

Molecular quantum dynamics: Exercise series 9

Read: Schatz and Ratner 5.4.1, 5.4.2 (previous lecture), 5.4.9 , Tannor 6.1.1, 6.1.2, 6.2.1, 6.2.2.

Problem 1: Collisional line broadening

In spectroscopy, broadening of lines can occur by several mechanisms. One origin of broadening is the finite collisional or natural lifetime of a state. Such broadening gives rise to a Lorentzian line shape function due to the effective damping of the oscillating dipole. Derive the Lorentzian line shape $\sigma(\omega)$ as the Fourier transform, $\sigma(\omega) = (2\pi)^{-1} \int_{-\infty}^{\infty} C(t) e^{i\omega t} dt$, of the correlation function

$$C(t) = C(0) e^{-\Gamma|t|}.$$

Problem 2: Properties of the Fourier transform and convolution.

a) Prove the inverse form of the convolution theorem:

$$\widetilde{f * g} = \sqrt{2\pi} \tilde{f} \tilde{g},$$

or, more explicitly,

$$\int_{-\infty}^{\infty} f(x') g(x - x') dx' = \int_{-\infty}^{\infty} \tilde{f}(k) \tilde{g}(k) e^{ikx} dk$$

b) Show that the convolution of any function with a δ -function is the function itself, i.e., that

$$f * \delta = f.$$