HW2.

2020년 9월 7일 월요일 오후 4:11

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Schrödinger eq.

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

(finite difference

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

$\equiv H$

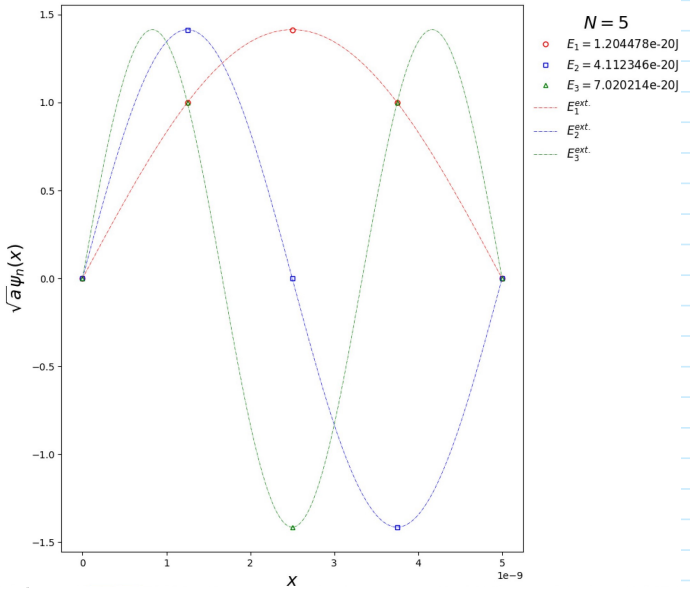
* Numerical solution : H 를 diagonalize $\Rightarrow$ eigenvalue : E_n
eigenvector : Normalized $\begin{pmatrix} \psi_2^{(n)} \\ \vdots \\ \psi_{N-1}^{(n)} \end{pmatrix}$

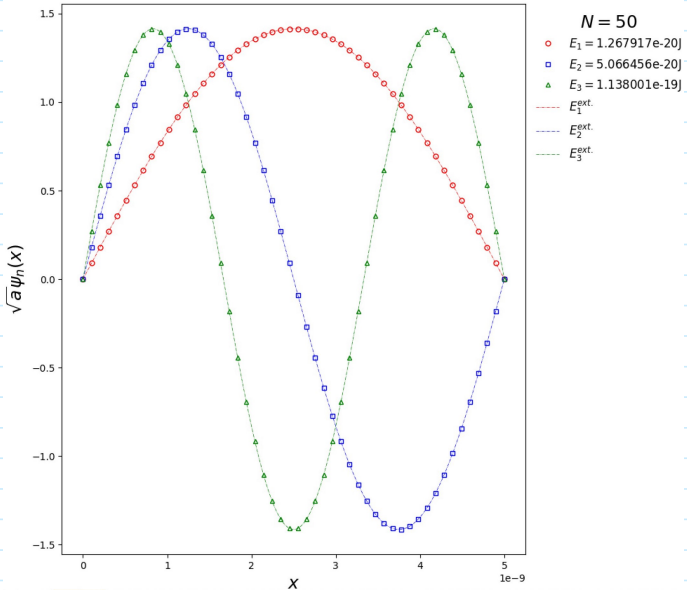
* Exact solution : $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$

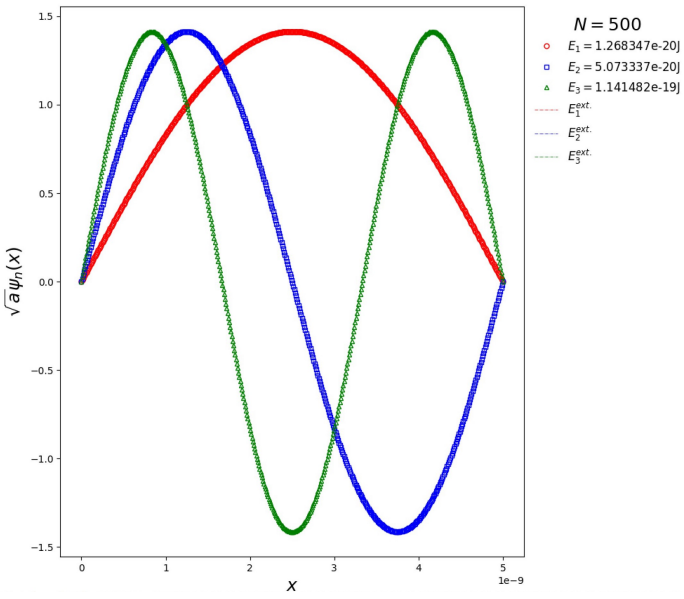
$\therefore N \to \infty$, $\sqrt{N-1}\,\psi_i^{(n)} = \sqrt{a}\,\psi_n(x_i)$ 가 된다. ($\sqrt{N-1}\,\psi_i^{(n)}$ 로 rescaling 필요)

Results

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







E_1 이 Ground state energy
E_2 이 1st excited state energy
⋮

* N이 커질수록 E_n이 정확한 값으로 수렴.

$N=5$

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Numertical 1th E : 1.204478e-20
Exact 1th E : 1.268351e-20

Numertical 2th E : 4.112346e-20
Exact 2th E : 5.073404e-20

Numertical 3th E : 7.020214e-20
Exact 3th E : 1.141516e-19
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$N=50$

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Numertical 1th E : 1.267917e-20
Exact 1th E : 1.268351e-20

Numertical 2th E : 5.066456e-20
Exact 2th E : 5.073404e-20

Numertical 3th E : 1.138001e-19
Exact 3th E : 1.141516e-19
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$N=500$

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Numertical 1th E : 1.268347e-20
Exact 1th E : 1.268351e-20

Numertical 2th E : 5.073337e-20
Exact 2th E : 5.073404e-20

Numertical 3th E : 1.141482e-19
Exact 3th E : 1.141516e-19
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