Chapt8Exercise1b.m

Quantum Well Wavefunction Probability

Fourier Transform Approach to Finite Barrier Tunneling

Semiconductor Physics Documentation

Abstract

This document provides a comprehensive analysis of `Chapt8Exercise1b.m`, which calculates the probability amplitude squared for a quantum well wavefunction as a function of a dimensionless parameter γ. The code uses sinc-function representations arising from Fourier transforms of finite-width barrier wavefunctions.

Contents

1 Theoretical Foundation

1.1 Quantum Confinement Axioms

Axiom 1 (Schrödinger Equation). *The time-independent behavior of a non-relativistic particle is governed by:*

$$\hat{H}\psi = E\psi \quad \text{where} \quad \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \tag{1}$$

Axiom 2 (Born Interpretation). *The probability density of finding a particle at position* $\mathbf{r}$ *is:*

$$P(\mathbf{r}) = |\psi(\mathbf{r})|^2 \tag{2}$$

Axiom 3 (Continuity Conditions). *At a potential discontinuity, the wavefunction* ψ *and its derivative* ψ' *(weighted by* $1/m^*$ *in heterostructures) must be continuous.*

1.2 Finite Quantum Well

Definition 1 (Finite Square Well Potential). *A one-dimensional finite quantum well is defined by:*

$$V(z) = \begin{cases} 0 & |z| \leq L/2 \\ V_0 & |z| > L/2 \end{cases} \tag{3}$$

where L *is the well width and* V_0 *is the barrier height.*

Theorem 1 (Bound State Solutions). *For* $0 < E < V_0$*, the bound state wavefunctions have the form:*

$$\psi(z) = \begin{cases} A\cos(kz) \text{ or } A\sin(kz) & |z| \leq L/2 \\ Be^{-\kappa|z|} & |z| > L/2 \end{cases} \tag{4}$$

where:

$$k = \sqrt{\frac{2mE}{\hbar^2}} \tag{5}$$

$$\kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \tag{6}$$

1.3 Fourier Transform Representation

Definition 2 (Sinc Function). *The cardinal sine function is defined as:*

$$sinc(x) = \frac{\sin(x)}{x} \tag{7}$$

with $sinc(0) = 1$ *by L'Hôpital's rule.*

Theorem 2 (Fourier Transform of Rectangular Function). *The Fourier transform of a rectangular pulse of width* $2a$ *centered at the origin is:*

$$\mathcal{F}\{rect(x/2a)\} = 2a \cdot sinc(ka) \tag{8}$$

1.4 Probability Amplitude in Momentum Space

For a quantum well of width related to the quantum number n, the probability amplitude in the basis of plane waves involves:

$$|A(\gamma)|^2 \propto \left| \frac{\sin(\pi(n/\gamma - 1))}{\pi(n/\gamma - 1)} - \frac{\sin(\pi(n/\gamma + 1))}{\pi(n/\gamma + 1)} \right|^2 \tag{9}$$

where γ is a dimensionless parameter representing the ratio of some characteristic scale to the well width.

2 Mathematical Derivation

2.1 The Amplitude Expression

The code computes:

$$a = \frac{1}{\sqrt{\gamma}} \left[\frac{\sin(\pi(n/\gamma - 1))}{\pi(n/\gamma - 1)} - \frac{\sin(\pi(n/\gamma + 1))}{\pi(n/\gamma + 1)} \right] \tag{10}$$

Let us define:

$$y_1 = \left(\frac{n}{\gamma} - 1 \right) \pi \tag{11}$$

$$y_2 = \left(\frac{n}{\gamma} + 1 \right) \pi \tag{12}$$

Then:

$$a = \frac{1}{\sqrt{\gamma}} \left[\frac{\sin(y_1)}{y_1} - \frac{\sin(y_2)}{y_2} \right] \tag{13}$$

2.2 Physical Interpretation

The expression represents the overlap integral between:

- A bound state wavefunction of quantum number n
- A plane wave basis state characterized by γ

The probability $|a|^2$ gives the momentum distribution of the confined particle.

2.3 Special Cases

Lemma 1 (Resonance Condition)**.** *When $\gamma = n$:*

$$y_1 = 0 \implies sinc(y_1) = 1 \tag{14}$$

$$y_2 = 2\pi \implies sinc(y_2) = 0 \tag{15}$$

Maximum probability occurs near these resonance points.

3 Line-by-Line Code Analysis

3.1 Initialization

```
clear
clf;
```

Clear workspace and figure.

```
err=0.00001;
```

$$\epsilon = 10^{-5} \tag{16}$$

Small offset to avoid division by zero when $y_1 = 0$ or $y_2 = 0$.

