Homework #2
Computational Microelectronics

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1 Results

We have calculated the ground state energy of the one-dimensional infinite potential well (IPW) problem with the mass $m = 0.19m_e$ by discretizing the well of $a = 5$ nm by $N - 1$ bins (N uniformly distributed points). Note that the exact ground state energy is given by

$$E_g = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 \simeq 79.1704 \text{ meV}. \tag{1}$$

The numerical results are provided in Table 1. One can also check the results by running the Python code provided. We see that the numerical value converges to the exact value as N increases. Even for $N = 5$ which is small, the error is about 5 %.

When the eigenvalue provide the energy, the eigenvector should provide the wave function. As we know the exact form $\psi_g = A \sin \frac{\pi x}{a}$, we compare the eigenvectors to ψ_g in Fig. 1. We find that the eigenvectors form the similar form to ψ_g, though we do not normalize them.

Table 1: Numerically obtained ground state energy for given N. The error is provided. For the graphical comparison, we rescale the function by arbitrary factor.

N	E_g (meV)	Error (%)
5	75.1835	5.04%
50	79.1434	0.034%
500	79.1702	3.3e-4

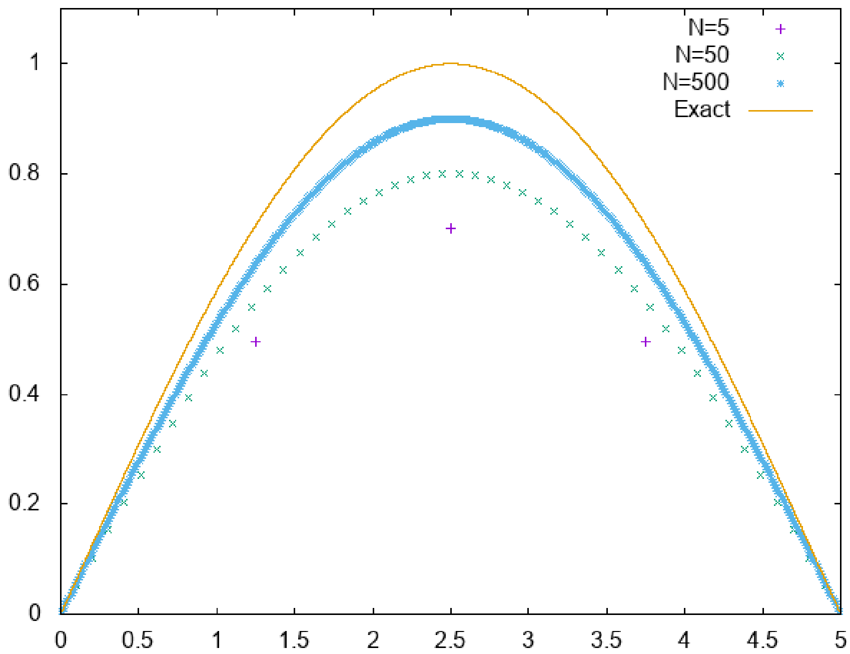

Figure 1: Unnormalized ground state wave function for given discretization parameter N. The exact form $f(x) = \sin \frac{pix}{a}$ is provided.