5.74 Introductory Quantum Mechanics II
Spring 2009

Absorption Lineshape for the Displaced Harmonic Oscillator Model

Investigate the low temperature lineshape for electronic transition coupled to a single harmonic mode.

We will perform calculations for three couplings: weak medium, and strong: $z := 0, 1 .. 2$

Lets work in units of $hbar := 1$ $\mu_{eg} := 1$ $m := 1$

Define the frequency of the electronic transition: $\omega_{eg} := 10$

and the vibrational frequency: $\omega_0 := 1$

Set up displacement grid $i := 0 .. 200$ $q_i := -5 + 0.05 \cdot i$

Set up time grid $t_i := i \cdot 0.1$

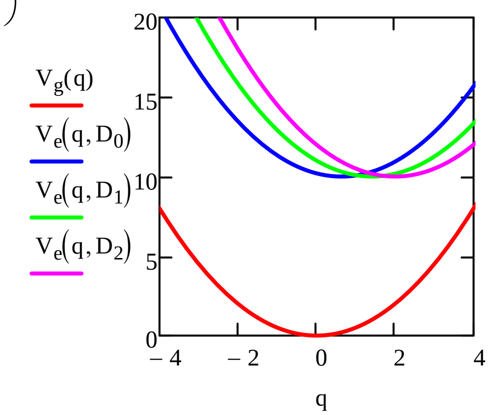
Set up frequency grid: $\omega_i := -4 + \omega_{eg} + 0.05 \cdot i$

The unitless displacement of the two harmonic wells is:

$$D_z := \begin{pmatrix} 0.2 \\ 1 \\ 2 \end{pmatrix}$$

Ground and excited state potential energy surfaces

$$V_g(qx) := \frac{1}{2} \cdot m \cdot \omega_0^{\,2} \cdot qx^2 \qquad V_e(q, D) := \omega_{eg} + \frac{1}{2} m \cdot \omega_0^{\,2} \cdot \left(q - \sqrt{\frac{2 \cdot D \cdot hbar}{m \cdot \omega_0}} \right)^2$$



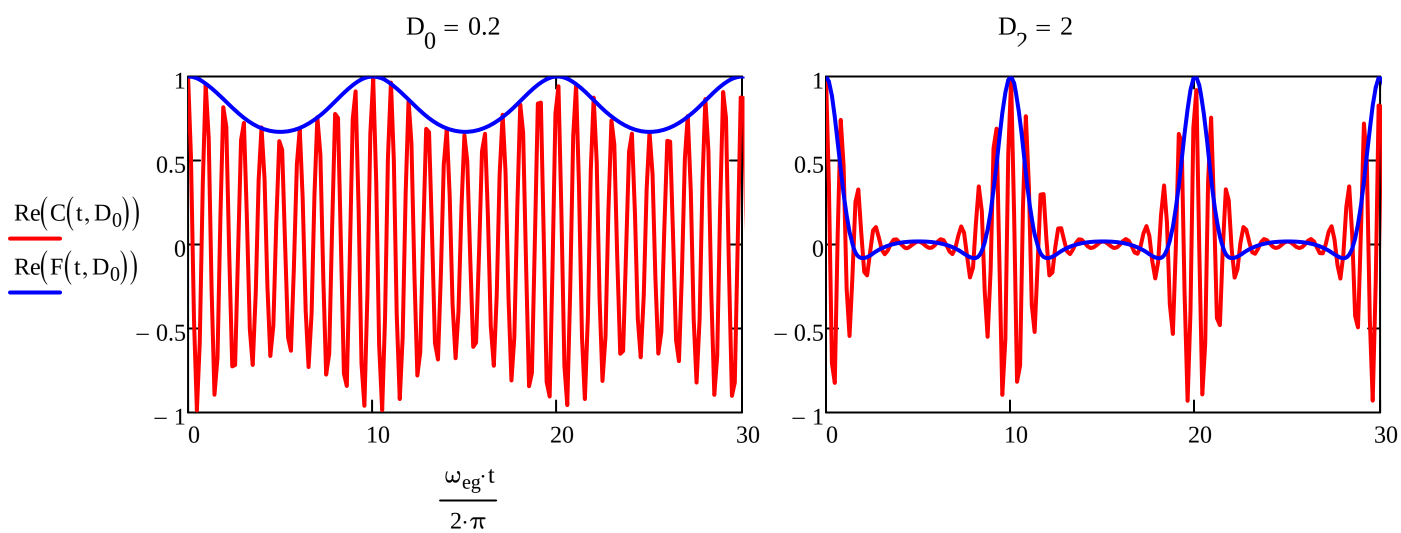
Lineshape function, Dephasing function and dipole correlation function

$$g(t, D) := -D \cdot \left(e^{-i \cdot \omega_0 \cdot t} - 1 \right)$$

$$F(t, D) := e^{-g(t, D)}$$

$$C(t, D) := \left(\left| \mu_{eg} \right| \right)^2 \cdot e^{-i \cdot \omega_{eg} \cdot t - g(t, D)}$$

