Supplementary Information for Exponential convergence of the local diabatic representation for nonadiabatic eigenvalue problems

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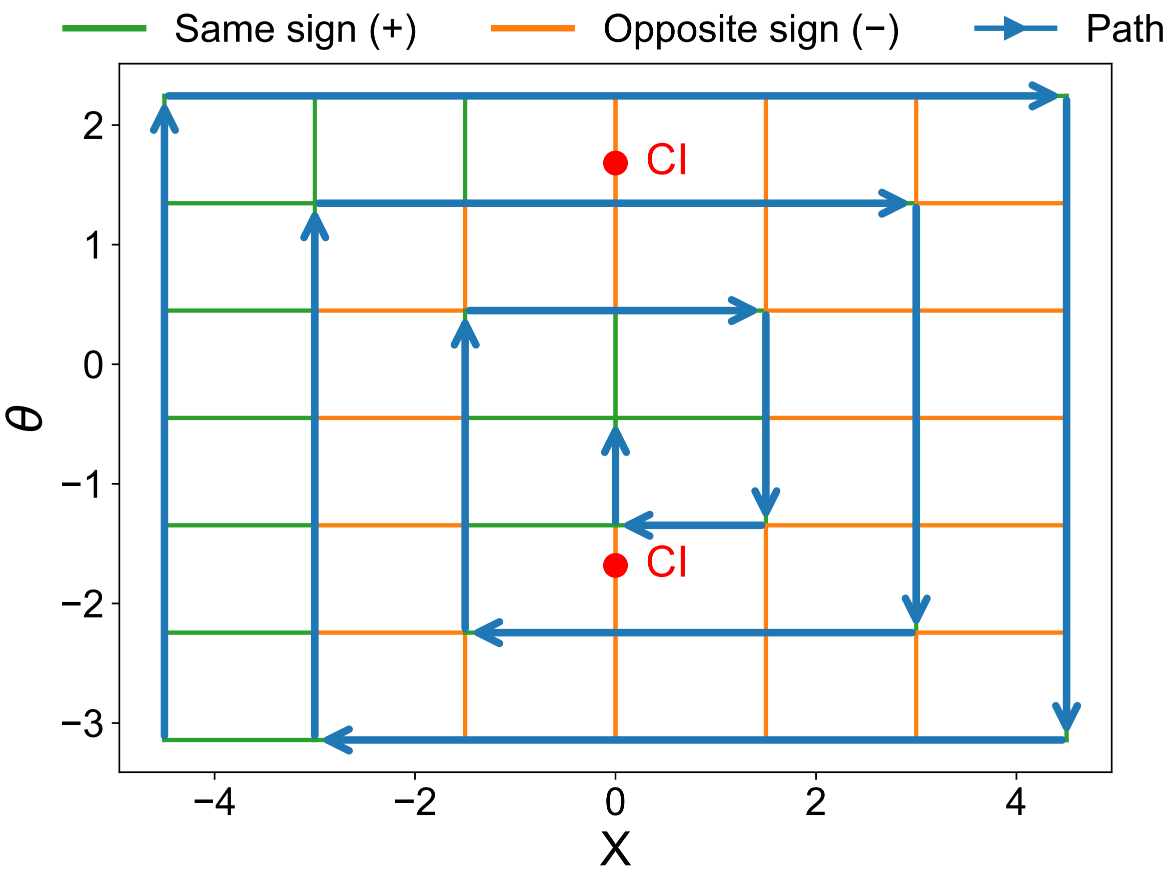

FIG. S1: Schematic of the parallel transport gauge construction for the conical intersection model. A 7×7 grid is displayed for clarity. The gauge is defined by scanning the 2D grid along a rectangular spiral path (blue arrows), starting from the bottom-left corner and winding clockwise inward. Positive overlaps are enforced between adjacent grid points along this path.

