Arrowhead Matrix and Berry Phase Calculations: Technical Documentation

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Abstract

This document provides a comprehensive technical overview of the Arrowhead matrix generation, Berry phase calculations, and visualization tools implemented in the project. We focus particularly on the `run_optimal_visualization.py` script, which generates comprehensive visualizations of Berry phases, eigenstate behavior, and parity flips using optimal parameters. We also discuss the physical significance of half-integer winding numbers and topological phase transitions observed in the system.

Contents

1 Introduction

The Arrowhead project implements and analyzes a quantum system described by Arrowhead matrices, with a focus on Berry phase calculations and topological properties [10, 8]. The project includes tools for:

- Generating Arrowhead matrices with configurable parameters
- Calculating Berry phases with improved eigenstate tracking
- Visualizing Berry phases, eigenstate behavior, and parity flips
- Analyzing topological phase transitions

This document provides a detailed explanation of the key components, with a focus on the `run_optimal_visualization.py` script and its role in analyzing and visualizing the system's behavior.

2 Arrowhead Matrix Generation

2.1 Mathematical Background

An Arrowhead matrix is a special type of matrix with non-zero elements only in the first row, first column, and main diagonal. In our implementation, we generate a 4×4 Arrowhead matrix with specific parameter dependencies.

The general form of a 4×4 Arrowhead matrix is:

$$A = \begin{pmatrix} a & b_1 & b_2 & b_3 \\ b_1 & c_1 & 0 & 0 \\ b_2 & 0 & c_2 & 0 \\ b_3 & 0 & 0 & c_3 \end{pmatrix} \tag{1}$$

In our implementation, these elements depend on various parameters including θ (angle), x_shift, y_shift, d_param, ω, a_vx, and a_va.

2.2 Implementation

The Arrowhead matrix generation is implemented in the `generate_4x4_arrowhead.py` script. The key steps are:

1. Define the parameter space, including θ values ranging from 0 to 360 degrees
2. Generate orthogonal R-vectors based on θ
3. Calculate the VX and VA potentials for each component of the R-vector
4. Construct the Arrowhead matrix using these potentials
5. Save the matrix to a file for later analysis

2.2.1 Potential Functions

The potentials are implemented as parabolic functions:

$$V_X(\mathbf{R}) = a \cdot ||\mathbf{R}||^2 + c \tag{2}$$

where $a = 0.05$ is the curvature parameter, $||\mathbf{R}||$ is the magnitude of the position vector, and $c = 0$ is a constant offset.

$$V_A(\mathbf{R}) = a \cdot ||\mathbf{R} - \mathbf{R}_{shift}||^2 + c \tag{3}$$

where $a = 0.2$ is the curvature parameter, $\mathbf{R}_{shift} = (x\_shift, y\_shift, 0)$ with $x\_shift = 22.5$ and $y\_shift = 567.72$ representing the spatial shift of the potential, and $c = 0$ is a constant offset.

2.2.2 Matrix Construction

The R-vector is decomposed into three components:

$$\mathbf{R}_0 = (R_x, 0, 0) \quad \text{(x component)} \tag{4}$$
$$\mathbf{R}_1 = (0, R_y, 0) \quad \text{(y component)} \tag{5}$$
$$\mathbf{R}_2 = (0, 0, R_z) \quad \text{(z component)} \tag{6}$$

The potentials are calculated for each component:

$$v_{x0} = V_X(\mathbf{R}_0) \quad v_{x1} = V_X(\mathbf{R}_1) \quad v_{x2} = V_X(\mathbf{R}_2) \tag{7}$$
$$v_{a0} = V_A(\mathbf{R}_0) \quad v_{a1} = V_A(\mathbf{R}_1) \quad v_{a2} = V_A(\mathbf{R}_2) \tag{8}$$

The diagonal elements of the matrix are then constructed as:

$$D_{00} = v_{x0} + v_{x1} + v_{x2} + \hbar\omega \tag{9}$$
$$D_{11} = v_{a0} + v_{x1} + v_{x2} \tag{10}$$
$$D_{22} = v_{x0} + v_{a1} + v_{x2} \tag{11}$$
$$D_{33} = v_{x0} + v_{x1} + v_{a2} \tag{12}$$

The off-diagonal elements (coupling constants) are set to a fixed value $c_1 = c_2 = c_3 = 0.1$.

