4.14: The Harmonic Oscillator Quantum Jump

This Mathcad worksheet determines whether an SHO spectroscopic transition is allowed assuming that the Bohr frequency condition is satisfied. It requires only the quantum numbers of the initial and final states.

The $v = 0$ to $v = 1$ transition is allowed because the position distribution function, $Y^{*}Y$, exhibits oscillating dipole character.

$$\text{Initial State:} \quad v_i = 0 \quad E_i = v_i + \tfrac{1}{2} \quad \text{Final state:} \quad v_f = 1 \quad E_f = v_f + \tfrac{1}{2}$$

$$\text{Set plot parameters:} \quad \text{Space} = 60 \quad \text{Time} = 10 \quad \text{Xmin} = 3$$

$$j = 0..\text{Space} \quad x_j = -\text{Xmin} + \frac{2\text{Xmin}j}{\text{Space}} \quad k = 0..\text{Time} \quad t_k = \frac{k20}{\text{Time}}$$

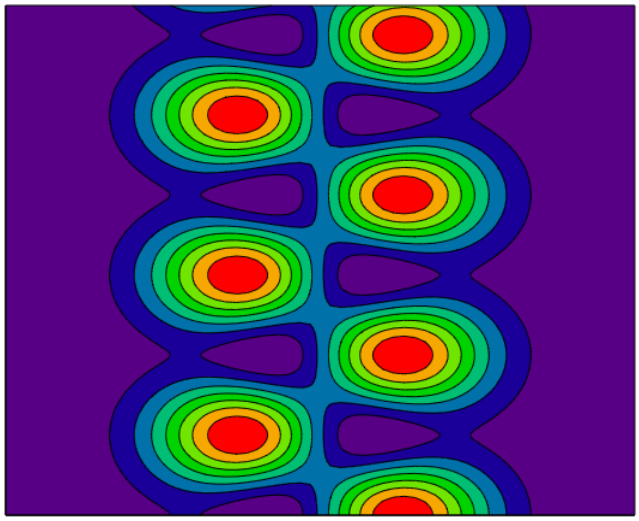
Construct time-dependent superposition of the initial and final states:

$$\Psi(x,\ t) = \exp\left(-\frac{x^2}{2}\right)\left(\text{Her}(v_i,\ x)\exp(-iE_i t) + \text{Her}(v_f,\ x)\exp(-iE_f t)\right)$$

Calculate and plot Y*Y:

$$\Psi\Psi_{(j,\,k)} = \overline{\Psi(x_j,\ t_k)}\,\Psi(x_j,\ t_k)$$

In this contour plot the horizontal axis is the spatial axis. Time is graphed on the veritcal axis. If $Y^{*}Y$ asymmetric in time the transition is allowed.



The v = 0 to v = 2 transition is allowed because the position distribution function, $Y^{*}Y$, does not exhibit oscillating dipole character.

$$\text{Initial State:} \quad v_i = 0 \quad E_i = v_i + \tfrac{1}{2} \quad \text{Final state:} \quad v_f = 1 \quad E_f = v_f + \tfrac{1}{2}$$

$$\text{Set plot parameters:} \quad \text{Space} = 60 \quad \text{Time} = 150 \quad \text{Xmin} = 3$$

$$j = 0..\text{Space} \quad x_j = -\text{Xmin} + \frac{2\text{Xmin}j}{\text{Space}} \quad k = 0..\text{Time} \quad t_k = \frac{k20}{\text{Time}}$$

Construct time-dependent superposition of the initial and final states:

$$\Psi(x,\ t) = \exp\left(-\frac{x^2}{2}\right)\left(\text{Her}(v_i,\ x)\exp(-iE_i t) + \text{Her}(v_f,\ x)\exp(-iE_f t)\right)$$

Calculate and plot Y*Y:

$$\Psi\Psi_{(j,\,k)} = \overline{\Psi(x_j,\,t_k)}\Psi(x_j,\,t_k)$$

In this contour plot the horizontal axis is the spatial axis. Time is graphed on the vertical axis. If $\Upsilon^*\Upsilon$ asymmetric in time the transition is allowed.