4.10: Another Look at the Quantum Jump

Consider an electron in a one-bohr, one-dimensional box. This tutorial will explore, in an elementary way, the selection rule for the transition of the electron from one allowed energy level to another. The condition for an allowed transition is two-fold: the photon exciting the transition must satisfy the Bohr frequency condition [hν = Ef - Ei] and the expectation value for the position of the electron must exhibit oscillatory dipole character as a function of time. This latter requirement provides a coupling mechanism between the oscillating electromagnetic field and the oscillating charge density of the electron in the box.

Assuming that the Bohr frequency condition is met we will look at the second at the second criterion for a number of possible electronic transitions or "quantum jumps." Consider first the transition from the ground state to the first excited state.

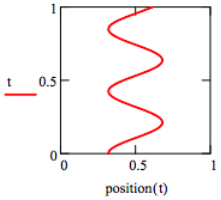
$$\text{Initial state:} \quad n_i = 1 \quad E_i = \frac{n_i^2 \pi^2}{2} \quad \text{Final state:} \quad n_f = 2 \quad E_f = \frac{n_f^2 \pi^2}{2}$$

Time-dependent superposition of initial and final states:

$$\Psi(x,\ t) = \sin(n_i \pi x) exp(-iE_i t) + \sin(n_f \pi x) exp(-iE_f t)$$

Time-dependent expectation value for position:

$$\text{position(t)} = \int_0^1 x(|\Psi(\text{x, t})|)^2 dx \quad t = 0, .001..1$$



Since the expectation value for position fluctuates in time (has time dependence) the transition between the n =1 and n = 2 states is allowed.

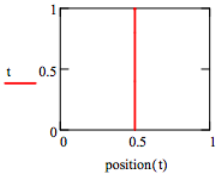
Now consider the n = 1 to n = 3 electronic transition.

$$\text{Initial state:} \quad n_i = 1 \quad E_i = \frac{n_i^2 \pi^2}{2} \quad \text{Final state:} \quad n_f = 3 \quad E_f = \frac{n_f^2 \pi^2}{2}$$

Time-dependent superposition of initial and final states:

$$\Psi(x,\ t) = \sin(n_i \pi x) exp(-iE_i t) + \sin(n_f \pi x) exp(-iE_f t)$$

$$\text{position}(t) = \int_0^1 x(|\Psi(x,\ t)|)^2 dx \quad t = 0, .002..1$$



For this case the expectation value for position does not fluctuate with time, providing no mechanism for coupling with the oscillating dipole character of the electromagnetic field. Therefore, the n = 1 to n = 3 electronic transition is not allowed. The selection rule that emerges after study of more cases is that Δn = an odd integer.

Simple Harmonic Oscillator

The same method is now used to look at allowed and forbidden transitions for the simple harmonic oscillator.

$$\text{Initial state:} \quad E_i = \nu_i + \tfrac{1}{2} \quad \text{Final state:} \quad E_f = \nu_f + \tfrac{1}{2} \quad nu = 0,\ 1, \text{etc.}$$

Time-dependent superposition of initial and final harmonic oscillator states:

$$\Psi(x,\ t,\ \nu_i,\ \nu_f) = \frac{1}{\sqrt{2}}\exp\left(-\frac{x^2}{2}\right)\left[\frac{\mathrm{Her}(\nu_i,\ x)\exp\left[-i\left(\nu_i+\frac{1}{2}\right)t\right]}{\sqrt{\nu_i!2^{\nu_i}\sqrt{\pi}}} + \frac{\mathrm{Her}(\nu_f,\ x)\exp\left[-i\left(\nu_f+\frac{1}{2}\right)t\right]}{\sqrt{\nu_f!2^{\nu_f}\sqrt{\pi}}}\right]$$

Time-dependent expectation value for position:

$$\mathrm{position}\,(t,\ \nu_i,\ \nu_f) = \int_{-\infty}^{\infty} x\left(\left|\Psi(x,\ t,\ \nu_i,\ \nu_f)\right|\right)^2 dx \quad t = 0,\ .05..20$$

Plot the time-dependent position expectation value for three transitions: 0-1; 0-2; 1-2. The 0-1 and 1-2 transitions are allowed and the 0-2 transition is forbidden.