A worksheet for generating trajectories for a Gaussian random process

This worksheet gnerates a trajectory of points for a Gaussian random process characterized by an arbitrary time-correlation function. The example specifically calculates a trajectory of instantaneous frequencies for a quantum system coupled to a bath.

The method makes use of the convolution theorem. The convolution of a set of Gaussian random time points with a time-correlation function can be evaluated by taking the product of their Fourier transforms and inverse Fourier transforming.

The number of points in the trajectory: $T := 2^{14}$ $\quad T = 1.638 \times 10^4$

Time-separation of points: $\delta t := 10$ femtoseconds

i

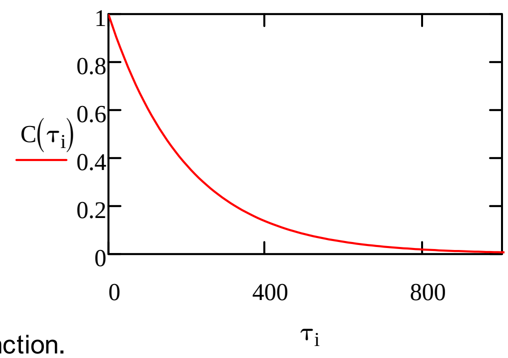
i

$i := 0 .. T - 1 \qquad \tau_i := \delta t \cdot i$

Define time-correlation function:

$A := 1 \qquad \tau_c := 200 \qquad C(t) := A \cdot \exp\left(\frac{-t}{\tau_c}\right)$

Fill data array with TCF: $E_i := C(\tau_i)$



Define Gaussian distribution:

Fill an array with a set of Gaussian distributed random numbers. Centered about ω_0=0 and width σ.

$\sigma := 180$ cm^{-1} $\qquad P := \mathrm{rnorm}(T, 0, \sigma)$

Convolute the random noise with the exponential correlation function.
Do in the frequency domain with FT.

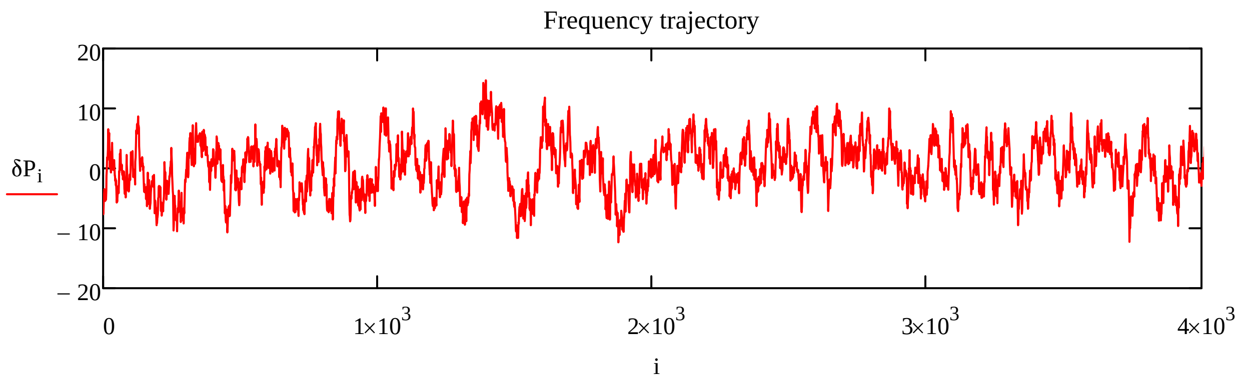
$P\omega := \mathrm{fft}(P) \qquad E\omega := \mathrm{fft}(E) \qquad P2 := \mathrm{ifft}\left[\overrightarrow{(P\omega \cdot E\omega)}\right]$

You may want to correct the average of the data set for imperfect sampling:

Frequency Fluctuations: $\delta P := \overrightarrow{(\mathrm{Re}(P2) - \mathrm{mean}(P2))}$

Add back a mean value for the fluctuations:

$\omega_0 := 1804$ cm^{-1} $\qquad Pt := \overrightarrow{(\omega_0 + \delta P)}$



Export data file:

WRITEPRN("D:\cf.dat") □ Pt

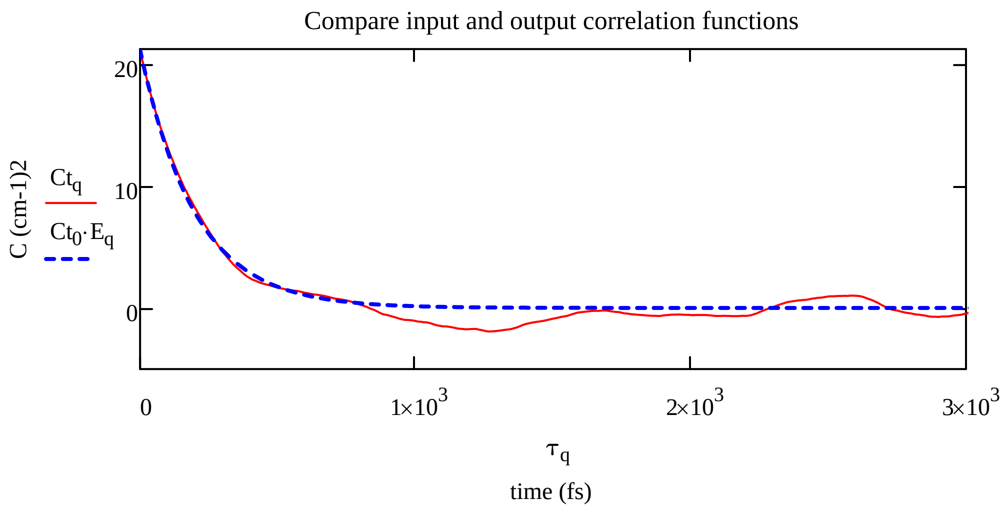
Calculate a correlation function from the trajectory:

We'll evaluate products of pairs of frequency separated by t, and normalize by the number of observations. Since we are interested in the short time behavior, let's not include all of the products for time delays >> τ_c.

Frequen

$q := 0 .. 600$

$$Ct_q := \frac{1}{T-q} \cdot \sum_{n=0}^{T-1-q} \left[\left(\delta P_{q+n} \right) \cdot \delta P_n \right]$$



Using more points in the trajectory will give a better correspondence.