3.2 Main Computation Loop

```
for n=1:5
```

Loop over quantum numbers $n = 1, 2, 3, 4, 5$ *(first five bound states).*

```
    for x=0:1000
        gamma=1.0+x*0.004+err;
```

$$\gamma = 1 + 0.004x + \epsilon \quad \text{for } x = 0, 1, \ldots, 1000 \tag{17}$$

Discretize γ *from 1 to 5 with step size 0.004.*

```
        y1=((n/gamma)-1.0)*pi;
```

$$y_1 = \left(\frac{n}{\gamma} - 1\right)\pi \tag{18}$$

First sinc argument.

```
        y2=((n/gamma)+1.0)*pi;
```

$$y_2 = \left(\frac{n}{\gamma} + 1\right)\pi \tag{19}$$

Second sinc argument.

```
        a=sqrt(1/gamma)*((sin(y1)/y1)-(sin(y2)/y2));
```

$$a = \frac{1}{\sqrt{\gamma}}\left[\operatorname{sinc}(y_1) - \operatorname{sinc}(y_2)\right] \tag{20}$$

Compute the probability amplitude using the difference of two sinc functions.

```
        a2(x+1)=a*a;
```

$$|a|^2 = a^2 \tag{21}$$

Store the probability (amplitude squared) in array.

```
    end
```

End of inner loop over γ *values.*

3.3 Plotting

```
    plot(1:0.004:5,a2), axis([1,5,0,1]), hold on
```

$$\text{Plot } |a|^2 \text{ vs } \gamma \in [1, 5] \tag{22}$$

Plot probability vs γ *with y-axis limited to* $[0, 1]$.

```
    xlabel('\gamma'),ylabel('Probability');
    title(['Chapt8Exercise1b']);
end
hold off;
```

Add labels and title; overlay all five curves.

4 Numerical Method: Direct Evaluation

4.1 Grid-Based Computation

This code uses direct numerical evaluation on a discrete grid:

1. **Grid Generation**: Create γ values from 1 to 5 with step 0.004

$$\gamma_k = 1 + 0.004k + \epsilon, \quad k = 0, 1, \ldots, 1000 \tag{23}$$

2. **Function Evaluation**: For each γ_k and quantum number n:

$$|a(\gamma_k, n)|^2 = \frac{1}{\gamma_k}\left[\text{sinc}\left(\frac{n\pi}{\gamma_k} - \pi\right) - \text{sinc}\left(\frac{n\pi}{\gamma_k} + \pi\right)\right]^2 \tag{24}$$

3. **Singularity Avoidance**: The small offset $\epsilon = 10^{-5}$ prevents evaluation exactly at points where denominators vanish.

4.2 Alternative: Using MATLAB's sinc Function

The code could be rewritten using MATLAB's built-in sinc function:

$$\text{sinc}_{\text{MATLAB}}(x) = \frac{\sin(\pi x)}{\pi x} \tag{25}$$

Note: MATLAB's definition differs by a factor of π:

$$\text{sinc}_{\text{code}}(y) = \frac{\sin(y)}{y} = \text{sinc}_{\text{MATLAB}}(y/\pi) \tag{26}$$

5 Physical Interpretation

5.1 Peak Locations

The probability $|a|^2$ peaks when the resonance condition $\gamma \approx n$ is satisfied:

- For $n = 1$: Peak near $\gamma = 1$
- For $n = 2$: Peak near $\gamma = 2$
- For $n = 3$: Peak near $\gamma = 3$
- And so on...

5.2 Physical Meaning of γ

The parameter γ represents a ratio of length scales or momentum scales:

$$\gamma = \frac{k_{\text{external}}}{k_{\text{well}}} \tag{27}$$

When $\gamma = n$, the external wavefunction matches the n-th bound state, maximizing the overlap.

5.3 Decay of Probability

Away from resonance ($\gamma \neq n$), the probability decays as:

$$|a|^2 \sim \frac{1}{\gamma(\gamma - n)^2} \quad \text{for } |\gamma - n| \gg 1 \tag{28}$$

This is the characteristic decay of sinc^2 functions.

6 Results Analysis

6.1 Expected Plot Features

1. Five curves, one for each quantum number $n = 1$ to 5
2. Each curve peaks near $\gamma = n$
3. Peak heights decrease with increasing n (due to $1/\sqrt{\gamma}$ factor)
4. Side lobes appear between peaks

6.2 Normalization

The $1/\sqrt{\gamma}$ factor ensures proper normalization:

$$\int_0^\infty |a(\gamma)|^2 \, d\gamma = 1 \tag{29}$$

7 Summary

This code calculates and plots the probability distribution in a dimensionless parameter space, showing how quantum well bound states project onto a continuous spectrum. The sinc function structure arises naturally from the Fourier transform of the localized wavefunction, and the resonance condition $\gamma = n$ identifies the dominant contribution of each bound state.