Plot the correlation function and dephasing function for low and high coupling



Absorption lineshape:

$$\delta(g) := \text{if}(g = 0, 1, 0)$$

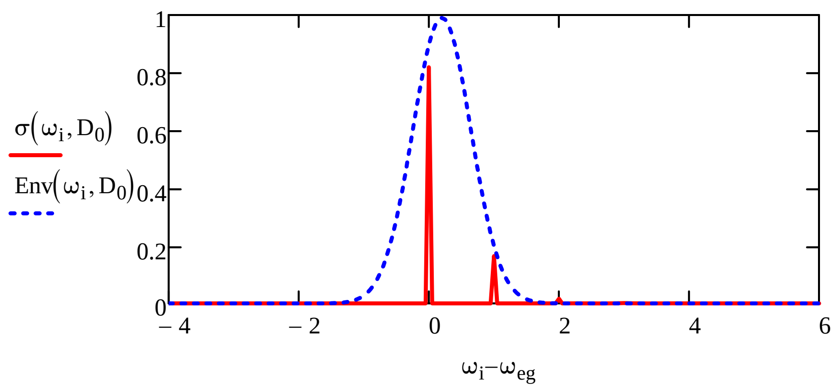
$$\sigma(\omega, D) := \left(\left|\mu_{eg}\right|\right)^2 \cdot e^{-D} \cdot \sum_{J=0}^{10} \left[\frac{D^J}{J!} \cdot \left(\delta\left(\omega - \omega_{eg} - J \cdot \omega_0\right)\right)\right]$$

Envelope of vibronic progression:

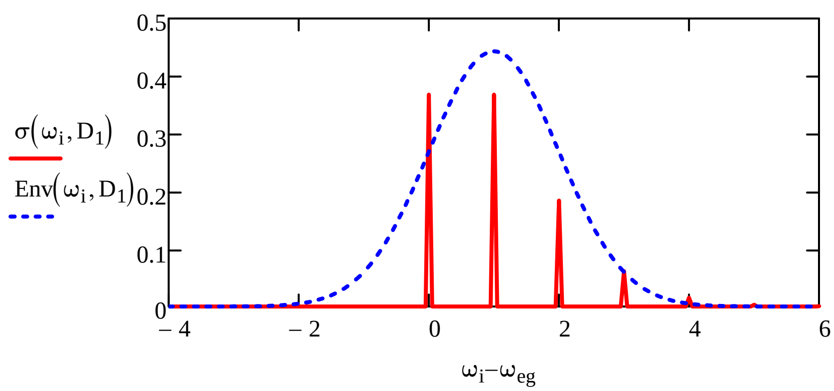
$$\text{Env}(\omega, D) := \sqrt{\frac{\pi}{D \cdot \omega_0{}^2}} \cdot 0.25 \cdot \left(\left|\mu_{eg}\right|\right)^2 \cdot \exp\left[\frac{-\left(\omega - \omega_{eg} - D \cdot \omega_0\right)^2}{2 \cdot D \cdot \omega_0{}^2}\right]$$

Plot lineshapes for low, mid and high coupling.

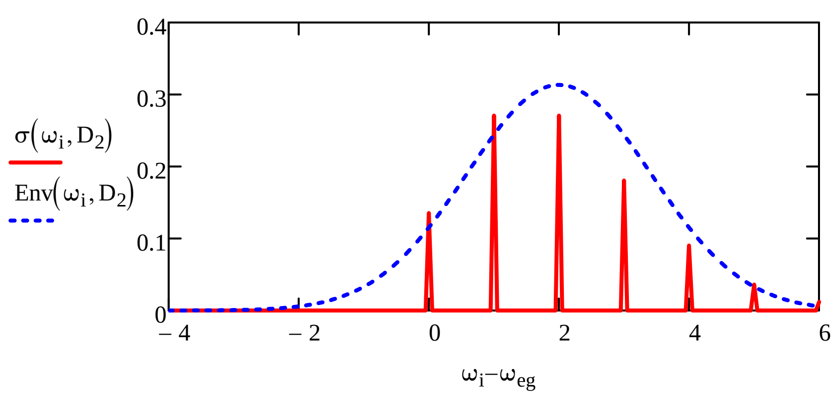
(a) $D_0 = 0.2$



(b) $D_1 = 1$



(c) $D_2 = 2$



$$D = \begin{pmatrix} 0.2 \\ 1 \\ 2 \end{pmatrix} \qquad \omega_0 = 1$$