EE683 Project Report

Semiconductors Nanostructures with Crystal Vibrations

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- Abstract -

Semiconductor crystals are known to have atoms arranged in a periodic fashion. These atoms are continuously vibrating about their mean position. These vibrations are caused when atoms absorb thermal energy ($\sim$ 26meV at room temperature) from the surrounding environment. To model these atoms and the vibrating behavior, we consider the crystal lattice points where atoms are present as points of infinite potential. The vibrations are then considered as time dependent perturbations of these 'infinite potential walls.' We use this simple model to study the effect of these vibrations on the probability density distribution of the electrons confined in these potential wells.

1 Introduction

The problem of moving walls of an infinite potential well has been looked into by several papers [1] [2]. However, the approach to the problem in these paper differ significantly depending on the kind of perturbation in consideration. For example, the problem where the one of the wall is moving with constant velocity i.e. $\frac{dL(t)}{dt} =$ constant, the solution can be found exactly using perturbation techniques [3]. In the case of semiconductor crystals, the vibrations can be approximated as time dependent sinusoidal oscillations about the mean position. The frequency of these oscillations is chosen to match the energy of the oscillations.

In this project, we solve the Schrodinger Equation for the infinite potential well with time varying length. We arrive at a set of infinite coupled differential equations for which we truncate our basis for simplification. The solutions for the coupled differential equation are obtained using Matlab. The relevant plots and codes are appended with this report.

2 Solving the Schrodinger Equation

We know that for an infinite potential well of length L(t), the normalised eigenfunctions take the form

$$\mathbf{u_n}(\mathbf{x},\mathbf{t}) = \sqrt{\frac{2}{L(t)}}\sin\left(\frac{n\pi x}{L(t)}\right), n = 1, 2, 3....$$

With energy

$$\mathbf{E_n}(\mathbf{t}) = \frac{\hbar^2 n^2 \pi^2}{2mL(t)^2}, n = 1, 2, 3....$$

Using these eigenfunctions, any wavefunction Ψ can be written by superimposing these eigenfunctions. A general wavefunction, expanded in the above mentioned basis can be written as

$$\mathbf{\Psi}(\mathbf{x},\mathbf{t}) = \sum_n b_n(t)u_n(x,t)\exp\left\{\frac{-i}{\hbar}\Big(\int_0^t E_n(\tau)d\tau\Big)\right\}$$

Substituting the wave function into the time dependent Schrodinger equation

$$i\hbar\Big(\frac{d\Psi}{dt}\Big) = \mathbf{H}\Psi$$

Where $\mathbf{H}$ is the Hamiltonian for the infinite potential well. Substituting the wavefunction $\mathbf{\Psi}(\mathbf{x},\mathbf{t})$ into the equation, we get

$$\sum_k \dot{b}_k(t)u_k(x,t)\exp\left\{\frac{-i}{\hbar}\Big(\int_0^t E_k(\tau)d\tau\Big)\right\} = -\sum_k b_n(t)\dot{u}_n(x,t)\exp\left\{\frac{-i}{\hbar}\Big(\int_0^t E_n(\tau)d\tau\Big)\right\}$$

As the eigenfunctions $u_k(x,t)$ are normalised, to get the rate equation for the coefficient $b_k(t)$, taking inner product with $u_k^*(x,t)$ to eliminate the summation on LHS.

$$\dot{b}_k(t) = -\sum_n b_n(t)\left(\int_0^{L(t)} u_k^* \frac{du_n}{dt} dx\right) \exp\left\{\frac{i}{\hbar}\Big(\int_0^t (E_k - E_n)d\tau\Big)\right\}$$

The integral on RHS can be solved separately to give:

$$\int_0^{L(t)} u_k^* \frac{du_n}{dt} dx = (-1)^{k+n} \frac{2kn}{k^2-n^2} \frac{1}{L(t)} \frac{dL(t)}{dt} (1-\delta_{n,k})$$

