Computational Microelectronics HW.2

EECS, 20204003

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1. Comparing normalized wavefunction with different N

*n=1일 때 wavefunction의 부호가 일반적으로 알려진 식과 반대로 나오지만, 실제로 부호는 영향이 없으므로, 이를 exact solution과 비교를 위해 그래프를 그릴 때 (-1)를 취해주었습니다.

1) N=5

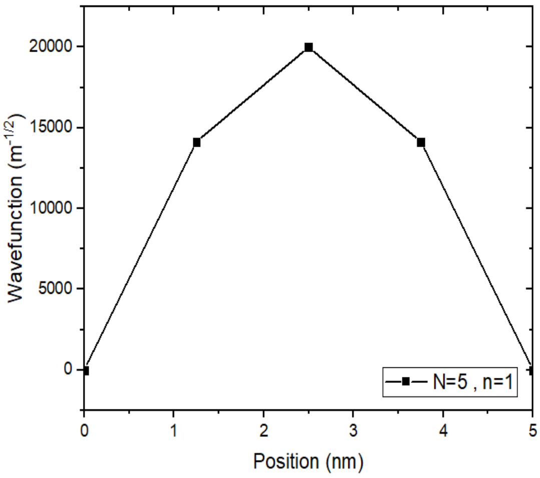

Fig 1. Position vs. Wavefunction when N=5 for the ground state.

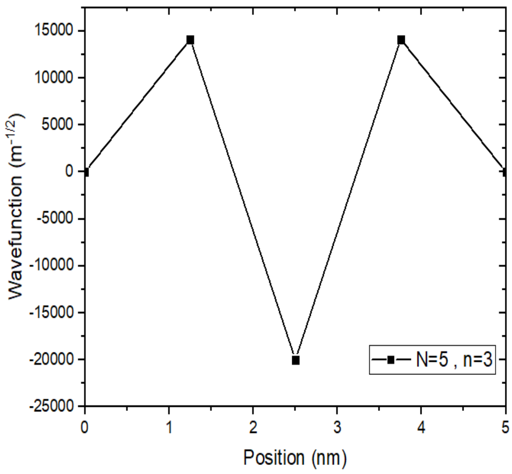

Fig 2. Position vs. Wavefunction when N=5 for the third state.

2) N=50

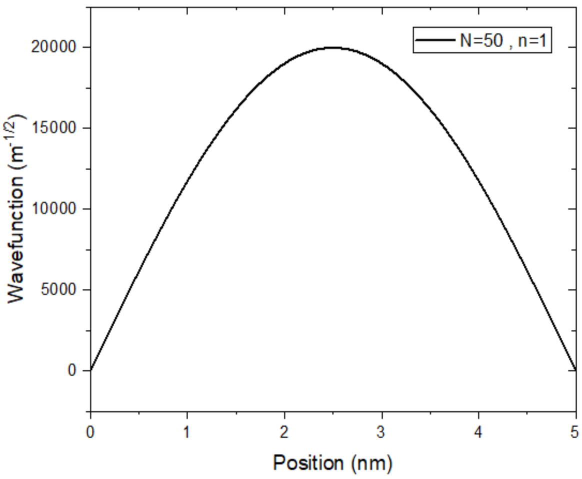

Fig 3. Position vs. Wavefunction when N=50 for the ground state.

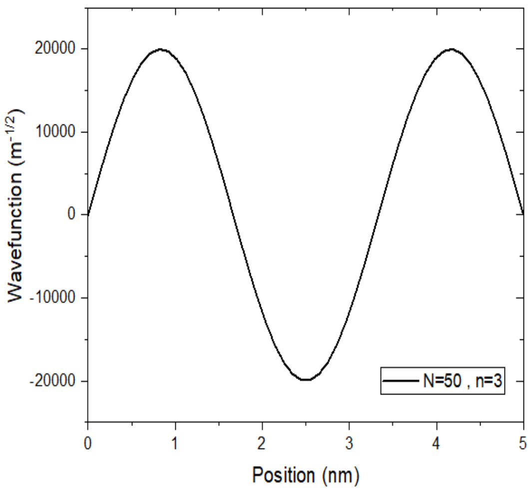

Fig 4. Position vs. Wavefunction when N=50 for the third state.

3) N=500 and exact solutions are compared.

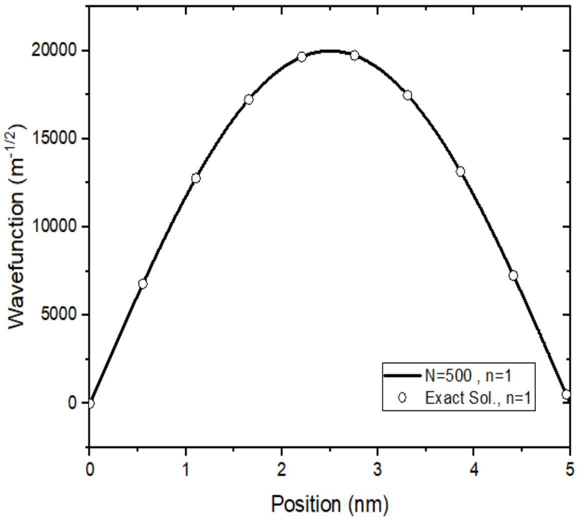

Fig 5. Position vs. Wavefunction when N=500 for the ground state and compared with exact solution.

