The Variational Method:

Often, perturbation theory is useless (e.g. problem not close to one we can solve exactly)

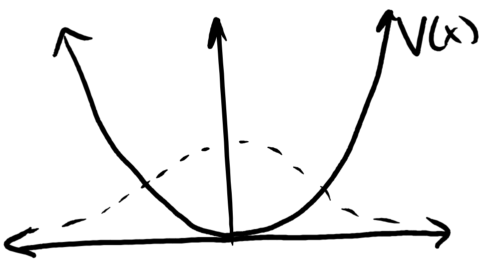
If we want to estimate the ground state energy E_0:

can use that E_0 = minimum of $\langle\psi|H|\psi\rangle$ over all $|\psi\rangle$

This is the avg. value of E we will measure. The average is always greater than the minimum possible value E_0

Strategy: ① pick a state $|\psi\rangle$
② calculate $\langle\psi|H|\psi\rangle$: this gives upper bound on E_0
③ repeat

e.g. Harmonic oscillator



Guess $\psi(x) = \dfrac{A}{x^2+b^2}$ we will vary this.

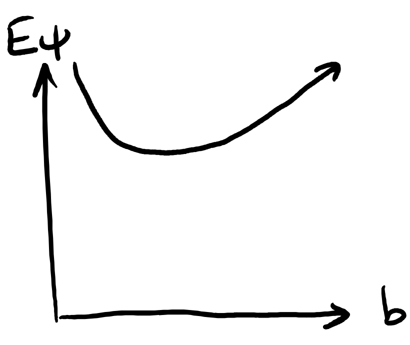
Normalization:

$$\int |\psi(x)|^2 dx = 1 \Rightarrow A = \sqrt{\frac{2b^3}{\pi}}$$

Calculate:

$$E_\psi = \langle\psi|H|\psi\rangle = \frac{2b^3}{\pi}\int dx \frac{1}{x^2+b^2}\left(-\frac{\hbar^2}{2m}\frac{d}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\frac{1}{x^2+b^2}$$

$$= \frac{1}{4}\frac{\hbar^2}{b^2m} + \frac{1}{2}m\omega^2b^2$$



Minimize over b $\longrightarrow E_\psi^{min} = \frac{\sqrt{2}}{2}\hbar\omega \approx 0.707\hbar\omega$

exact result: $0.5\hbar\omega$

In practice:

1. Choose trial state with some arbitrary parameters
$$|\psi(a_i)\rangle$$
2. Normalize: $\langle\psi(a_i)|\psi(a_i)\rangle = 1$
3. Evaluate $E_\psi(a_i) = \langle\psi(a_i)|\, H\, |\psi(a_i)\rangle$
4. Minimize over $a_i \longrightarrow E^{\psi}_{min}$

E_ψ^{min} is an upper bound on E_0

$\longrightarrow$ More accurate results for better guess

$\longrightarrow$ Hard to tell how close we are

$\longrightarrow$ Only tells us about ground state energy (but a related approach works more generally).

Next time: apply to 2 electrons in a Helium atom

apply to 1 electron H_2^+ molecule.