Non-adiabatic dynamics is a research topic that has been intensively investigated. In a typical non-adiabatic system:

- There are multiple close-lying electronic states
- The Born-Oppenheimer approximation becomes invalid
- The nuclear wave's have components along the multiple electronic states

Non-adiabatic dynamics problem can be decomposed into two parts:

1. Part 1: Construction of the vibronic Hamiltonian

\[
\hat{H}_{\text{vibronic}} = \hat{F}_1 \cdot \text{N.A.C} \cdot \hat{T}_1 + \hat{E}_1(\hat{R}) \cdot 0
\]

2. Part 2: Solve the quantum dynamics problem of the vibronic model Hamiltonian

\[
\frac{d}{dt} |\Psi(t)\rangle = \hat{H}_{\text{vibronic}} |\Psi(t)\rangle
\]

The vibronic model Hamiltonian can be expressed in terms of second quantized bosonic construction operators:

\[
\hat{H} = \sum_{ij} a_i^\dagger a_j^\dagger a_i a_j + \sum_i b_i^\dagger b_i^\dagger b_i + \sum_{ij} c_{ij}^\dagger c_{ij} + \cdots
\]

The full wavefunction is a linear combination of all electronic states:

\[
|\Psi(t)\rangle = \sum_k \chi_k |\psi_k(t)\rangle
\]

We apply the mixed CC / CI ansatz to parameterize the time dependent wavefunction:

\[
|\psi_k(t)\rangle = \sum_j |\phi_j\rangle \chi_{jk} e^{i\lambda_{jk}t}
\]

Substitute the ansatz into the TDSE and solve CC EOM:

\[
i \frac{\partial |\phi_j\rangle}{\partial t} = -\sum_k \epsilon_{jk} |\phi_j\rangle \chi_{jk}
\]

The excitation energy is derived by expanding the Hamiltonian in terms of diabatic states:

\[
\epsilon_{ij} = \sum_k \chi_{ik}^\dagger \chi_{jk} (H_{ij}^\dagger x |0\rangle)
\]

The EHrenfest (taking state average) parameterization of the EOM for \( \hat{T} \):

\[
i \frac{\partial |\phi_j\rangle}{\partial t} = -\sum_k \epsilon_{jk} |\phi_j\rangle \chi_{jk} (H_{ij}^\dagger x |0\rangle)
\]

Apply modified projection manifold to parameterize EOM for \( \hat{Z} \):

\[
i \frac{\partial |\phi_j\rangle}{\partial t} = \sum_k \chi_{ik}^\dagger \chi_{jk} (H_{ij}^\dagger x |0\rangle) \chi_{jk}
\]

Compute the auto-correlation function (ACF) from the CC amplitudes:

\[
ACF(t) = \langle \Psi(0)|\Psi(t)\rangle = \sum_{i,j} \chi_{ij}^\dagger \chi_{ij}
\]