HW2.

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V=∞ ; V=∞ (potential well diagram with walls at $x=0$ and $x=a$)

Schrödinger eq.

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

(finite difference

$$-\frac{\hbar^2}{2m}\frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & & 0 \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ 0 & & & \ddots \end{pmatrix}\begin{pmatrix} \psi_2^{(n)} \\ \vdots \\ \psi_{N-1}^{(n)} \end{pmatrix} = E_n \begin{pmatrix} \psi_2^{(n)} \\ \vdots \\ \psi_{N-1}^{(n)} \end{pmatrix}$$
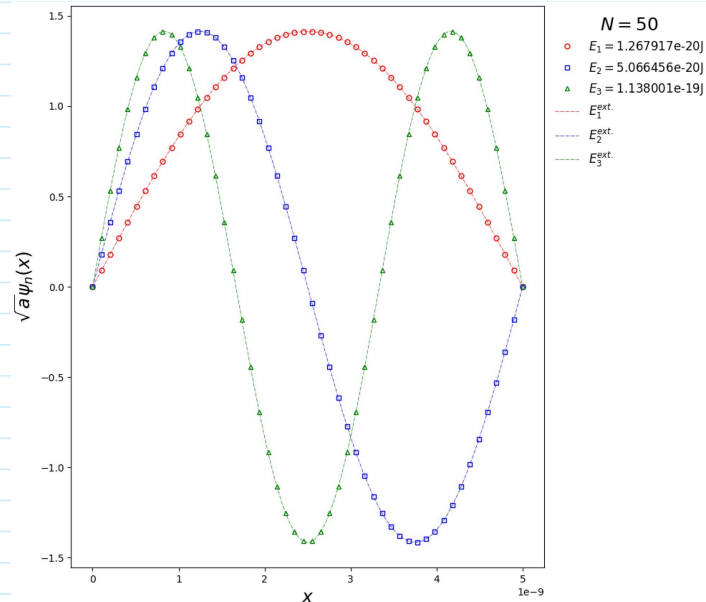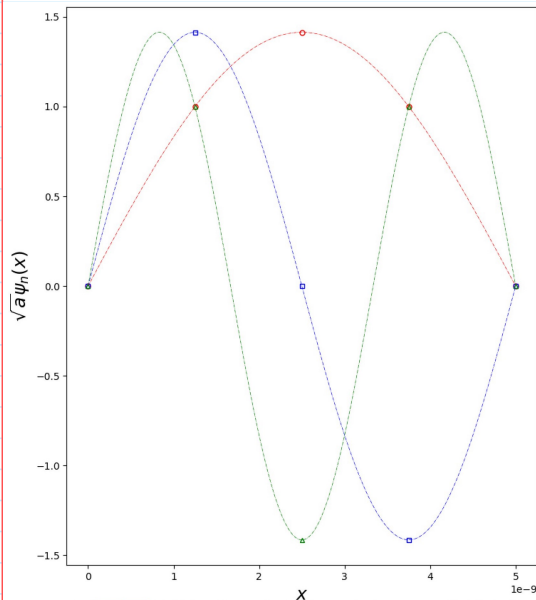
$\equiv H$

* Numerical solution : H를 diagonalize ⇒ eigen value : E_n

eigen vector : Normalized $\begin{pmatrix} \psi_2^{(n)} \\ \vdots \\ \psi_{N-1}^{(n)} \end{pmatrix}$

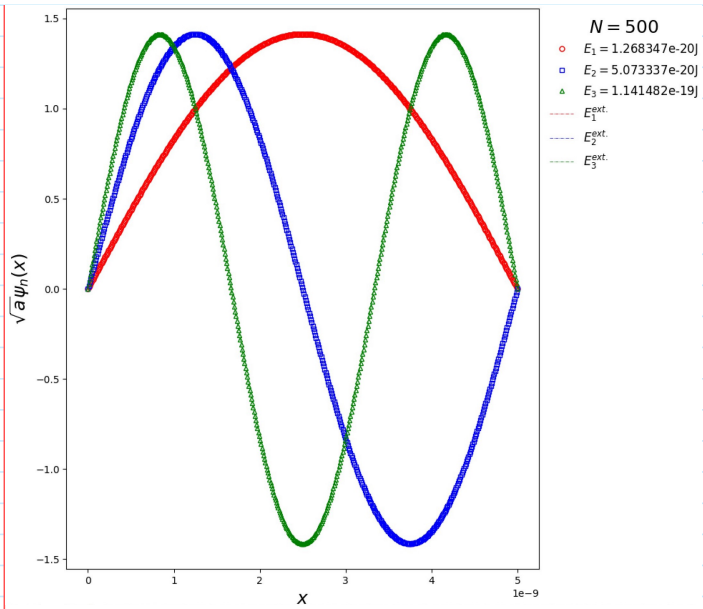* Exact solution : $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$

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

Results

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

$N=5$
$E_1 = 1.204478e{-}20J$
$E_2 = 4.112346e{-}20J$
$E_3 = 7.020214e{-}20J$
$E_1^{ext.}$
$E_2^{ext.}$
$E_3^{ext.}$

$N=50$
$E_1 = 1.267917e{-}20J$
$E_2 = 5.066456e{-}20J$
$E_3 = 1.138001e{-}19J$
$E_1^{ext.}$
$E_2^{ext.}$
$E_3^{ext.}$

$N = 500$
- ○ $E_1 = 1.268347\text{e-}20J$
- □ $E_2 = 5.073337\text{e-}20J$
- △ $E_3 = 1.141482\text{e-}19J$
- ----- $E_1^{ext.}$
- ----- $E_2^{ext.}$
- ----- $E_3^{ext.}$

E_1 이 Ground state energy

E_2 이 1st excited state energy

⋮

＊ N 이 커질 수록 E_n 이 정확한 값으로 수렴.