RESOLUTION OF TWO DEBYE LOSS PEAKS OF EQUAL AMPLITUDE

Consider two Debye peaks of equal amplitude with relaxation times τ / R and τR so that their ratio is R^2. This ensures that the geometric average relaxation time of their sum is $\langle\tau\rangle = 1$ and that when plotted against $\log_{10}(\omega\tau)$ the two peaks, if resolved, appear an equal number of decades on each side of $\ln\langle\tau\rangle = 0$. This symmetry and the equality of amplitudes make the mathematics tractable (otherwise an 18th order polynomial (!) would have to be solved, see below). For convenience place $\omega\tau = x$ so that the sum of the two Debye peaks is

$$f = \frac{x/R}{1+x^2/R^2} + \frac{Rx}{1+R^2x^2}. \quad (1)$$

The extrema in f are then obtained from

$$\frac{df}{dx} = 0 = \frac{1/R}{1+x^2/R^2} - \frac{x/R\left(2x/R^2\right)}{\left(1+x^2/R^2\right)^2} + \frac{R}{1+R^2x^2} - \frac{Rx\left(2R^2x\right)}{\left(1+R^2x^2\right)^2} \quad (2a)$$

$$= \frac{1/R\left(1-x^2/R^2\right)}{\left(1+x^2/R^2\right)^2} + \frac{R\left(1-R^2x^2\right)}{\left(1+R^2x^2\right)^2} \quad (2b)$$

$$= \frac{1/R\left(1-x^2/R^2\right)\left(1+R^2x^2\right)^2 + R\left(1-R^2x^2\right)\left(1+x^2/R^2\right)^2}{\left(1+x^2/R^2\right)^2\left(1+R^2x^2\right)^2} \quad (2c)$$

$$= \frac{1/R\left[\left(1-x^2/R^2\right)\left(1+R^2x^2\right)^2 + R^2\left(1-R^2x^2\right)\left(1+x^2/R^2\right)^2\right]}{\left(1+x^2/R^2\right)^2\left(1+R^2x^2\right)^2}. \quad (2d)$$

Defining $r = R^2$ and $z = x^2$ and placing the numerator of eq. (2d) equal to zero yields

$$\left(1-z/r\right)\left(1+2rz+r^2z^2\right) + r\left(1-rz\right)\left(1+2z/r+z^2/r^2\right) = 0. \quad (3)$$

Rearranging eq. (3) yields

$$-\left(r+1\right)z^3 + \left[\frac{1}{r}\left(r+1\right)\left(r^2-3r+1\right)\right]z^2 - \left[\frac{1}{r}\left(r+1\right)\left(r^2-3r+1\right)\right]z + \left(r+1\right) = 0; \quad (4a)$$

$$-\left[r\left(r+1\right)\right]z^3 + \left[\left(r+1\right)\left(r^2-3r+1\right)\right]z^2 - \left[\left(r+1\right)\left(r^2-3r+1\right)\right]z + \left[r\left(r+1\right)\right] = 0; \quad (4b)$$

$$-\left(r^2+r\right)z^3 + \left(r^3-2r^2-2r+1\right)z^2 - \left(r^3-2r^2-2r+1\right)z + \left(r^2+r\right) \quad (4c)$$

$$a_3z^3 + a_2z^2 + a_1z + a_0 = 0 \quad (4d)$$

Equation (4) is appropriately a cubic equation in z whose solutions for resolved peaks correspond to the two maxima and the intervening minimum. The condition for no resolution is that eq. 4 has one real root and two complex conjugate roots. The condition for borderline resolution is that there are three identical solutions, i.e that eq. (4) is a perfect cube. For eq. (4c) to have three equal roots it is required that $3a_3 = -a_2 = a_1 = -3a_0$ and indeed $a_3 = -a_0$ and $a_2 = -a_1$. For $3a_3 = -a_2$

$$a_2 = \frac{1}{r}(r+1)(r^2-3r+1) = -3a_3 = 3(r+1) \tag{5a}$$

$$\Rightarrow (r^2-3r+1) = 3r \tag{5b}$$

$$\Rightarrow r^2-6r+1=0. \tag{5c}$$

The quadratic solutions to eq. (5c) are

$$r = \frac{6 \pm (36-4)^{1/2}}{2} = \frac{6 \pm (32)^{1/2}}{2} = 3 \pm 2^{3/2}, \tag{6}$$

so that $R = \left[3 \pm 2^{3/2}\right]^{1/2} = \left(1 \pm 2^{1/2}\right)$. Note that $\left(1+2^{1/2}\right) = 1\Big/\left[\left(1-2^{1/2}\right)\right]$, consistent with the equivalence of R and $1/R$ in eq (1). On a logarithmic scale the ratio of the relaxations times $R^2 = r$ is $\log_{10}\left(3+2^{3/2}\right) = 0.7656$ decades.

preliminary analysis of unequal amplitudes

To illustrate the intractability of solving for two peaks of unequal amplitude (but still symmetrically placed around $\omega\tau = 1$) we now show that the Cardano method for solving a cubic equation indicates that an 18th order polynomial in r would have to be solved. Consider the following:

$$f = \frac{x/R}{1+x^2/R^2} + \frac{ARx}{1+R^2x^2} = \frac{Rx}{R^2+x^2} + \frac{ARx}{1+R^2x^2}. \tag{7}$$

Equation (4c) then becomes

$$-\left(r^2+Ar\right)z^3 + \left(r^3-2Ar^2-2r+A\right)z^2 - \left(Ar^3-2r^2-2Ar+1\right)z + \left(Ar^2+r\right) = 0. \tag{8}$$

Note that for A = 1 eq. (8) is the same as eq. (4c). Borderline resolution occurs when eq. (8) has two equal and real roots and one different real root. The first step to solving eq. (8) is to make the substitution $z = y - \dfrac{a_2}{3a_3}$ that converts the cubic form of eq. (4d) into one of the form

$$y^3 + A_1 y + A_0 = 0, \tag{9}$$

where

$$A_1 = -\frac{a_2^2}{3a_3^2} + \frac{a_1}{a_3} = \frac{1}{a_3^2}\left(-\frac{a_2^2}{3} + a_1 a_3\right) \tag{10a}$$

and

$$A_0 = \frac{2a_2^3}{27a_3^2} - \frac{a_1 a_2}{3a_3^2} + \frac{a_0}{a_3} = \frac{1}{a_3^3}\left(2a_2^3 a_3 - \frac{a_1 a_2 a_3}{3} + a_0 a_3^2\right). \tag{10b}$$

For there to be two equal real roots the cubic equivalent of the quadratic determinant must be zero and this yields

$$\frac{A_0^2}{4} + \frac{A_1^3}{27} = 0\,. \tag{11}$$

Multiplying eq. (11) through by a_3^6 (that cannot be zero for eq. (4d) to be cubic) yields an 18th order polynomial in *r*. For example the term a_2^2 in eq. (10a) for A_1 is a 6th order polynomial in *r* (eq. 4c)) that is raised to the 3rd power in eq. (11), and a_2^3 in eq. (10b) for A_0 is a 9th order polynomial in *r* (eq. 4c)) that is raised to the 2nd power in eq. (11)).

Placing the second derivative of eq. (7) equal to zero appears to require the solution of another intractable polynomial of order much greater than 4.