

What is the mapping?

One electron state: spin- $1/2$ system

Map each degree of freedom to
a semiclassical model of a spin system

$$\mathbf{S}_x/\hbar = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mapsto \sqrt{\sigma^2 - \left(n - \frac{1}{2}\right)^2} \cos(q)$$

$$\mathbf{S}_y/\hbar = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \mapsto \sqrt{\sigma^2 - \left(n - \frac{1}{2}\right)^2} \sin(q)$$

$$\mathbf{S}_z/\hbar = \frac{1}{2} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \mapsto n - \frac{1}{2}$$

Molecular Electronic Devices