Substituting this back,

$$\dot{b}_k(t) = \sum_n (-1)^{k+n} \frac{2kn}{k^2-n^2} \frac{1}{L(t)} \frac{dL(t)}{dt} \exp\left\{\frac{i\hbar\pi^2(k^2-n^2)}{2m} \int_0^t \frac{d\tau}{L^2(\tau)}\right\} (1-\delta_{n,k}) b_n(t)$$

Now we move on to consider the variation of the length of the infinite potential well. Considering time varying sinusoidal oscillations, the length of the well can be written as:

$$L(t) = L_o(1 + \lambda \sin(\omega t))$$

Where we know that $\lambda \ll 1$. To find the appropriate range of values of λ, we consider the energy associated with the vibrations. The unperturbed energy is in the order of 1000 meV whereas the vibrations are about 1 - 10 meV in energy. Mathematically,

$$\mathbf{E_n(t)} = \frac{\hbar^2 n^2 \pi^2}{2mL(t)^2} = \frac{\hbar^2 n^2 \pi^2}{2mL_o^2(1+\lambda\sin(\omega t))^2} \approx \frac{\hbar^2 n^2 \pi^2}{2mL_o^2}\Big(1 - 2\lambda\sin(\omega t)\Big)$$

The first term represents the unperturbed energy whereas the second term represents the vibration in the energy of the unperturbed energy states. Therefore, λ equals to the ratio of the vibrational energy and the unperturbed energy. So, $\lambda \sim 10^{-3}$.

With this in place, we move on to use the expression of $L(t)$ to evaluate the other unknown quantities present in the coupled differential equation.

$$\frac{1}{L(t)}\frac{dL(t)}{dt} = \frac{L_o \lambda\omega\cos(\omega t)}{L_o(1+\lambda\sin(\omega t))} \approx \lambda\omega\cos(\omega t)(1-\lambda\sin(\omega t)) \approx \lambda\omega\cos(\omega t)$$

$$\int_0^t \frac{d\tau}{L^2(\tau)} = \int_0^t \frac{d\tau}{L_o^2(1+\lambda\sin(\omega t))^2} \approx \frac{1}{L_o^2}\int_0^t \Big(1 - 2\lambda\sin(\omega\tau)\Big)d\tau \approx \frac{1}{L_o^2}\left(t - \frac{2\lambda}{\omega}(1-\cos(\omega t))\right)$$

The final simplified coupled differential equations are:

$$\dot{b}_k(t) = \sum_n (-1)^{k+n} \frac{2kn\lambda\omega\cos(\omega t)}{k^2-n^2} \exp\left\{\frac{i\hbar\pi^2(k^2-n^2)}{2mL_o^2}\Big(t - \frac{2\lambda}{\omega}(1-\cos(\omega t))\Big)\right\}(1-\delta_{n,k})b_n(t)$$

3 Code and Plots

We first restrict the basis to only two eigenfunctions. This is later justified by the plots obtained. Reducing the basis limits down the equation to a pair of coupled differential equation thus rendering it exactly solvable. The equations become:

$$= \begin{cases} \dot{b}_1(t) = & \frac{4\lambda\omega\cos(\omega t)}{3} \exp\left\{\frac{-3i\mathbf{E}}{\hbar}\Big(t - \frac{2\lambda}{\omega}(1-\cos(\omega t))\Big)\right\} b_2(t) \\ \dot{b}_2(t) = & -\frac{4\lambda\omega\cos(\omega t)}{3} \exp\left\{\frac{3i\mathbf{E}}{\hbar}\Big(t - \frac{2\lambda}{\omega}(1-\cos(\omega t))\Big)\right\} b_1(t) \end{cases}$$

