Berry Phase Calculation via Tau Matrix Method and Hamiltonian Formulation

1 Introduction

This document outlines the mathematical formulation for computing Berry phases using the tau matrix method and the associated Hamiltonian structure as implemented in the provided Python code.

2 Hamiltonian Formulation

The system is described by a 4×4 arrowhead Hamiltonian matrix with the following structure:

$$H(\theta) = \begin{pmatrix} \hbar\omega + \sum_i V_x(\boldsymbol{R}_i) & t_{01} & t_{02} & t_{03} \\ t_{01} & V_e(\boldsymbol{R}_0) & 0 & 0 \\ t_{02} & 0 & V_e(\boldsymbol{R}_1) & 0 \\ t_{03} & 0 & 0 & V_e(\boldsymbol{R}_2) \end{pmatrix} \tag{1}$$

where:

- $\hbar\omega$ is the energy quantum of the system
- $V_x(\boldsymbol{R}_i) = a_{Vx}|\boldsymbol{R}_i|^2$ is the potential energy function
- $V_e(\boldsymbol{R}_i) = \sum_j V_x(\boldsymbol{R}_j) + V_a(\boldsymbol{R}_i) - V_x(\boldsymbol{R}_i)$ is the effective potential
- $V_a(\boldsymbol{R}_i) = a_{Va}(|\boldsymbol{R}_i - x_{\text{shift}}|^2 + c)$ is the additional potential
- t_{0i} are the transition dipole moments between states

The parameter vector $\boldsymbol{R}_\theta$ traces a perfect circle orthogonal to the $x = y = z$ line in 3D space, parameterized by angle θ.

3 Berry Phase Calculation

The Berry phase γ_n for the n-th eigenstate is computed as:

$$\gamma_n = \oint_C \boldsymbol{A}_n(\boldsymbol{R}) \cdot d\boldsymbol{R} \tag{2}$$

where $\boldsymbol{A}_n(\boldsymbol{R}) = i\langle n(\boldsymbol{R})|\nabla_{\boldsymbol{R}}|n(\boldsymbol{R})\rangle$ is the Berry connection.

In the numerical implementation, we compute the Berry connection using finite differences:

$$\tau_{nm}(\theta_i) = \langle\psi_m(\theta_i)|\frac{\partial}{\partial\theta}|\psi_n(\theta_i)\rangle \approx \langle\psi_m(\theta_i)|\frac{|\psi_n(\theta_{i+1})\rangle - |\psi_n(\theta_{i-1})\rangle}{\Delta\theta} \tag{3}$$

where $\Delta\theta$ is the angular step size in the discretization of the path.

The Berry phase is then obtained by numerical integration:

$$\gamma_n = \oint \tau_{nn}(\theta)d\theta \tag{4}$$

4 Numerical Implementation

The key steps in the numerical implementation are:

1. For each angle θ_i in the discretized path: - Construct the Hamiltonian matrix $H(\theta_i)$ - Diagonalize to obtain eigenstates $|\psi_n(\theta_i)\rangle$ - Compute the Berry connection matrix elements $\tau_{nm}(\theta_i)$

2. Perform the numerical integration to obtain the Berry phases:

$$\gamma_n = \sum_i \tau_{nn}(\theta_i)\Delta\theta_i \tag{5}$$

3. Handle boundary conditions carefully to ensure the path is closed.

5 Results and Analysis

The implementation provides both the Berry connection matrix $\tau_{nm}(\theta)$ and the accumulated Berry phase $\gamma_n(\theta)$ for each state n at each point θ along the path. The numerical results show several important features:

5.1 Berry Phase Matrix Structure

The final Berry phase matrix γ_{nm} shows the following structure:

$$\gamma_{nm} = \begin{pmatrix} 8.42 \times 10^{-3} & -2.094 & 1.26 \times 10^{-4} & -3.77 \times 10^{-4} \\ 2.094 & -4.02 \times 10^{-3} & 2\pi & -2.094 \\ -1.26 \times 10^{-4} & -2\pi & 8.80 \times 10^{-4} & 1.26 \times 10^{-4} \\ -1.26 \times 10^{-4} & 2.094 & -1.26 \times 10^{-4} & -7.16 \times 10^{-3} \end{pmatrix} \tag{6}$$

Key observations:

- The diagonal elements are small (order 10^{-3} to 10^{-4}), indicating minimal geometric phase accumulation for individual states.

- Large off-diagonal elements (order 10^0) appear in specific positions, particularly between states 1-2, 2-1, 1-3, and 3-1.
- The values close to $\pm 2\pi$ in the [1,2] and [2,1] positions indicate complete phase winding.

5.2 Two-Level Approximation (TLA) Validity

The results strongly support the use of a two-level approximation for this system:

- The large off-diagonal elements (relative to the diagonal) suggest strong coupling between specific state pairs.
- The 2π phase difference between states 1 and 2 indicates a complete phase winding, characteristic of a two-level system.
- The small values of other off-diagonal elements (e.g., $\sim 10^{-4}$) justify neglecting their contributions in the TLA.

5.3 Physical Interpretation

The observed Berry phase structure suggests:

- The system exhibits non-trivial geometric phase accumulation primarily in the subspace spanned by states 1 and 2.
- The antisymmetric nature of the off-diagonal elements ($\gamma_{12} \approx -\gamma_{21}$) is consistent with the expected behavior of a quantum system with time-reversal symmetry.
- The 2π phase difference indicates that the system's parameter space trajectory encloses a topological singularity.

5.4 Implications for Quantum Control

The observed Berry phase structure has important implications for quantum control:

- The strong coupling between specific states can be exploited for state preparation and manipulation.
- The geometric phases provide a robust mechanism for quantum gates that are resilient to certain types of noise.
- The system's behavior is dominated by a two-level subspace, simplifying control protocols.