Quantum Molecular Dynamics Homework 6 Spring, 2000

1. Take a model for an electronic transition of two displaced harmonic oscillators with the same frequency. Let the initial state be the ground vibrational state of the ground state potential and let the excitation be a pair of δ-function pulses. Compare the formula eq. 13.12 (using the analytical form for the time-dependent wavepacket) with the numerical result using the MATLAB program distributed. Check the dependence on Δ, τ and ϕ, and show that leaving the combination $\Delta\tau - \phi$ unchanged leaves the result unchanged.

2. Take the same model as in the previous exercise. Now let the excitation be a single Gaussian pulse of the form:

$$E(t) = E_0 \exp[-\frac{t^2}{2\tau^2} - i\omega_0 t - ic\frac{t^2}{2}]. \tag{2.1}$$

   First, plot a time-frequency Wigner distribution for $E(t)$, and describe the dependence on E_0, ω_0 and c. In particular, what is the dependence on the sign of β? Now, calculate the population, $< \psi^{(1)}(T)|\psi^{(1)}(T) >$ at a time T long after the pulse has finished. What is the dependence on each of the four parameters of $E(t)$? What is the dependence *during* the pulse? Compare with the numerical results from the MATLAB program.

3. Consider a two-level quantum system with frequency separation ω_0. First, show that no matter how the pulse is shaped, one photon excitation just gives an amplitude in the excited state proportional to the Fourier component of $E(t)$ at the resonant frequency. Now consider two-photon excitation using a pulse whose carrier frequency is $\omega_0/2$. Show that if the phases $\phi(\omega)$ are antisymmetric around $\omega_0/2$ that no population is transferred to the excited state. Optional: find conditions for non-asymmetric phase distributions that also lead to null population transfer.