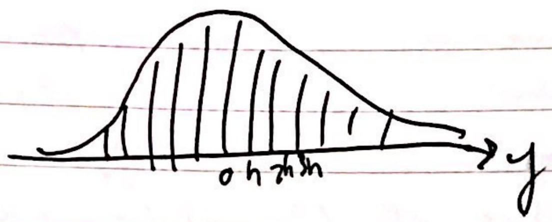
10/11 From last time: Finite differences co method

$$\epsilon\psi(y) = -\frac{d^2}{dy^2}\psi(y) + v(y) = \psi(y)$$



$$\epsilon\psi(y_n) = -\left(\frac{\partial^2\psi}{\partial y^2}\right)_n + V(y_n)\psi(y_n)$$

$y_n = nh = n\Delta y$

$\psi(y_n) \to \psi_n$

$$\epsilon\psi_n = -\left(\frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h^2}\right) + V_n\psi_n + O(h^2)$$

$$\epsilon\left(\frac{\psi_{n+1} + 10\psi_n + \psi_{n-1}}{12}\right) = -\left(\frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h^2}\right) + \frac{V_{n+1}\psi_{n+1} + 10V_n\psi_n + V_{n-1}\psi_{n-1}}{12} + O(h^4)$$

$$O(h^2) = -\frac{1}{12}\left(\frac{d^4\psi}{dy^4}\right)_n$$

$$\frac{d^4\psi}{dy^4} \approx \frac{1}{h^2}\left(\left(\frac{d^2\psi}{dy^2}\right)_{n+1} - 2\left(\frac{d^2\psi}{dy^2}\right)_n + \left(\frac{d^2\psi}{dy^2}\right)_{n-1}\right)$$

$$\frac{d^2\psi}{dy^2} = (v(y) - \epsilon)\psi$$

~~Shooting method~~

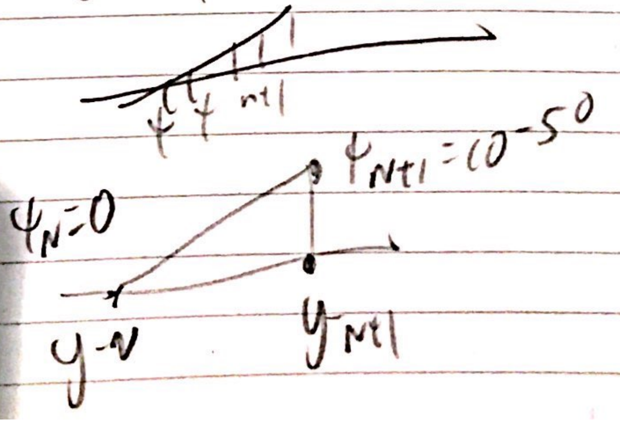
Code

boundary conditions

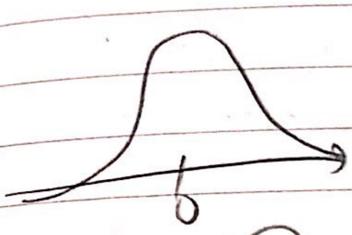
Somewhere is range of 15 or so.

use large #s

double precision

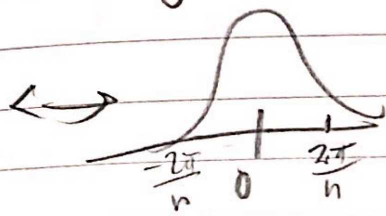


Error estimates



$F(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$

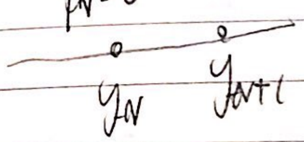
$F(0) = \int_{-\infty}^{\infty} f(x) k$

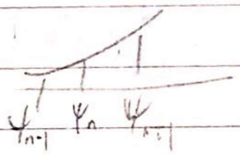


$h \sum f(nh) = \int_{-\infty}^{\infty} f(x)dx + F\left(\frac{2\pi}{h}\right) + F\left(-\frac{2\pi}{h}\right) \ldots$

