

Born-Oppenheimer approximation

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huge scale difference of scales of electronic vs. nuclear degrees of freedom

B.O 1927: keep the nuclei fixed

ansatz for wf: product of electronic & nuclear wf.

$$\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, \vec{R}) = \underbrace{\phi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)}_{\text{all electrons}} \cdot \underbrace{\psi(\vec{R})}_{\text{all nuclei}}$$

$$= \phi(\vec{r}) \cdot \psi(\vec{R})$$

e.g. for diatomic molecule $\vec{R} \Rightarrow R_{AB} \leftarrow$ parameter

S.E $\hat{H} \Psi = W \Psi$ is solved for many R

→ typical molecular potential