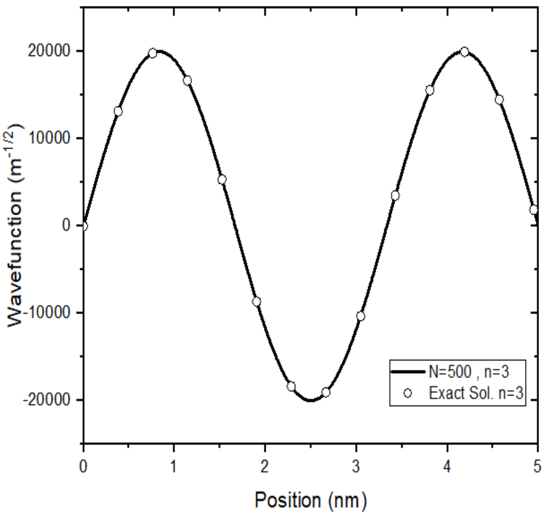

Fig 6. Position vs. Wavefunction when N=500 for the third state and compared with exact solution.

As it can be seen, the more we discretize, the smoother graphs become. Also, the numerical solutions seem to be quite consistent with the exact solutions when discretization level rises as represented in Fig. 5 and 6. To get the exact solution, an equation right below was used.

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) \quad for\ 0 \leq x \leq L = 5nm$$

2. Comparing energies with different N and exact solutions

1) Ground state energy error for each N=5, 50 ,500

	N=5	N=50	N=500	Exact sol.
Ground state Energy(eV)	0.07519	0.07915	0.07917	0.07917
Error rate(%)	5.03588	0.03425	3.30307E-4	

Error rate calculation(%) : $\frac{|Exact\ sol. - Numerical\ sol.|}{Exact\ sol.} \times 100(\%)$

2) Energy vs. Error rate for N=50 and 500.

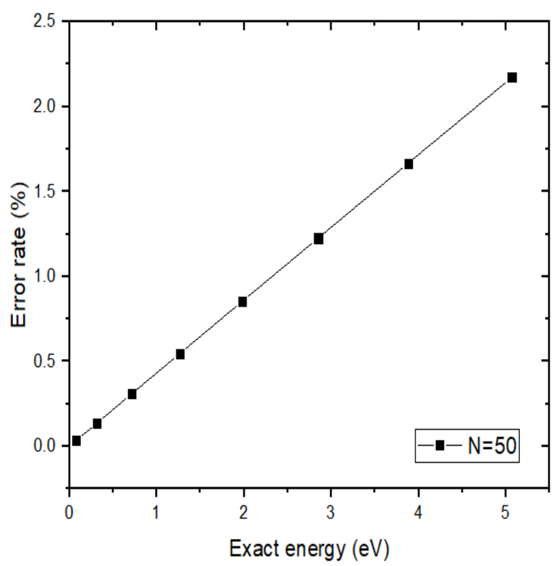

Fig 7. Exact solution vs. error rate when N=50 .

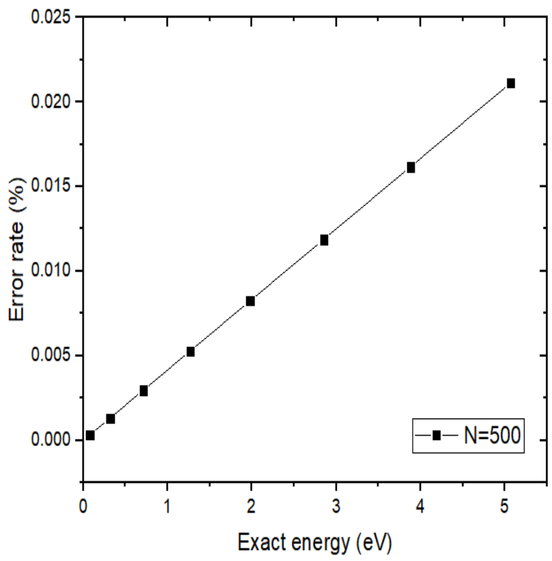

Fig 8. Exact solution vs. error rate when N=500.

As the case of wave function, energy also become closer to exact solution as discretization level rises. Error range is about 0~2% when N=50 at energy range 0~5eV. When N=500, it is much smaller about hundred times (0~0.02%). However, the time which takes to simulate will highly increase when the system becomes more complicated. As a result, we should choose a reasonable level when trade off happens significantly. For exact solution, below equation was used.

$$E_n = \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{L}\right)^2 \quad n = 1,2,3 \ldots.$$