

We have shown that everything fits up with SE:

$$\hat{H}\Psi = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(\vec{r})\Psi = E\Psi$$

$$E \sim \frac{\hbar^2}{m} \quad \text{or} \quad E \sim \frac{\hbar^2}{mr^2}$$

It all depends on mass and size of the particle.

$$m_H \sim 1.67 \cdot 10^{-27} \text{ kg}$$

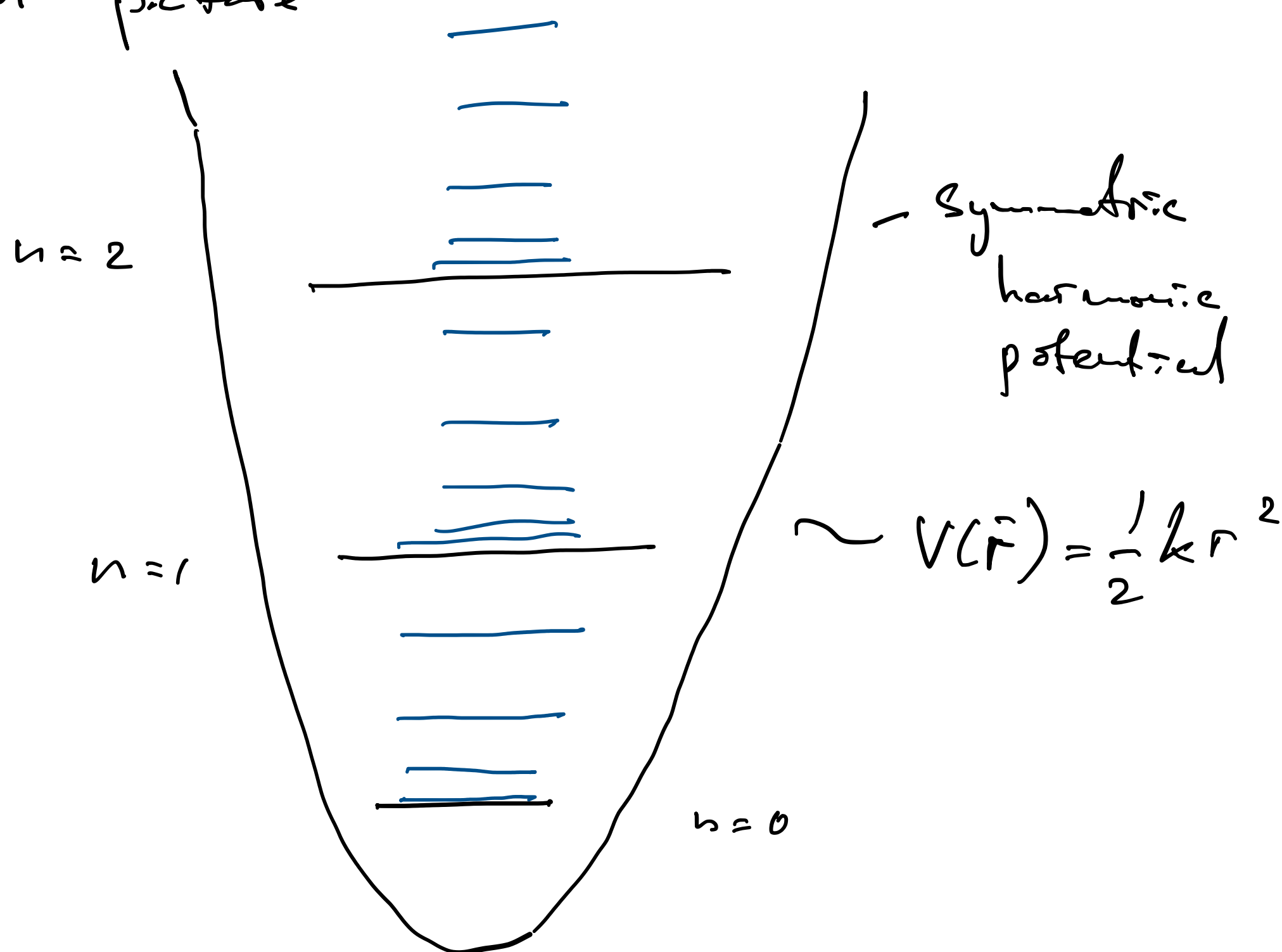
$$m_e \sim 9.11 \cdot 10^{-31} \text{ kg} \quad 10^4 !$$