Where, $\mathbf{E} = \dfrac{\hbar^2\pi^2}{2mL_0^2}$ is the energy of ground state of the infinite potential of length L_0. These equations can be simplified by substituting:

$$\begin{cases} b_1(t) = & \tilde{b}_1(t) \exp\left\{\frac{-3i\mathbf{E}}{2\hbar}\Big(t - \frac{2\lambda}{\omega}(1-\cos(\omega t))\Big)\right\} \\ b_2(t) = & \tilde{b}_2(t) \exp\left\{\frac{3i\mathbf{E}}{2\hbar}\Big(t - \frac{2\lambda}{\omega}(1-\cos(\omega t))\Big)\right\} \end{cases}$$

giving,

$$\begin{cases} \dot{\tilde{b}}_1(t) = & \frac{3i\mathbf{E}}{\hbar}\Big(1-2\lambda\sin(\omega t)\Big)\tilde{b}_1(t) + \frac{4\lambda\omega\tilde{b}_2(t)}{3}\cos(\omega t) \\ \dot{\tilde{b}}_2(t) = & -\frac{3i\mathbf{E}}{\hbar}\Big(1-2\lambda\sin(\omega t)\Big)\tilde{b}_2(t) - \frac{4\lambda\omega\tilde{b}_1(t)}{3}\cos(\omega t) \end{cases}$$

The advantage of this substitution is that the probability of finding the electron in the ground or excited same can be calculated by taking modulus square of the coefficients.
The code for solving the above equation is written in Matlab for both the original and the simplified differential equation.

```
%% Constants and System Parameters
hbar = 1.0545718*10^-34;
energy = 1000*1.6*10^-22;
lambda = 0;
omega = energy*lambda/hbar;

%% Solving the coupled differential equation
tbegin = 0;
tend = 100*6.62607004*10^(-34)/(lambda*energy) % 100 cycles of oscillations;
steps = 100;
initial = [1; 0];

tspan = linspace(tbegin, tend, steps);
[t, B] = ode45(@solver, tspan, initial);

%% Plotting the result
B = B';
ground = B(1, :);
first = B(2, :);


prob_ground = conj(ground).*ground;
prob_first = conj(first).*first

figure();
subplot(2,1,1);
plot(t,prob_ground);
xlabel('time (s)');
ylabel('Ground State Population');
subplot(2,1,2);
plot(t,prob_first);
xlabel('time (s)');
ylabel('First Excited State Population');

%% Defining the equation
function B_dot = solver(t, B)

hbar = 1.0545718*10^-34;
energy = 1000*1.6*10^-22;
lambda = 0;
omega = energy*lambda/hbar;

B_dot = zeros(2, 1);

% Comment out any one of the two pair of coupled differential equation to
% obtain the solution

% Differential equation after substitution and simplification
B_dot(1) = 3i*energy*(1-2*lambda*sin(omega*t))*B(1)/(hbar - 4*lambda*omega*B(2)*
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```
cos(omega*t)/(3*(1 + lambda*sin(omega*t)));

B_dot(2) = -3i*energy*(1-2*lambda*sin(omega*t))*B(2)/(hbar) + 4*lambda*omega*B(1)*
cos(omega*t)/(3*(1 + lambda*sin(omega*t)));

% Original differential equation
B_dot(1) = 4*lambda*omega*B(2)*cos(omega*t)*exp(-3i*energy*(t -
2*lambda*(1-cos(omega*t))/omega)/hbar)/(3*(1 + lambda*sin(omega*t)));

B_dot(2) = -4*lambda*omega*B(1)*cos(omega*t)*exp(3i*energy*(t -
2*lambda*(1-cos(omega*t))/omega)/hbar)/(3*(1 + lambda*sin(omega*t)));
end
```

The plots obtained by solving the original differential equation obtained by solving the Schrodinger equation are:

