

Hamiltonian describing an electron interacting with a nucleus in the presence of a magnetic field  $\mathbf{B}_0$

$$\begin{aligned}
 \mathcal{H} = & -\frac{\hbar^2}{2m} \nabla^2 && \text{electron kinetic energy} \\
 + & V_0 && \text{electron potential energy in the field of the nucleus and of other electrons} \\
 + & V_{cryst} && \text{electron potential energy due to charges outside the atom} \\
 + & \frac{e\hbar}{2m^2c^2} \mathbf{S} \cdot \left[ \mathbf{E} \times \left( \mathbf{p} + \frac{e}{c} \mathbf{A}_0 \right) \right] && \text{electron spin-orbit coupling} \\
 + & \gamma_e \hbar \mathbf{B}_0 \cdot \mathbf{S} && \text{electron spin Zeeman energy} \\
 + & \frac{e}{2mc} (\mathbf{p} \cdot \mathbf{A}_0 + \mathbf{A}_0 \cdot \mathbf{p}) + \frac{e^2}{2mc^2} \mathbf{A}_0^2 && \text{coupling of electron orbital motion to } \mathbf{B}_0 \\
 + & \frac{e}{2mc} (\boldsymbol{\pi} \cdot \mathbf{A}_n + \mathbf{A}_n \cdot \boldsymbol{\pi}) && \text{coupling of nuclear momentum to electron orbital motion} \\
 + & \frac{\gamma_e \gamma_n \hbar^2}{r^3} \left[ \frac{3(\mathbf{I} \cdot \mathbf{r})(\mathbf{S} \cdot \mathbf{r})}{r^2} - \mathbf{I} \cdot \mathbf{S} \right] && \text{coupling of nuclear moment with electron spin moment for non s-states} \\
 + & \frac{8\pi}{3} \gamma_e \gamma_n \hbar^2 \mathbf{I} \cdot \mathbf{S} \delta(\mathbf{r}) && \text{coupling of nuclear moment with electron spin moment for s-states} \\
 + & \mathcal{H}_Q && \text{coupling of nuclear quadrupole moment to field gradient due to electron and external charges} \\
 + & -\gamma_n \hbar \mathbf{B}_0 \cdot \mathbf{I} && \text{nuclear Zeeman energy}
 \end{aligned}$$