$$\text{rotation} \rightarrow 10^{-1} - 10^2 \text{ cm}^{-1} \text{ (THz)}$$

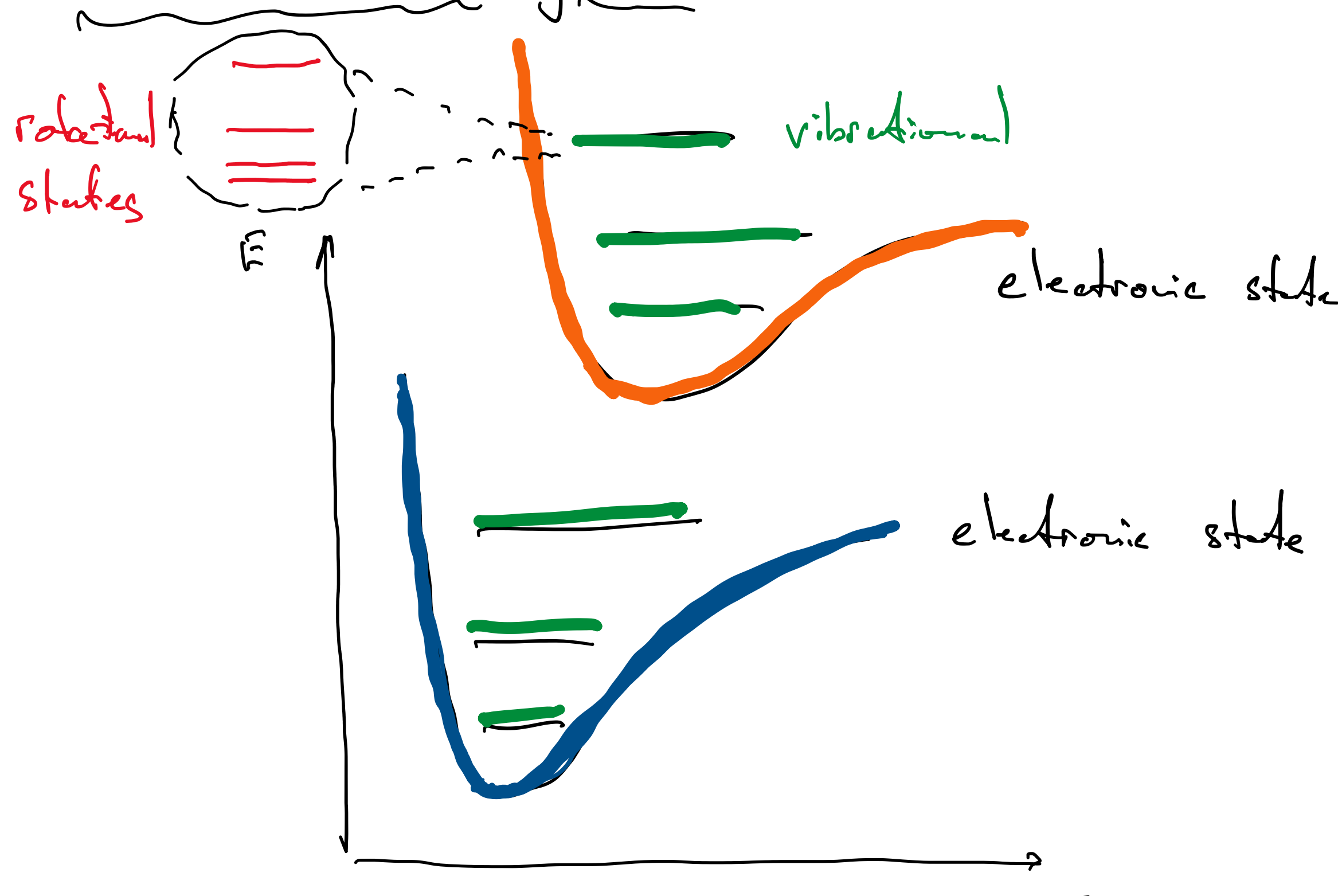
$$\text{vibration} \rightarrow 10^2 - 10^3 \text{ cm}^{-1} \text{ (IR)}$$