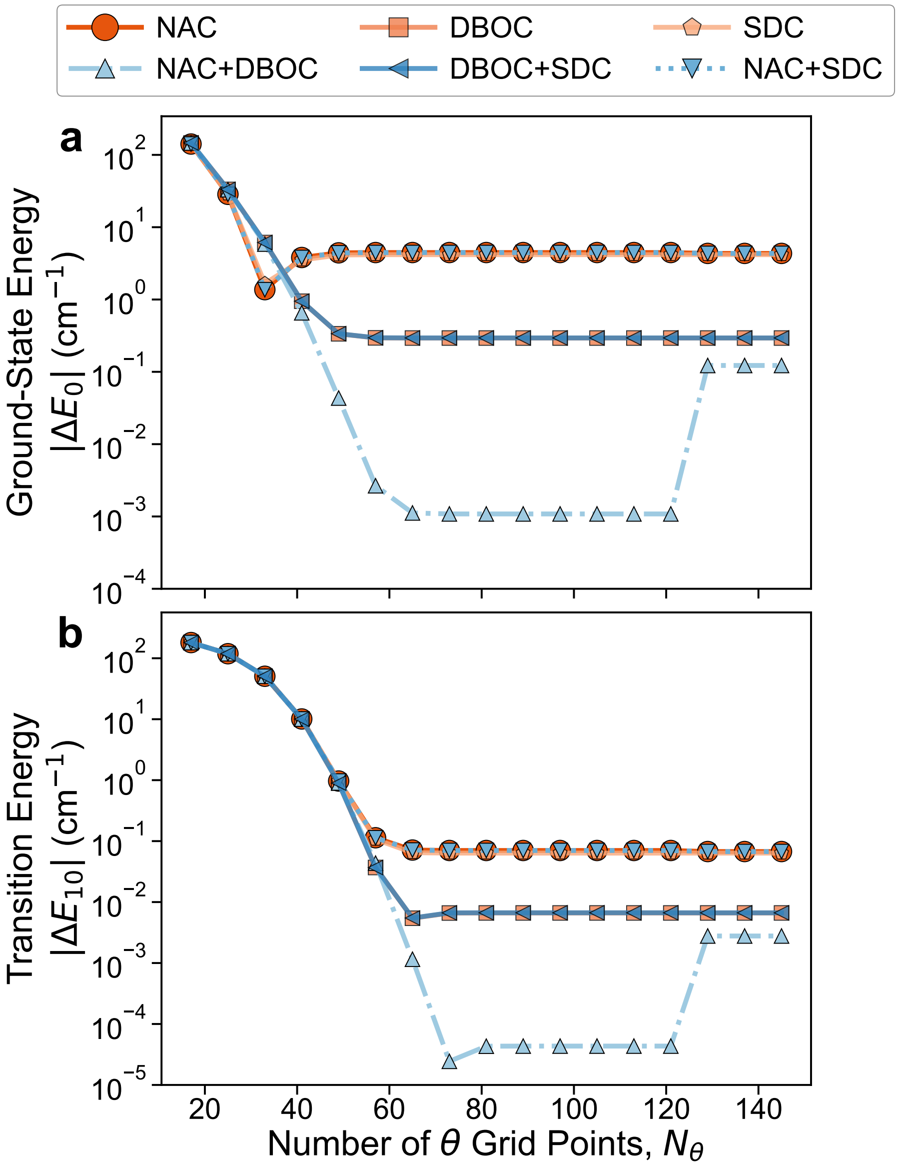

FIG. S2: Convergence analysis of individual nonadiabatic coupling contributions for the conical intersection model. The panels show the results for (a) ground state energy error $|\Delta E_0|$ and (b) transition energy error $|\Delta E_{10}|$ with two electronic states ($N_s = 2$) with N_x fixed at 63. Calculations lacking the DBOC exhibit non-monotonic convergence and result in substantial errors. The NAC+DBOC method yields lower errors initially, but the error increases as the grid becomes denser. In contrast, only the DBOC and DBOC+SDC methods sustain convergence, even at high grid densities.

