HW2.

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Schrödinger eq.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

finite difference

$$-\frac{\hbar^2}{2m}\frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & & 0 \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ 0 & & -1 & \ddots \end{pmatrix}\begin{pmatrix} \psi_1^{(n)} \\ \vdots \\ \psi_{N-1}^{(n)} \end{pmatrix} = E_n \begin{pmatrix} \psi_1^{(n)} \\ \vdots \\ \psi_{N-1}^{(n)} \end{pmatrix}$$

$\equiv H$

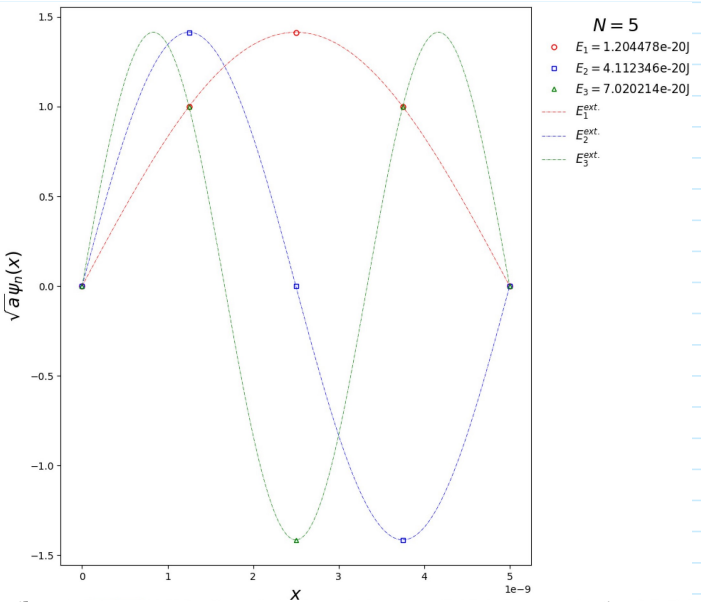
* Numerical solution : H 를 diagonalize ⇒ eigenvalue : E_n, eigenvector : Normalized $\begin{pmatrix} \psi_1^{(n)} \\ \vdots \\ \psi_{N-1}^{(n)} \end{pmatrix}$

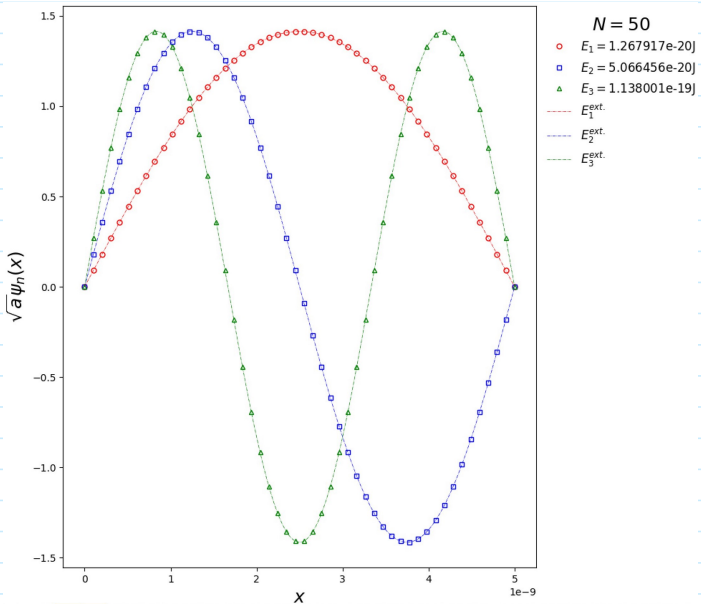
* Exact solution : $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$

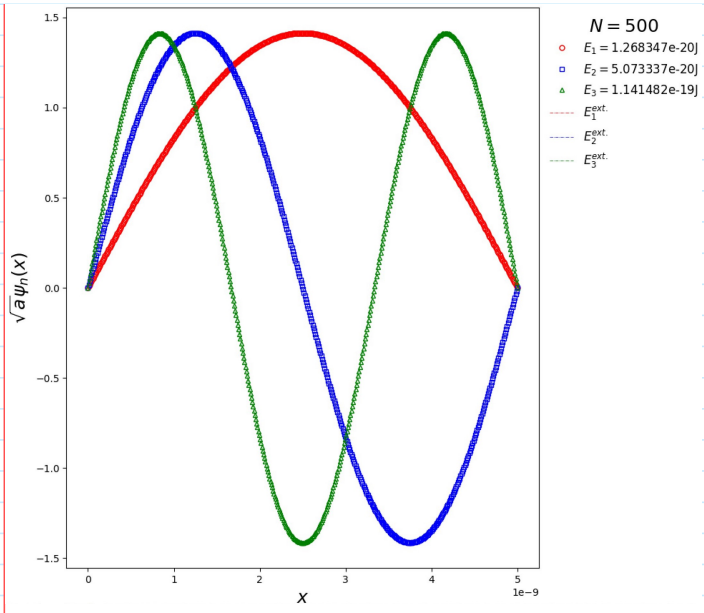
$\therefore N \to \infty$, $\sqrt{N-1}\,\psi_i^{(n)} = \psi_n(x_i)$ 가 된다. ($\sqrt{N-1}\,\psi_i^{(n)}$ 로 rescaling 필요)

Results

$a = 5\,nm$, $m = 0.19\,m_e$







E_1이 Ground state energy

E_2이 1st excited state energy

⋮

*N이 커질수록 E_n이 정확한 값으로 수렴.