1 Hamiltonian Formulation

The Hamiltonian $H(\boldsymbol{R}_\theta)$ is a 4x4 arrowhead matrix defined as:

$$H(\boldsymbol{R}_\theta) = \begin{pmatrix} E_0(R_{\theta,i}) & c_{10} & c_{20} & c_{30} \\ c_{10} & E_1(R_{\theta,i}) & 0 & 0 \\ c_{20} & 0 & E_2(R_{\theta,i}) & 0 \\ c_{30} & 0 & 0 & E_3(R_{\theta,i}) \end{pmatrix} \tag{1}$$

where $E_0(R_{\theta,i}) = \hbar\omega + \sum_{i=0}^{2} V_x^{(i)}(R_{\theta,i})$ and $E_{i+1}(R_{\theta,i}) = E_0(R_{\theta,i}) + V_a^{(i)}(R_{\theta,i}) - V_x^{(i)}(R_{\theta,i})$ for $i = 0, 1, 2$.

Here ω is a frequency parameter, and V_x and V_a are potential terms that depend on the parameter vector $R(\theta)$. These potential terms are defined as follows:

$$V_x^{(i)}(R_{\theta,i}) = a \cdot (R_{\theta,i})^2 + c \tag{2}$$

$$V_a^{(i)}(R_{\theta,i}) = a \cdot (R_{\theta,i} - x_{\text{shift}})^2 + c \tag{3}$$

The coupling constants c_{10}, c_{20}, and c_{30} are calculated using the transitional dipole moment between the ground state and excited states. The transitional dipole moment is computed as:

$$c_{i0} = c_{i0} = \langle \psi_i | \hat{\boldsymbol{r}} | \psi_0 \rangle \tag{4}$$

where ψ_0 is the ground state eigenvector, ψ_i is the i^{th} excited state eigenvector, and $\hat{\boldsymbol{r}}$ is the position operator. These couplings are then used in the Hamiltonian matrix:

$$H(\boldsymbol{R}_\theta) = \begin{pmatrix} E_0(R_{\theta,i}) & c_{10} & c_{20} & c_{30} \\ c_{10} & E_1(R_{\theta,i}) & 0 & 0 \\ c_{20} & 0 & E_2(R_{\theta,i}) & 0 \\ c_{30} & 0 & 0 & E_3(R_{\theta,i}) \end{pmatrix} \tag{5}$$

2 $\boldsymbol{R}_\theta$ generation

The $\boldsymbol{R}_\theta$ vector traces a perfect circle orthogonal to the $x = y = z$ line using the `create_perfect_orthogonal_vectors` function from the Arrowhead/generalized package.

3 Berry Connection

The Berry connection $A(\boldsymbol{R}_\theta)$ is calculated using:

$$A_n(\boldsymbol{R}_\theta) = \langle n(\boldsymbol{R}_\theta) | i\partial_{\boldsymbol{R}_\theta} | n(\boldsymbol{R}_\theta) \rangle \tag{6}$$

where $|n(\boldsymbol{R}_\theta)\rangle$ are the eigenstates of $H(\boldsymbol{R}_\theta)$.

4 Berry Phase

The Berry phase γ_n for state n is obtained by integrating the Berry connection:

$$\gamma_n = \int_0^{2\pi} A_n(\boldsymbol{R}_\theta) d\boldsymbol{R}_\theta \tag{7}$$

5 Verification

We verify the eigenvalue equation $H(\boldsymbol{R}_\theta)|n(\boldsymbol{R}_\theta)\rangle = E_n(\boldsymbol{R}_\theta)|n(\boldsymbol{R}_\theta)\rangle$ by comparing:

$$H(\boldsymbol{R}_\theta)|n(\boldsymbol{R}_\theta)\rangle \quad \text{vs} \quad E_n(\boldsymbol{R}_\theta)|n(\boldsymbol{R}_\theta)\rangle \tag{8}$$

6 Visualization

For each state n, we plot:

- Magnitude of $H(\boldsymbol{R}_\theta)|n(\boldsymbol{R}_\theta)\rangle$ and $E_n(\boldsymbol{R}_\theta)|n(\boldsymbol{R}_\theta)\rangle$
- Real and imaginary components separately
- All four vector components

7 References

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