Computational Microelectronics Report (Homework #2)

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Code

1-1. Captured code

HW2.m

```
function [E] = HW2(N) % Point values (5, 50, 500)

x = 5*10^-9/(N-1); % Length of the box (unit: m)
m0 = (0.511*10^6)/(3*10^8)^2; % Electron rest mass
h = 6.582*10^-16; % h-bar (unit: eV*s)

% Matrix form with the boundary conditions %
A = zeros(N-2,N-2);
for i = 2:N-3
    A(i,i-1) = 1;
    A(i,i) = -2;
    A(i,i+1) = 1;
end
A(1,1) = -2; A(1,2) = 1;
A(N-2,N-3)=1; A(N-2,N-2)= -2;
[V,D] = eig(A);

a = D(1,1);
for k=1:N-2
    if abs(a) > abs(D(k,k))
        a=abs(D(k,k));
    end
end

ksquare = a/x^2;
E = h^2*ksquare/(2*m0*0.19); % Ground state energy (unit: eV)
```

1-2. Explanation

In order to solve the infinite potential well problem, the SchÖdinger equation is absolutely essential. In the case of I dimensional problem, it is easy to calculate it by the eigenvalue/eigenfunction of the Laplacian operator. Based on this, computational methods allow us to get the analytic solution by discretization, that means the second derivative can be approximated in this case.

Furthermore, the higher the data are, the more exact the ground state energy values are. By drawing the error of them as a function of N, it can be evaluated how much drastic influence the number of data points has.

1. Results

2-1. Results of N (5, 50, and 500)

N = 5

```
>> HW2(5)

ans =

    0.0753
```

0.0753 eV

N = 50

```
>> HW2(50)

ans =

    0.0792
```

0.0792 eV

N = 500

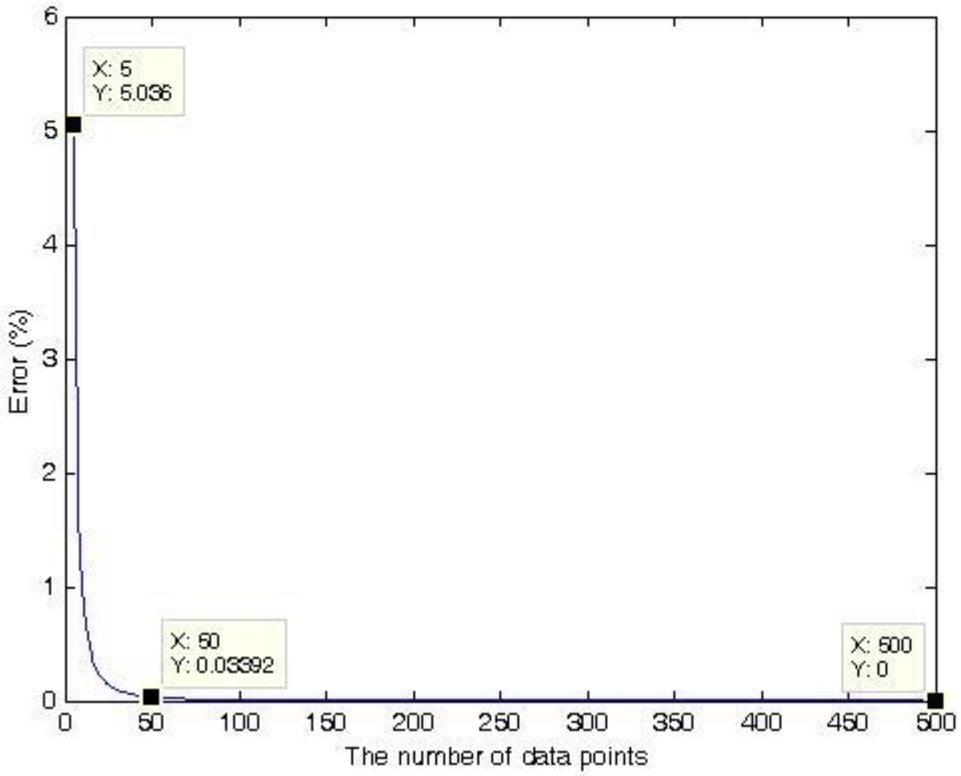
```
>> HW2(500)

ans =

    0.0793
```

0.0793 eV

2-2. Error of the ground state energy (<u>assumed as real value when N is 1000</u>)



N = 5	N = 50	N = 500
5.036%	0.03392%	0%

As the number of data points were larger, difference from real value dwindled to nothing. In five to twenty, the error fell markedly. After that, it was approaching zero (N = 0). In brief, it is very significant to evaluate the ground state energy.