5.74 Introductory Quantum Mechanics II
Spring 2009

Gaussian-stochastic model for the absorption lineshape

This worksheet plots the frequency correlation function $C\omega\omega$, dephasing function F, and absorption lineshape σ. The parameters that determine the lineshape are the width of the frequency distribution Δ and the frequency correlation time τ_c. Defining $\kappa = \Delta\tau_c$, we will investigate the fast (κ>1), intermediate (κ=1) and slow (κ <1) modulation cases.

First define variables. Range variables for the time and frequency axes : $ma := 2^{12}$ $\quad i := 0..\, ma - 1$ $\quad ii := 0..\, 2^{13} - 1$

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

We will perform all calculations for a fixed value of Δ, and calculate for three correlation times: $z := 0, 1..\, 2$

$\Delta := 1$

$\tau_{c_z} :=$

0.2
1
10

$\kappa_z := \tau_{c_z} \cdot \Delta$ $\quad \kappa = \begin{pmatrix} 0.2 \\ 1 \\ 10 \end{pmatrix}$

Define the lineshape function and dephasing function:

$$g(t, \tau_c) := \left[\Delta^2 \cdot \tau_c^{\,2} \cdot \left(\exp\left(\frac{-t}{\tau_c} \right) + \frac{t}{\tau_c} - 1 \right) \right] \qquad F(t, \tau_c) := \exp(-g(t, \tau_c))$$

Evaluate the correlation function and lineshape function

$$C\omega_{fast_i} := \exp\left(\frac{-t_i}{\tau_{c_0}} \right) \qquad C\omega_{slow_i} := \exp\left(\frac{-t_i}{\tau_{c_2}} \right) \qquad C\omega_{mid_i} := \exp\left(\frac{-t_i}{\tau_{c_1}} \right)$$

$$F_{fast_{ii}} := 0 \qquad F_{slow_{ii}} := 0 \qquad F_{mid_{ii}} := 0$$

$$F_{fast_i} := F(t_i, \tau_{c_0}) \quad F_{slow_i} := F(t_i, \tau_{c_2}) \quad F_{mid_i} := F(t_i, \tau_{c_1})$$

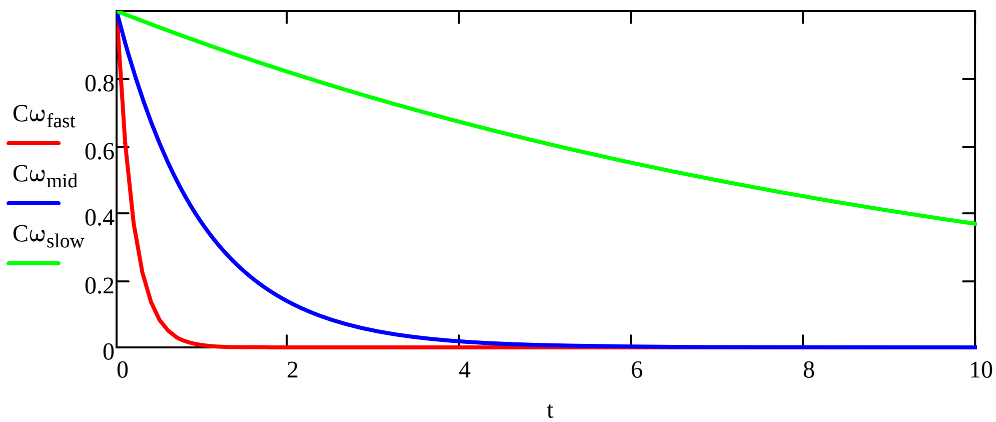
$$\Delta = 1 \qquad \tau_c = \begin{pmatrix} 0.2 \\ 1 \\ 10 \end{pmatrix} \qquad \kappa = \begin{pmatrix} 0.2 \\ 1 \\ 10 \end{pmatrix}$$

fast

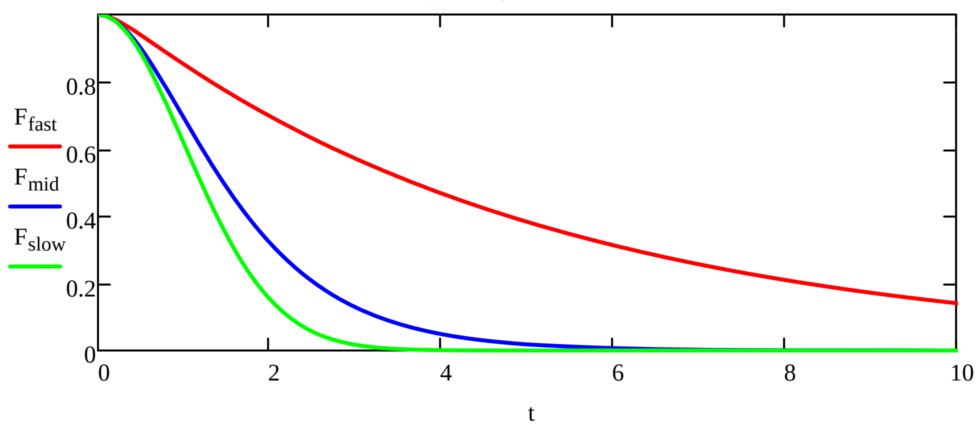
mid

slow

Frequency Correlation Function C(t)



Dephasing Function F(t)



Now Fourier transform the dipole correlation function $C_{\mu\mu}$ and use the real part to obtain the lineshape.

$$C\mu_{fast_i} := F\left(t_i, \tau_{c_0}\right) \qquad C\mu_{slow_i} := F\left(t_i, \tau_{c_2}\right) \qquad C\mu_{mid_i} := F\left(t_i, \tau_{c_1}\right)$$

$$S_{fast} := \mathrm{cfft}\left(C\mu_{fast}\right) \qquad S_{slow} := \mathrm{cfft}\left(C\mu_{slow}\right) \qquad S_{mid} := \mathrm{cfft}\left(C\mu_{mid}\right)$$

Some manipulations to wrap and normalize the Fourier transform:

$$\sigma_{fast} := \frac{\mathrm{stack}\left(S_{fast}, S_{fast}\right)}{\max\left(\mathrm{Re}\left(S_{fast}\right)\right)} \qquad \sigma_{slow} := \frac{\mathrm{stack}\left(S_{slow}, S_{slow}\right)}{\max\left(\mathrm{Re}\left(S_{slow}\right)\right)} \qquad \sigma_{mid} := \frac{\mathrm{stack}\left(S_{mid}, S_{mid}\right)}{\max\left(\mathrm{Re}\left(S_{mid}\right)\right)}$$

Determine the frequency axis for the Fourier transform

$$freq := \frac{1}{t_1 - t_0} \qquad t_{max} := t_{ma-1} \qquad \omega_{ii} := \frac{ii \cdot freq}{\pi \cdot t_{max}} \qquad \Omega := \omega_{ma-1}$$