Particle in a box

$$x \in [0, L]$$

$$\hat{H}\varphi_n(x) = E_n\varphi_n(x) \qquad \hat{H} = \frac{1}{2m}\hat{p}^2 = -\frac{\hbar}{2m}\frac{d^2}{dx^2}$$

then,

$$\varphi_n(x) = ce^{ikx} \qquad E_n = \frac{\hbar^2 k^2}{2m}$$

$$\varphi_n(x) = \varphi_n(x+L) \rightarrow \text{Periodic boundary condition}$$

Also

$$\exp(ikL) = 1 \rightarrow kL = 2\pi n$$

$$k = \frac{2\pi n}{L} \quad ; \; n = 0, \pm 1, \pm 2, \ldots$$

$$\frac{2\pi}{L} \rightarrow 0 \quad \text{if} \quad L \rightarrow \infty$$

$$\sum_k f(k) \rightarrow \int \frac{dk}{\frac{2\pi}{L}} f(k) = \frac{L}{2\pi}\int dk\, f(k)$$

In 3D

$$\varphi(\vec{r}) = c\exp(i\vec{k}\cdot\vec{r})$$

$$\vec{k} = \frac{2\pi}{L_1} m_1 \hat{e}_x + \frac{2\pi}{L_2} m_2 \hat{e}_y + \frac{2\pi}{L_3} m_3 \hat{e}_z$$

$$E_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m} \quad \text{and} \quad \sum_k f(\vec{k}) \rightarrow \frac{V}{(2\pi)^3}\int d^3\vec{k}\, f(\vec{k})$$

$$E_j := E_{\vec{k},\sigma} = \frac{\hbar^2 k^2}{2m} \qquad j := (\vec{k}, \sigma)$$

$$E_j := E_{\vec{k},\sigma} = \frac{\hbar^2 k^2}{2m} - \mu_B H_\sigma \qquad \sigma = \pm 1$$

Bohr magneton

$$\hat{H}_{mol} = \hat{H}_{tr} + \hat{H}_{el} + \hat{H}_{rot} + \hat{H}_{vib} + \ldots$$

molecules

$$E_j = E_{\vec{k},J,n} = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^3}{2I}J(J+1) + \hbar\omega\left(n + \frac{1}{2}\right)$$