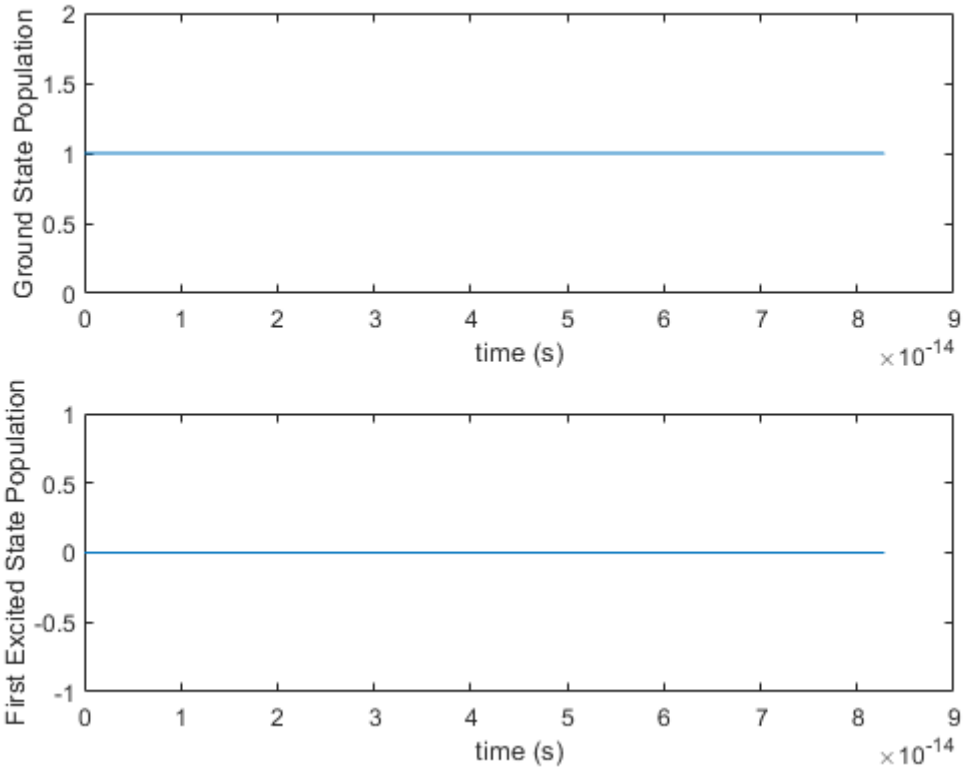

Figure 1: $\lambda = 0$

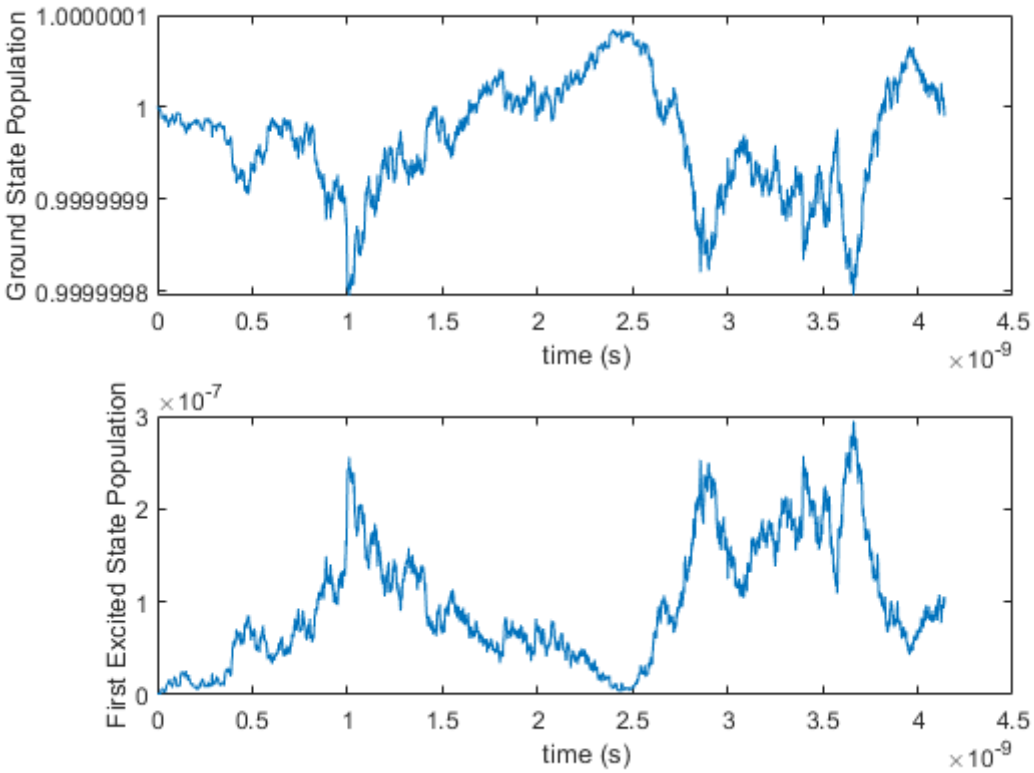

Figure 2: $\lambda = 10^{-4}$

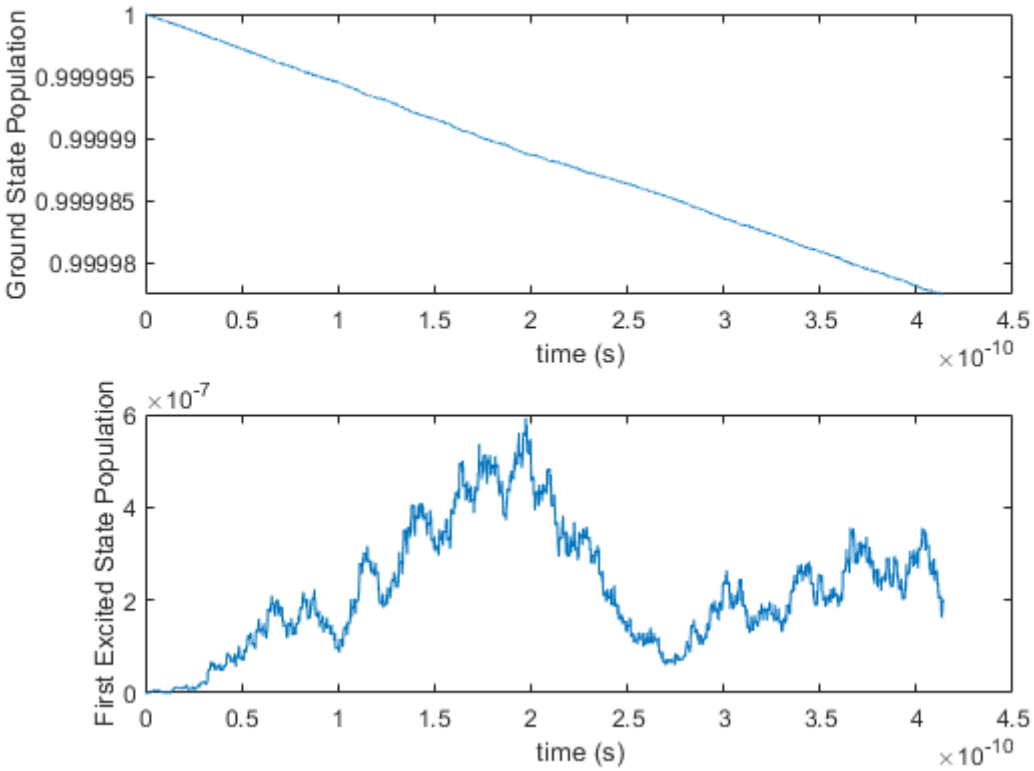

Figure 3: $\lambda = 10^{-3}$

References

[1] M. Glasser, J. Mateo, J. Negro, and L. Nieto, "Quantum infinite square well with an oscillating wall," *Chaos, Solitons Fractals*, vol. 41, no. 4, pp. 2067 – 2074, 2009.

[2] A. Munier, J. R. Burgan, M. Feix, and E. Fijalkow, "Schrödinger equation with time-dependent boundary conditions," *Journal of Mathematical Physics*, vol. 22, no. 6, pp. 1219–1223, 1981.

[3] S. W. Doescher and M. H. Rice, "Infinite square-well potential with a moving wall," *American Journal of Physics*, vol. 37, no. 12, pp. 1246–1249, 1969.