$A_n \psi_{n+1} + B_n \psi_n + C_n \psi_{n-1} = 0$

$\psi_N = 0 \quad \psi_{N+1} = 10^{-50}$

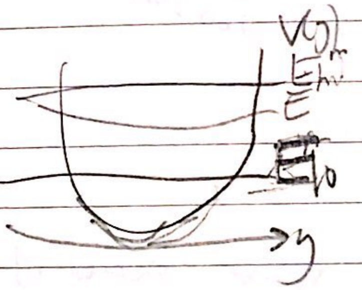


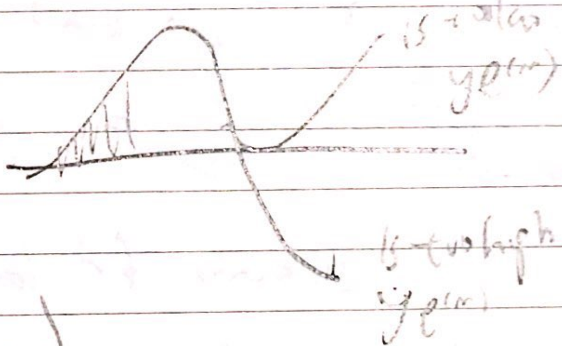


$\psi_{n+1} = -\frac{1}{A_n}(B_n \psi_n + C\psi_{n-1})$

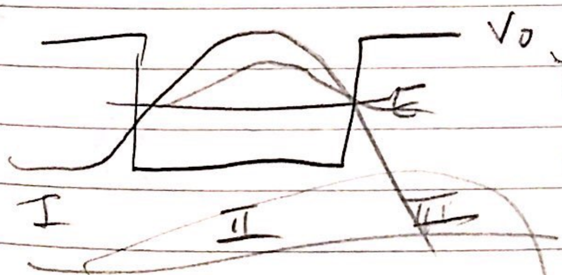
dont want integrate down?

$E\psi(y) = -\frac{d^2}{dy^2}\psi(y) + v(y)\psi(y)$





$E^{m+1} = \frac{1}{2}(E_{high} + E_{low})$



$\psi_I = a e^{qx}$

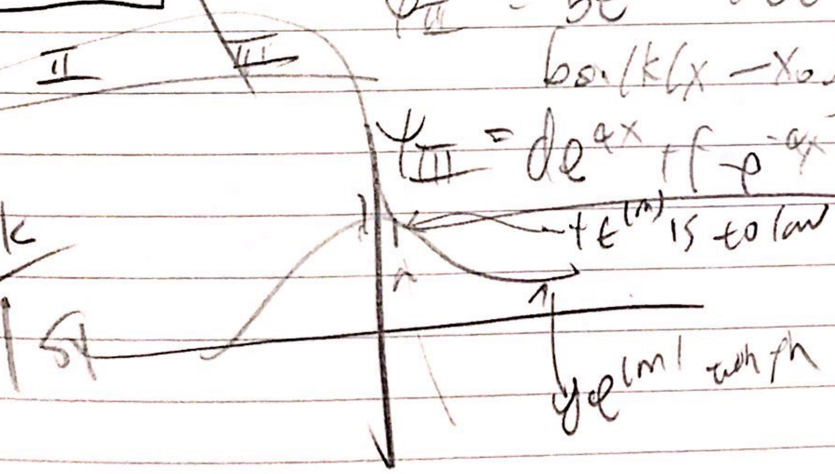
$\psi_{II} = b e^{ikx} + c e^{-ikx}$ or

$b \sin(k(x - x_0))$

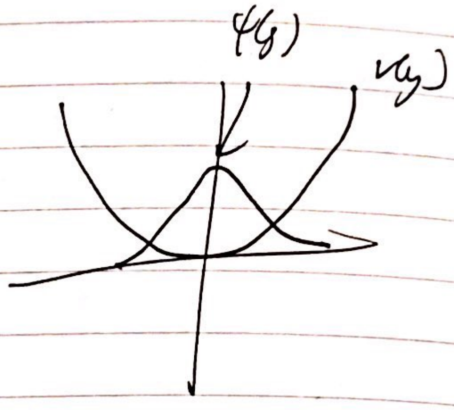
$\psi_{III} = d e^{qx} + f e^{-qx}$

Trick

Symm



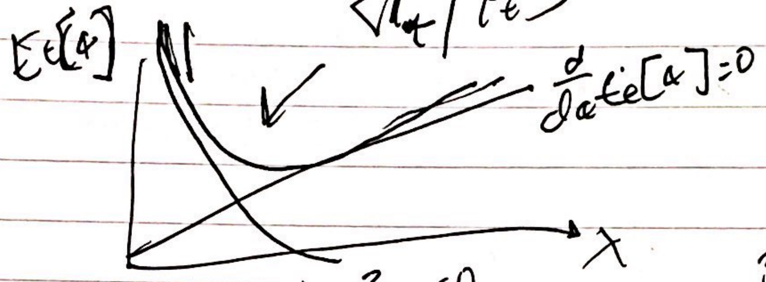
Variational Method



$$\epsilon \psi(y) = -\frac{d^2}{dy^2}\psi(y) + y^4 \psi(y)$$

guess : $\psi_\alpha(y) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha y^2}$

