Calculation of the dynamics of nonadiabatic transitions with multiple vibrational modes KUNIO ISHIDA, Corporate research and development center, Toshiba Corporation, KEIICHIRO NASU, Institute of Materials Structure Science, KEK — We propose a new calculation method of the dynamics of nonadiabatic transition which is applicable to study coherent control of photoisomerizations. We show that we can obtain a good approximation of the real dynamics of the system with less computational cost by switching fully quantum mechanical (QM) calculation and classical (CM) calculation at every time step by evaluating a "switching factor" defined by

$$\eta = \max_{\phi_i, z_i} |\langle z_1 e^{i\phi_1}, z_2 e^{i\phi_2}, ..., z_N e^{i\phi_N} |U|\Phi\rangle|^2, \tag{1}$$

where N is the number of the vibrational modes relevant to the photoisomerization, and $|\Phi\rangle$ shows the quantum mechanical state each wavepacket in the system. $|z_1 e^{i\phi_1}, z_2 e^{i\phi_2}, ..., z_N e^{i\phi_N}\rangle$ and U denote the coherent state in N-dimensional space and a translation operator, respectively. The switching rule is:
"When η exceeds a threshold value η_c, we perform a QM calculation, and *vice versa*."
By choosing an appropriate value of η_c we obtain a approximated wavefunction at each time step which well-reproduces that derived by QM calculation.

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