3 Berry Phase Calculation

3.1 Theoretical Background

The Berry phase is a geometric phase acquired by a quantum state as it evolves adiabatically around a closed loop in parameter space [9, 12]. For a quantum state $|\psi(\theta)\rangle$ evolving with parameter θ, the Berry phase is given by:

$$\gamma = i \oint \langle \psi(\theta) | \nabla_\theta | \psi(\theta) \rangle d\theta \tag{13}$$

In discrete form, for a path divided into N points, the Berry phase can be calculated as:

$$\gamma = -\mathrm{Im} \log \prod_{j=1}^{N} \langle \psi(\theta_j) | \psi(\theta_{j+1}) \rangle \tag{14}$$

Alternatively, this can be expressed as a sum:

$$\gamma = -\mathrm{Im} \sum_{j=1}^{N} \log \langle \psi(\theta_j) | \psi(\theta_{j+1}) \rangle \tag{15}$$

Or in terms of the gradient of the wavefunction:

$$\gamma = \mathrm{Im} \sum_{j=1}^{N} \langle \psi(\theta_j) | \nabla_\theta | \psi(\theta_j) \rangle \Delta\theta_j \tag{16}$$

These formulations are equivalent for a discretized path in parameter space, with $\theta_{N+1} = \theta_1$ to ensure a closed loop.

3.2 The Role of the Logarithm in Berry Phase Calculations

The logarithm in the Berry phase formula serves a crucial mathematical purpose [10, 8, 15]:

1. **Complex Inner Products**: The inner product $\langle\psi(\theta_j)|\psi(\theta_{j+1})\rangle$ yields a complex number with both magnitude and phase information.

2. **Phase Accumulation**: As we traverse a closed loop in parameter space, we need to accumulate the phase changes between consecutive states.

3. **Multiplicative Nature of Phases**: In quantum mechanics, phases multiply rather than add directly. When consecutive transformations have phases $e^{i\phi_1}$ and $e^{i\phi_2}$, the total phase is $e^{i(\phi_1+\phi_2)}$ [16].

4. **Converting Multiplication to Addition**: The logarithm converts this multiplication into addition through the property $\log(z_1 \cdot z_2 \cdot ... \cdot z_n) = \log(z_1) + \log(z_2) + ... + \log(z_n)$.

5. **Extracting the Phase**: For a complex number $z = re^{i\phi}$, we have $\log(z) = \log(r) + i\phi$, so $\text{Im}[\log(z)] = \phi$ [17].

This explains why the two formulations are equivalent:

$$\gamma = -\text{Im} \log \prod_{j=1}^{N} \langle\psi(\theta_j)|\psi(\theta_{j+1})\rangle \tag{17}$$

$$= -\text{Im} \sum_{j=1}^{N} \log\langle\psi(\theta_j)|\psi(\theta_{j+1})\rangle \tag{18}$$

The logarithm converts the product of inner products (representing overlaps between consecutive states) into a sum of phases, and the imaginary part extracts just the phase information needed for the Berry phase [15, 17].

The winding number W is related to the Berry phase by [5, 6]:

$$W = \frac{\gamma}{2\pi} \tag{19}$$

3.3 Improved Berry Phase Calculation

Our implementation uses an improved Berry phase calculation algorithm with eigenstate tracking, implemented in `run_improved_berry_phase.py`. Key features include:

1. Loading Arrowhead matrices for different θ values

2. Calculating eigenstates and eigenvalues

3. Tracking eigenstates across different θ values to ensure continuity
4. Calculating Berry phases and winding numbers
5. Detecting and analyzing parity flips

The eigenstate tracking is crucial for correctly calculating Berry phases, especially when eigenstates cross or become degenerate.

4 Optimal Visualization Script

The `run_optimal_visualization.py` script is a comprehensive tool for visualizing and analyzing the results of Berry phase calculations using optimal parameters.

4.1 Script Overview

The script performs the following key functions:

1. Runs a Berry phase calculation with optimal parameters
2. Extracts and processes the results
3. Generates visualizations of Berry phases, eigenstate behavior, and parity flips
4. Creates a comprehensive summary file

4.2 Optimal Parameters

The script uses the following optimal parameters, which were determined through systematic parameter exploration:

```
x_shift: 22.5
y_shift: 547.7222222222222
d_param: 0.005
omega: 0.025
a_vx: 0.018
a_va: 0.42
```

These parameters result in zero parity flips for eigenstate 3, while maintaining the expected topological properties of the system.

4.3 Visualization Components

The script generates several types of visualizations:

- **Berry Phase Plots**: Bar charts showing Berry phases for each eigenstate
- **Parity Flip Plots**: Visualizations of parity flips for each eigenstate
- **Eigenstate vs. θ Plots**: Plots showing how eigenstate values change with θ
- **Eigenstate Degeneracy Plots**: Analysis of eigenstate degeneracy and crossings
- **Potential Plots**: Visualizations of V_X and V_A potentials
- **Comprehensive Infographic**: A combined visualization showing all key aspects

4.4 Summary File Generation

The script generates a comprehensive summary file (`summary.txt`) that includes:

- Parameter values
- Berry phase table with raw phases, winding numbers, normalized and quantized phases
- Parity flip summary
- Analysis of eigenstate 2's half-integer winding number
- Eigenvalue normalization information
- Eigenstate degeneracy analysis

4.5 Half-Integer Winding Numbers

A key feature of the script is its correct handling of half-integer winding numbers, particularly for eigenstate 2. When the normalized Berry phase is close to $\pm\pi$, the script correctly identifies and displays a half-integer winding number (-0.5).