$$\epsilon_t[\alpha] = \frac{\langle \psi_t | -\frac{d^2}{dy^2} + v(y) | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle} = \alpha + \frac{3}{16\alpha^2}$$



$$\frac{d}{d\alpha}\epsilon_t[\alpha] = 1 - \frac{3}{8\alpha^3} = 0$$

$$\epsilon_t^*[\alpha_{opt}] = \left(\frac{3}{4}\right)^{4/3} = 1.081687\ldots$$

$$\alpha_{opt} = \left(\frac{3}{8}\right)^{1/3} \qquad \epsilon_{exact} = 1.060362\ldots$$

Tryna get an estimate for lowest ground state of ground state energy

Can only overestimate ground state energies

Heisenberg estimate

$$E\psi = -\frac{d^2}{dy^2}\psi + y^4\psi \qquad E = \langle \hat{k}^2\rangle + \langle y^4\rangle$$

$\hat{k}^2$

$$\Delta k \Delta y \sim \frac{1}{2}$$

$$\langle \hat{k}^2 \rangle = \langle \hat{k} \rangle^{2\,\nearrow 0} + (\Delta k)^2 \qquad \langle y^4 \rangle \to \Delta y^4$$

kinda of
developed
estimate
itself

$\delta k \Delta y \sim \frac{1}{2}$

$$E[\Delta y] = \frac{1}{4\Delta y^2} + \Delta y^4 \to \frac{3}{4}$$

$$\frac{\partial}{\partial \Delta y} E = \frac{-1}{2\Delta y^3} + 4\Delta y^3 = 0 \qquad \Delta y = \frac{1}{\sqrt{2}}$$

a benchmark

Why does it work

Start with $E\psi = \hat{H}\psi \qquad E_j\phi_j = \hat{H}\phi_j$

$$\phi_t = \sum_j a_j \phi_j$$

$$E_t = \frac{\langle \psi_t | \hat{H} | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle}$$

$$\langle \psi_t | \psi_t \rangle = \left\langle \sum_j a_j \phi_j \middle| \sum_j a_j \phi_j \right\rangle$$

$$= \sum_j |a_j|^2$$

$$\langle \psi_t | \hat{H} \psi_t \rangle = \left\langle \sum_j a_j \phi_j \middle| \hat{H} \middle| \sum_j a_j \phi_j \right\rangle$$

$$= \left\langle \sum_j a_j \phi_j \middle| \sum_{j'} a_{j'} E_{j'} \phi_{j'} \right\rangle$$

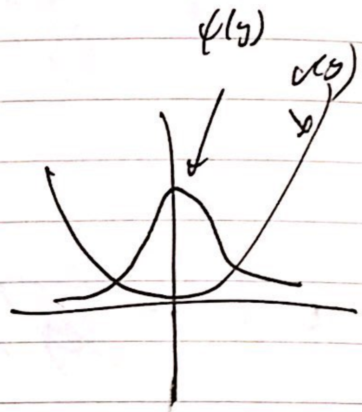
$$E_t = \sum_j |a_j|^2 E_j$$

$$E_t = \frac{\sum_j |a_j|^2 E_j}{\sum_j |a_j|^2}$$

$\psi_t = \phi_0 + \beta\phi_1$ $\qquad E_t = \dfrac{E_0 + \beta^2 E_1}{1+\beta^2} \approx E_0 + \beta^2(E_1 - E_0) + \dots$

garbage in $\Longrightarrow$ $\boxed{\text{Variational method}}$ $\Longrightarrow$ gold out

1 more example



$\psi_t = e^{-\sqrt{\alpha y^4 + \beta y^6}}$

$$E_t[\alpha,\beta] = \frac{\langle \psi_t | -\frac{d^2}{dy^2} + y^4 | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle}$$

$E_t = 1.0603638$

$E_{exact} = 1.0603$ etc.