

## Graph of Franck-Condon factors

The Franck-Condon factors are defined as the overlaps of vibrational eigenstates of two Born-Oppenheimer Hamiltonians corresponding to the electronic states of some transition. The simplest model is the displaced harmonic oscillator (HO). The first Hamiltonian is the HO centered at the origin,

$$\hat{H}_0 = -\frac{1}{2m} \frac{d^2}{dx^2} + \frac{m\omega^2 x^2}{2} = \omega(\hat{a}^\dagger \hat{a} + \frac{1}{2}). \quad (1)$$

The second Hamiltonian has its potential minimum displaced by a distance  $r$ ; it is given by

$$\hat{H}_1 = \omega(\hat{a}^\dagger \hat{a} + \frac{1}{2}) + \frac{r}{\sqrt{2}}(\hat{a}^\dagger + \hat{a}). \quad (2)$$

The program `franck-condon-graph.py` graphs the square of the overlap of the eigenstate  $|n\rangle$  of  $H_0$  with the eigenstate  $|m\rangle$  of  $H_1$ ,

$$|\langle n|m\rangle|^2. \quad (3)$$

Note that the parameter  $\Lambda$  in the program is related to the displacement  $r$  by  $\Lambda = r/\sqrt{2}$ .

The Python program requires a number of libraries. It has been tested under the Enthought distribution `epd-7.3-2-macosx-i386.dmg` of the Python libraries, together with the `MacTeX.pkg` distribution of Latex. Without the graphics, the program only needs the `numpy.py` library to run. The command

```
$python franck-condon-plot.py
```

will run the program for  $\Lambda = 10$ . The output graph is `fc.pdf`.

### Credits

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