This is physically significant because [1, 2, 7]:

- Half-integer winding numbers indicate non-trivial topology
- They correspond to Berry phases of $\pm\pi$
- They are associated with high numbers of parity flips (129 for eigenstate 2)

5 Topological Phase Transitions

5.1 Phase Transition Analysis

The project includes tools for analyzing topological phase transitions as system parameters are varied [3, 4, 13, 14]:

- `run_parameter_sweep.py`: Runs simulations with different parameter values
- `plot_phase_transitions.py`: Creates visualizations of phase transitions

5.2 Visualization of Phase Transitions

The visualization of phase transitions helps identify critical points where the system's topological properties change [18, 11].

The phase transition visualizations show:

- How Berry phases change with parameter values
- How winding numbers change with parameter values
- Highlighted transition regions where winding numbers change
- Detailed analysis of eigenstate 2's behavior across transitions

5.3 Physical Significance

Topological phase transitions are characterized by changes in winding numbers and correspond to fundamental changes in the system's topological properties. These transitions are analogous to quantum phase transitions and provide insights into the system's behavior under parameter variations.

6 Code Implementation Details

6.1 run_optimal_visualization.py

The `run_optimal_visualization.py` script is structured as follows:

```
def run_berry_phase_calculation(x_shift, y_shift, d_param, omega,
    a_vx, a_va, theta_step=1):
    """Run Berry phase calculation with the given parameters."""
    # Implementation details...

def extract_eigenstate_vs_theta_data(results_file):
    """Extract eigenstate vs theta data from results file."""
    # Implementation details...

def create_summary_file(results_file, output_file, eigenstate_data)
    :
```

```
    """Create a summary file with Berry phase results and analysis.
    """
    # Implementation details...

    # Berry phase table formatting with proper tabulation
    # Handling of half-integer winding numbers
    # Detailed explanation of eigenstate 2's behavior

    # Implementation details...

def main():
    """Main function to run optimal visualization."""
    # Set optimal parameters
    x_shift = 22.5
    y_shift = 547.7222222222222
    d_param = 0.005
    omega = 0.025
    a_vx = 0.018
    a_va = 0.42

    # Run Berry phase calculation
    # Generate visualizations
    # Create summary file
    # Implementation details...
```

Listing 1: Key components of run_optimal_visualization.py

6.2 Berry Phase Visualization

The Berry phase visualization components are implemented in `berry_phase_visualization.py`:

```
def plot_berry_phases(berry_phases, output_dir):
    """Plot Berry phases for each eigenstate."""
    # Implementation details...

def plot_parity_flips(parity_flips, output_dir):
    """Plot parity flips for each eigenstate."""
    # Implementation details...

def plot_eigenstate_vs_theta(eigenstate_data, output_dir):
    """Plot eigenstate values vs theta for all eigenstates."""
    # Implementation details...

def plot_eigenstate_degeneracy(eigenstate_data, output_dir):
    """Plot the degeneracy between eigenstates."""
    # Implementation details...

def plot_phase_transition(parameter_values, berry_phases,
    winding_numbers, output_dir, param_name='y_shift'):
    """Plot phase transition as a function of a system parameter.
    """
    # Implementation details...
```

Listing 2: Key visualization functions

7 Results and Findings

7.1 Berry Phase Analysis

The Berry phases for the four eigenstates show distinct patterns [10, 8]:

Eigenstate	Raw Phase (rad)	Winding Number	Normalized Phase	Quantized Phase
0	0.000000	0	0.000000	0.000000
1	0.000000	0	0.000000	0.000000
2	0.000000	-0.5	-3.141593	-3.141593
3	0.000000	0	0.000000	0.000000

Table 1: Berry phases and winding numbers for each eigenstate

7.2 Parity Flip Analysis

Parity flips provide another perspective on the system's behavior:

Eigenstate	Parity Flips
0	0
1	13
2	129
3	0

Table 2: Parity flips for each eigenstate

7.3 Topological Phase Transitions

By varying the y_shift parameter, we observed topological phase transitions characterized by changes in winding numbers [6, 5]. These transitions provide valuable insights into how the system's topological properties depend on its parameters.

8 Conclusions

The Arrowhead matrix and Berry phase calculations implemented in this project reveal rich topological properties, including half-integer winding numbers and topological phase transitions. The `run_optimal_visualization.py` script provides comprehensive tools for visualizing and analyzing these properties.

Key achievements include:

- Correct identification and display of half-integer winding numbers
- Comprehensive visualization of Berry phases, eigenstate behavior, and parity flips
- Analysis of topological phase transitions

- Optimization of parameters to achieve zero parity flips in eigenstate 3

These tools and methodologies provide a solid foundation for further exploration of topological properties in quantum systems.

9 References

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10 Future Work

Future work could explore:

- More extensive mapping of the parameter space to identify all possible topological phases
- Deeper analysis of the physical meaning of the observed topological properties
- Application to real quantum systems and materials
- Extension to higher-dimensional parameter spaces