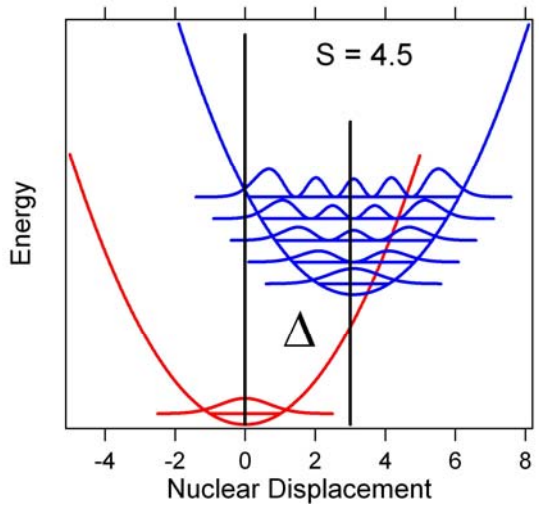
A. Sketch the potential energy surfaces of HF in the ground state and excited state assuming that the dimensionless displacement is Δ = 3. Label Δ on the sketch.



Δ is the displacement along the nuclear coordinate.
Note that the electron-phonon coupling $S = \Delta^2/2$ so $S = 4.5$.

B. Calculate the "stick spectrum" of the HF HOMO → LUMO transition assuming the T = 0 K approximation and that the vibrational mode is a Franck-Condon active mode. Make a table shows the individual bands.

$$FC = \sum_{v=0}^{\infty} \frac{S^v e^{-S}}{v!} \delta(\varepsilon - \varepsilon_{0-0'} - v\hbar\omega)$$

Solution: make a table to show the individual transitions

n'	FC factor	Plugged-in value	numerical value
0'	e^{-S}	$e^{-4.5}$	0.011
1'	Se^{-S}	$4.5e^{-4.5}$	0.05
2'	$S^2e^{-S}/2$	$20.25e^{-4.5}/2$	0.112
3'	$S^3e^{-S}/6$	$91.125e^{-4.5}/6$	0.168
4'	$S^4e^{-S}/24$	$410e^{-4.5}/24$	0.189
5'	$S^5e^{-S}/120$	$1845e^{-4.5}/120$	0.170
6'	$S^7e^{-S}/720$	$8303e^{-4.5}/720$	0.128

Note that for S=4.5, 1 → 4' and 1 → 5' bands are approximately equal in intensity.