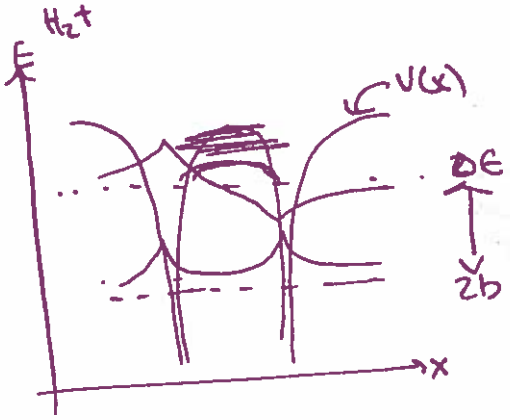
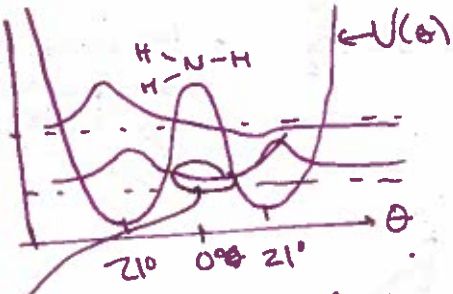
Tunneling in Chemistry



ex: Ammonia = NH_3



Not very different from the classical potential well

tunneling

Ammonia = a Schrödingers cat molecule

In the lowest E state, the Hs in ammonia simultaneously point up and down

Bonding occurs b/c the e⁻ has a high probability in the classically forbidden region

e⁻ between nuclei

where $K = E - V < 0 \Rightarrow p$ is imaginary

so $\frac{p^2}{2m} < 0$!

However $\langle \psi | \hat{K} | \psi \rangle$

$= \int dx \, \psi^*(x) \left(\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \right) \psi(x)$

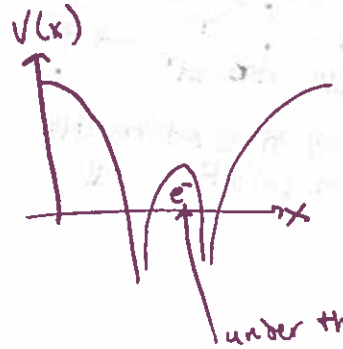
> 0 always

Fourier principles:

$\Delta x \cdot \Delta p = \frac{\hbar}{2}$

$\Delta \omega \cdot \Delta t = \frac{1}{2}$

$\Delta E \cdot \Delta t = \frac{\hbar}{2}$ → for a very short instant energy conservation can be violated when the e^- is under the barrier



under the barrier, called an "instanton"

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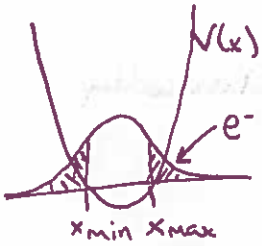
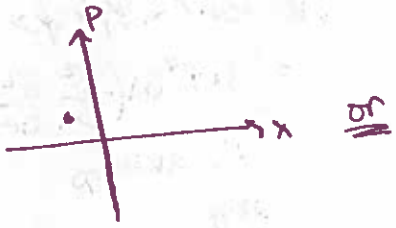
spring



$\rightarrow 0$ as $x \rightarrow \pm\infty$

$E = \frac{\hbar\omega}{2} = \frac{\hbar}{2}\sqrt{\frac{k}{m}}$

Hwk: $P_{\text{forbidden}} = 2 \cdot \int_{x_{max}}^{\infty} dx\, \psi_0^*(x)\, \psi_0(x)$



or