\sqrt{1 + i\Omega_{\Delta}k_{\Delta}/2k_{av}^2)} \approx i\,k_{av}\,(1 + i\Omega_{\Delta}k_{\Delta}/4k_{av}^2)$$

We then get

$$d_{\pm} = - k_{av} - \lambda + i\,\Omega_{av} \pm iR = - k_{av} - \lambda + i\,\Omega_{av} \mp k_{av}(1 + i\Omega_{\Delta}k_{\Delta}/4k_{av}^2)$$

$$= (- k_{av} - \lambda \mp k_{av}) + i\,(\Omega_{av} \mp \Omega_{\Delta}k_{\Delta}/4k_{av})$$

We really care only about the surviving d_- peak for which we get

$$d_- = -\lambda + i\,(\Omega_{av} + \Omega_{\Delta}k_{\Delta}/4k_{av})$$

This suggests that the surviving peak appears at this frequency

the surviving - peak is here: $\Omega_{av} + \Omega_{\Delta}k_{\Delta}/4k_{av}$ // large k, k' limit

Also, we see that this peak is "narrow" because it has only its natural λ width. The other peak which has no height has the width $\lambda + 2k_{av}$ which is infinitely wide. So, I have an estimate for the **"Knight shift"** in a system of A,B species with TE defined by K = k/k':

$$\Omega_{shift} = \Omega_{\Delta}k_{\Delta}/4k_{av}$$

If we take the limit k = k', then $k_{\Delta} = 0$ and we get zero shift in the large k limit, so that is good. My amplitudes above suggest that one amplitude only survives in this limit still, and that is the final narrow peak.

Let's now look at the **small k limit** of this same problem. We go back to:

$$s(t) = \{\,[(\varepsilon_+ + k) + (- K\varepsilon_- + k)]\,e^{d+t} - [(\varepsilon_- + k) + (-K\varepsilon_+ + k)]\,e^{d-t}\}\,/2iR$$

where, once again, we have

$$\varepsilon_{\pm} = i\,\Omega_{\Delta}'/2 \pm iR$$

$d_{\pm} = - k_{av} - \lambda + i\,\Omega_{av} \pm iR$

$R = \sqrt{(\Omega_{\Delta}'/2)^2 - k'k}$ $\qquad \Omega_{\Delta}' = \Omega_{\Delta} - ik_{\Delta}$ $\qquad (k'-k) = k_{\Delta}$

In the small k limit, we can crudely say that $R = (\Omega_{\Delta}/2)$ and then

$\varepsilon_{\pm} = i\,\Omega_{\Delta}'/2 \pm iR = i\,\Omega_{\Delta}/2 \pm i(\Omega_{\Delta}/2) = i\,\Omega_{\Delta}/2\,[\,1 \pm 1]$

$\varepsilon_{+} = i\,\Omega_{\Delta}$

$\varepsilon_{-} = 0$

Then we find: (set k = 0)

$s(t) = \{\,[(\varepsilon_{+} + k) + (-K\varepsilon_{-} + k)]\,e^{d+t} - [(\varepsilon_{-} + k) + (-K\varepsilon_{+} + k)]\,e^{d-t}\}\,/2iR$

$= \{\, i\,\Omega_{\Delta}\,e^{d+t} + K\,i\,\Omega_{\Delta}\,e^{d-t}\,\}/2iR$

$= i\,\Omega_{\Delta}\,\{\, e^{d+t} + K\,e^{d-t}\,\}\,/\,2i(\Omega_{\Delta}/2) = (1/2i)\,\{\, e^{d+t} + K\,e^{d-t}\,\}$

and here we see our desired effect that there are **two peaks with unequal amplitude** since $k \neq k'$