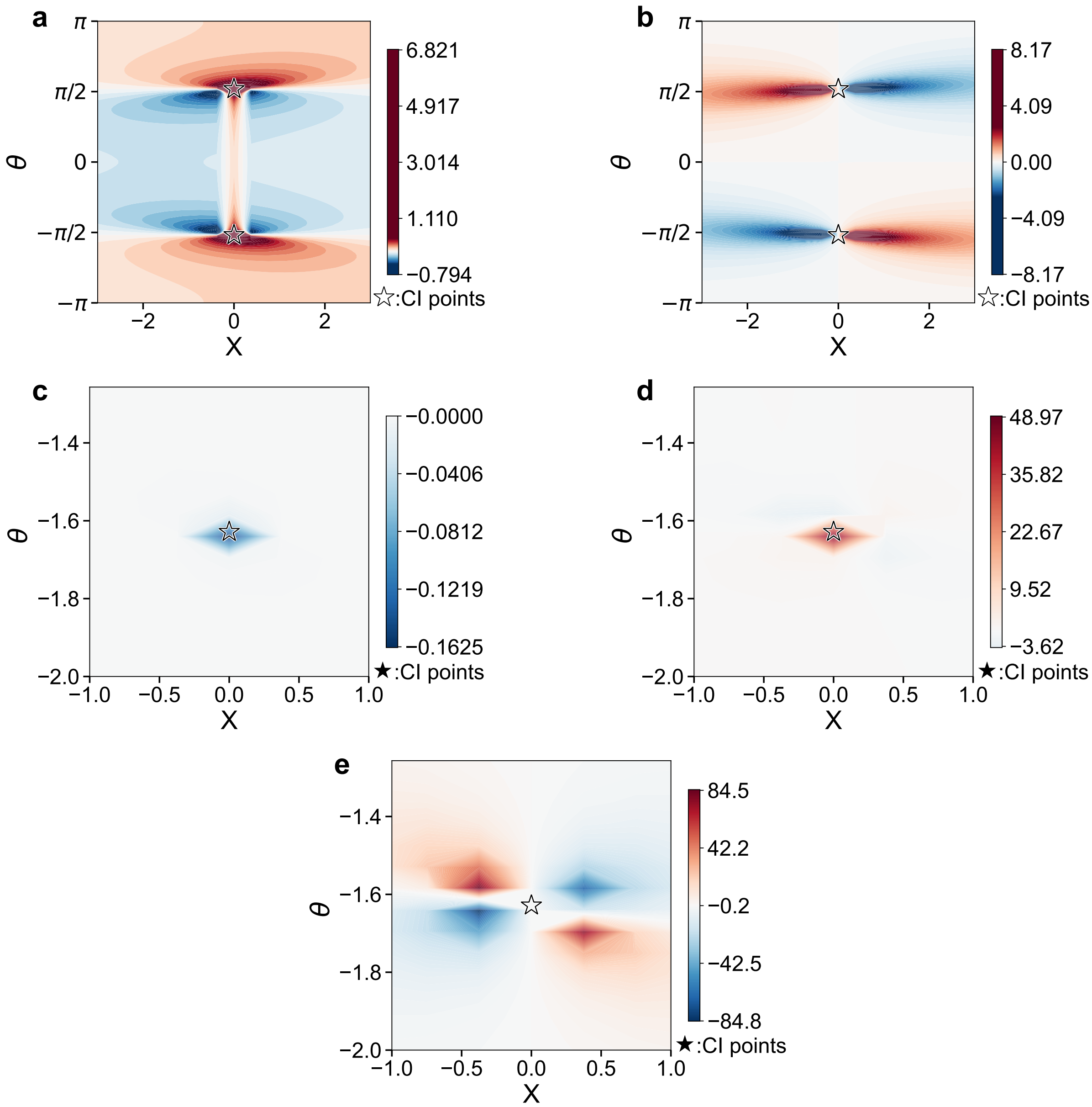

FIG. S3: Nonadiabatic coupling terms for the conical intersection model ($N_x = 31$, $N_\theta = 113$). (a, b) First-order NAC elements F_{01} along x and θ. (c) The ground state DBOC. (d, e) The off-diagonal SDC G_{01} along x and θ. With this grid density, the grid does not clearly resolve the singular features of the couplings near the CIs.