$$\text{electronic} \rightarrow 10^3 - 10^5 \text{ cm}^{-1} \text{ (UV-VIS)}$$

Final picture



Jablonski diagram



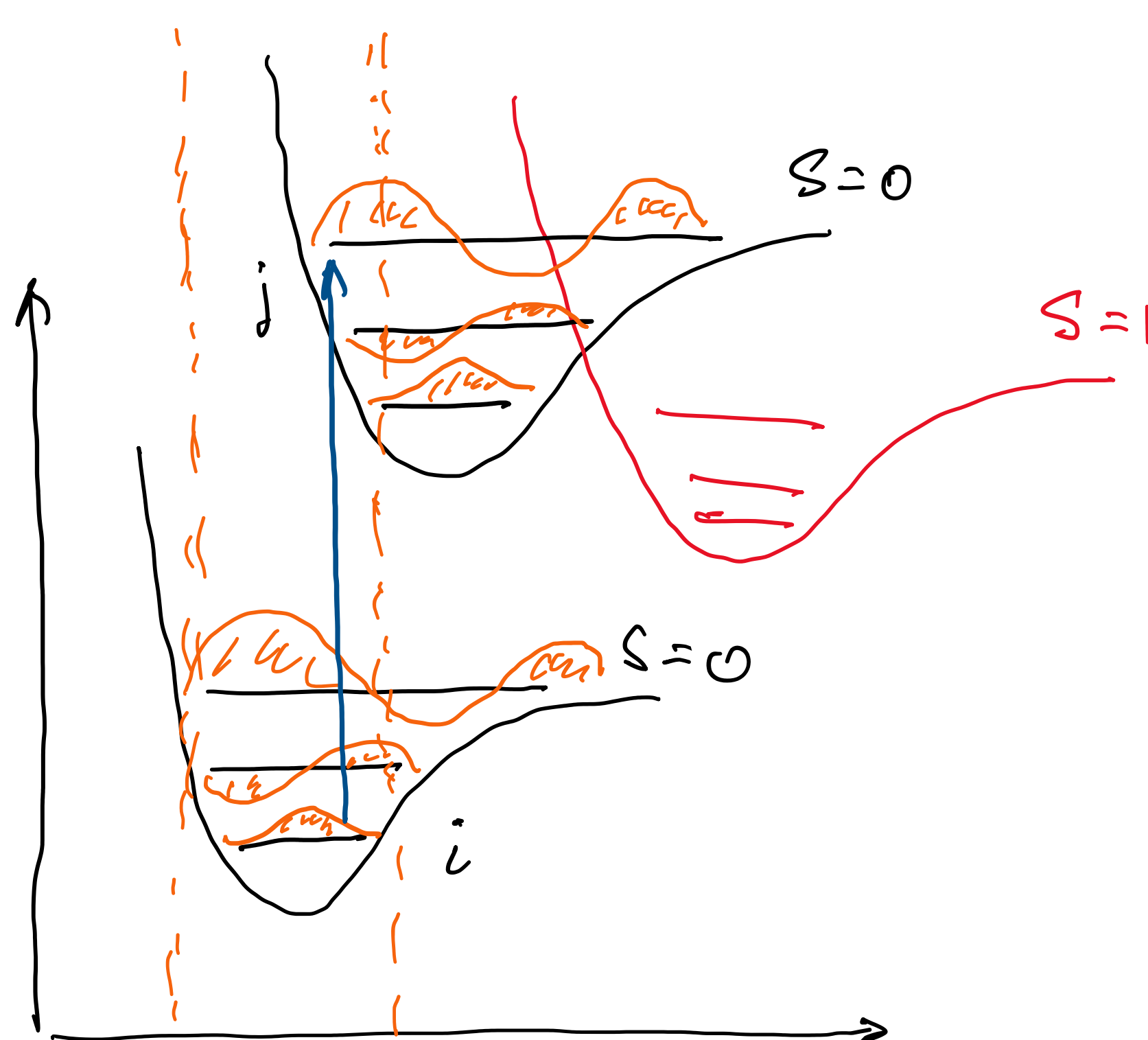
Which transitions will be allowed?

Rotation and vibration selection rules:

$$\Delta n = \pm 1 \quad \Delta l = \pm 1 \quad \Delta m = 0$$

Electronic states:

$$\Delta S = 0 - \text{spin}$$



Besides selection rules

$$\begin{cases} \Delta n = \pm 1 \\ \Delta l = \pm 1 \\ \Delta m = 0 \\ \Delta S = 0 \end{cases}$$

we need to see where wavefunctions overlap:

$$\int \psi_i^* \psi_j \neq 0$$

Franck-Condon principle:

1) Overlap between two wavefunctions must exist in $\vec{r}$

2) Only vertical transitions are allowed

This has two reasons:

a) transition bond length to remain constant

or

b) time of transitions infinitely shorter than vibration.