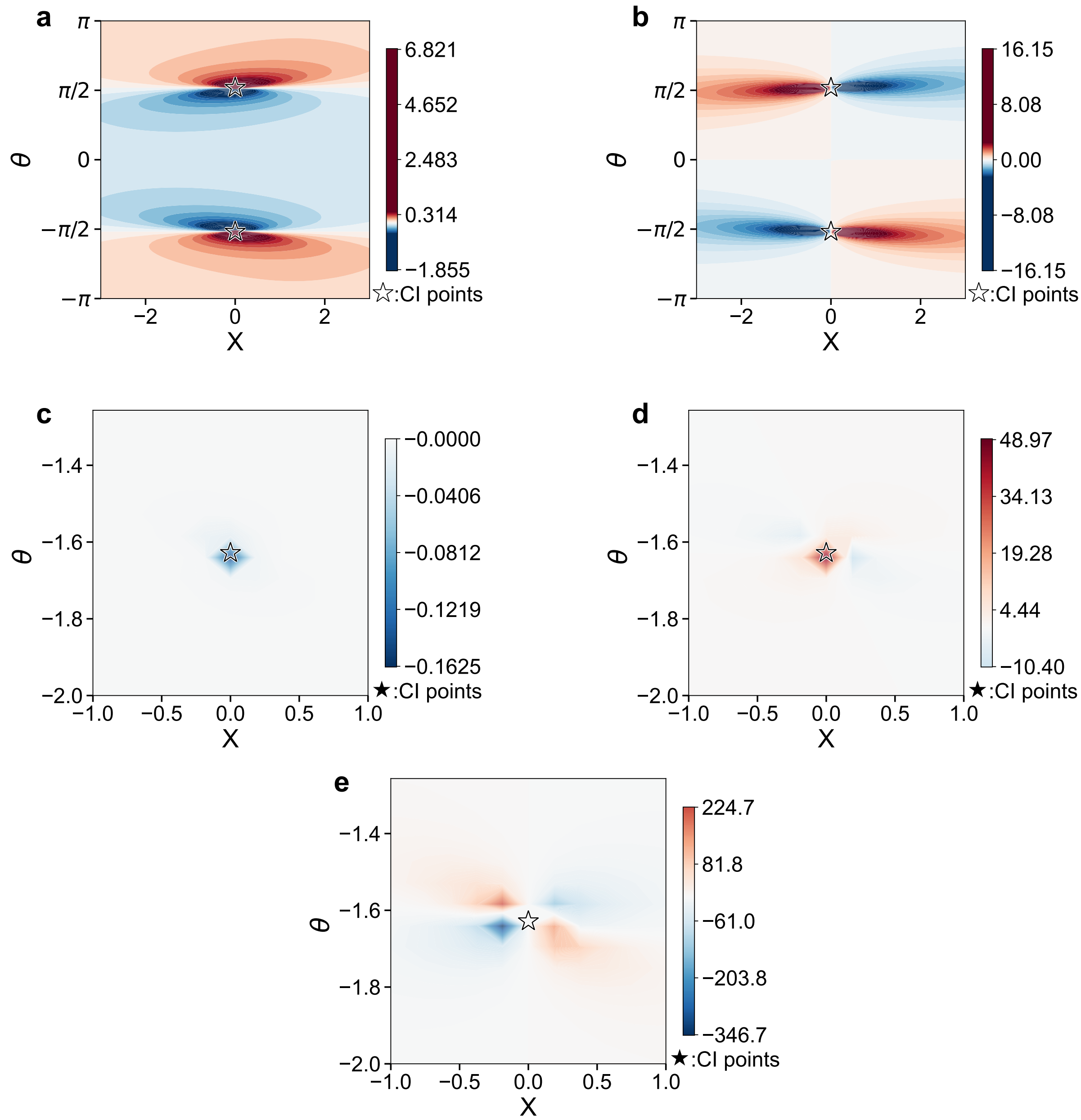

FIG. S4: Nonadiabatic coupling terms for the conical intersection model ($N_x = 63$, $N_\theta = 113$). (a, b) First-order NAC elements F_{01} along x and θ. (c) The ground state DBOC. (d, e) The off-diagonal SDC G_{01} along x and θ. With increased grid density, the resolution of singular features improves. The NAC and SDC along the θ-mode exhibit stronger localized singularities near the CIs.

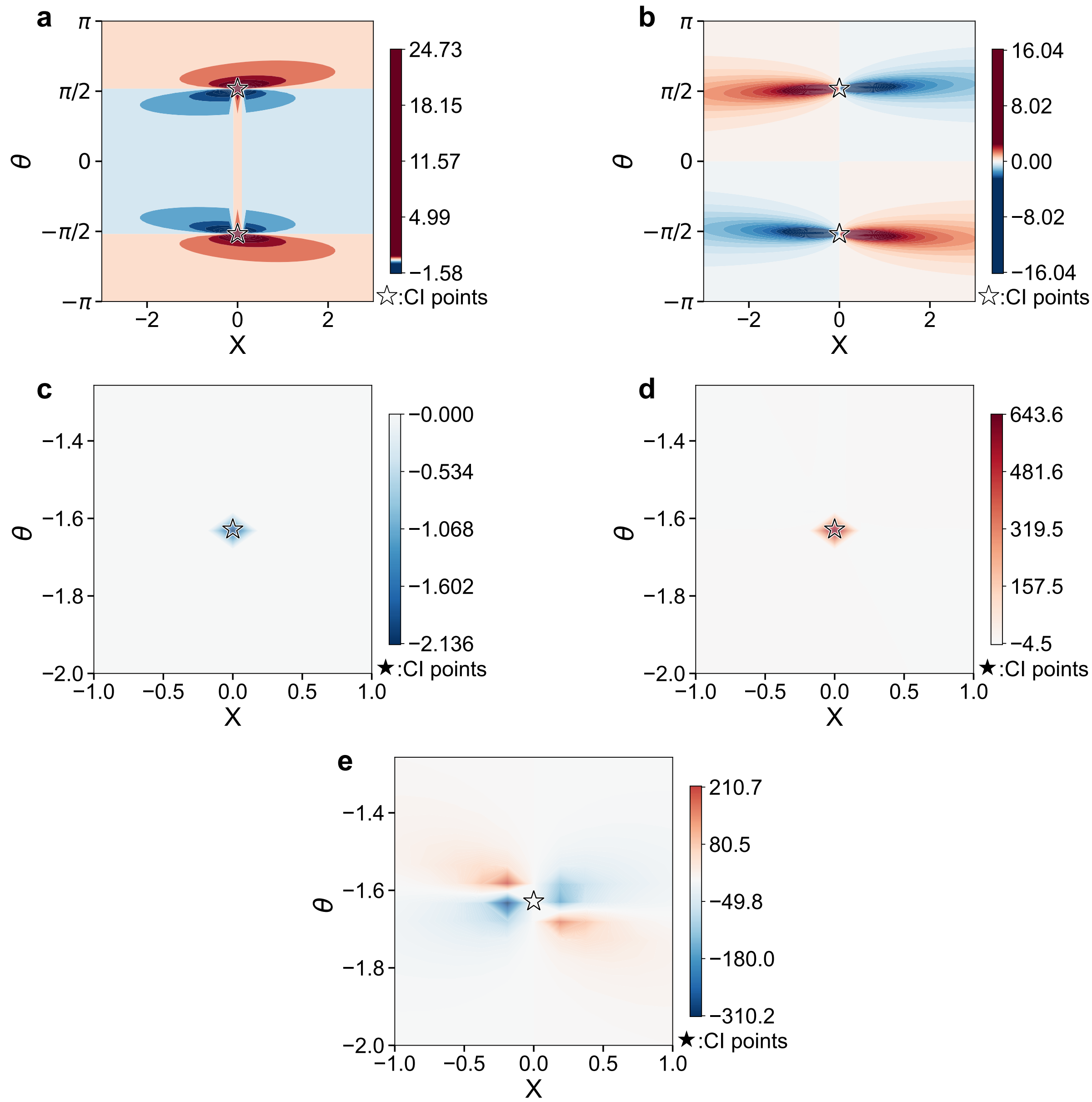

FIG. S5: Nonadiabatic coupling terms for the conical intersection model ($N_x = 63$, $N_\theta = 129$). (a, b) First-order NAC elements F_{01} along x and θ. (c) The ground state DBOC. (d, e) The off-diagonal SDC G_{01} along x and θ. With this high grid density, sampling points fall into the vicinity of the CIs, leading to large diverging amplitudes in all coupling terms.