Coherences in Nonadiabatic Dynamics

Tully Model 1
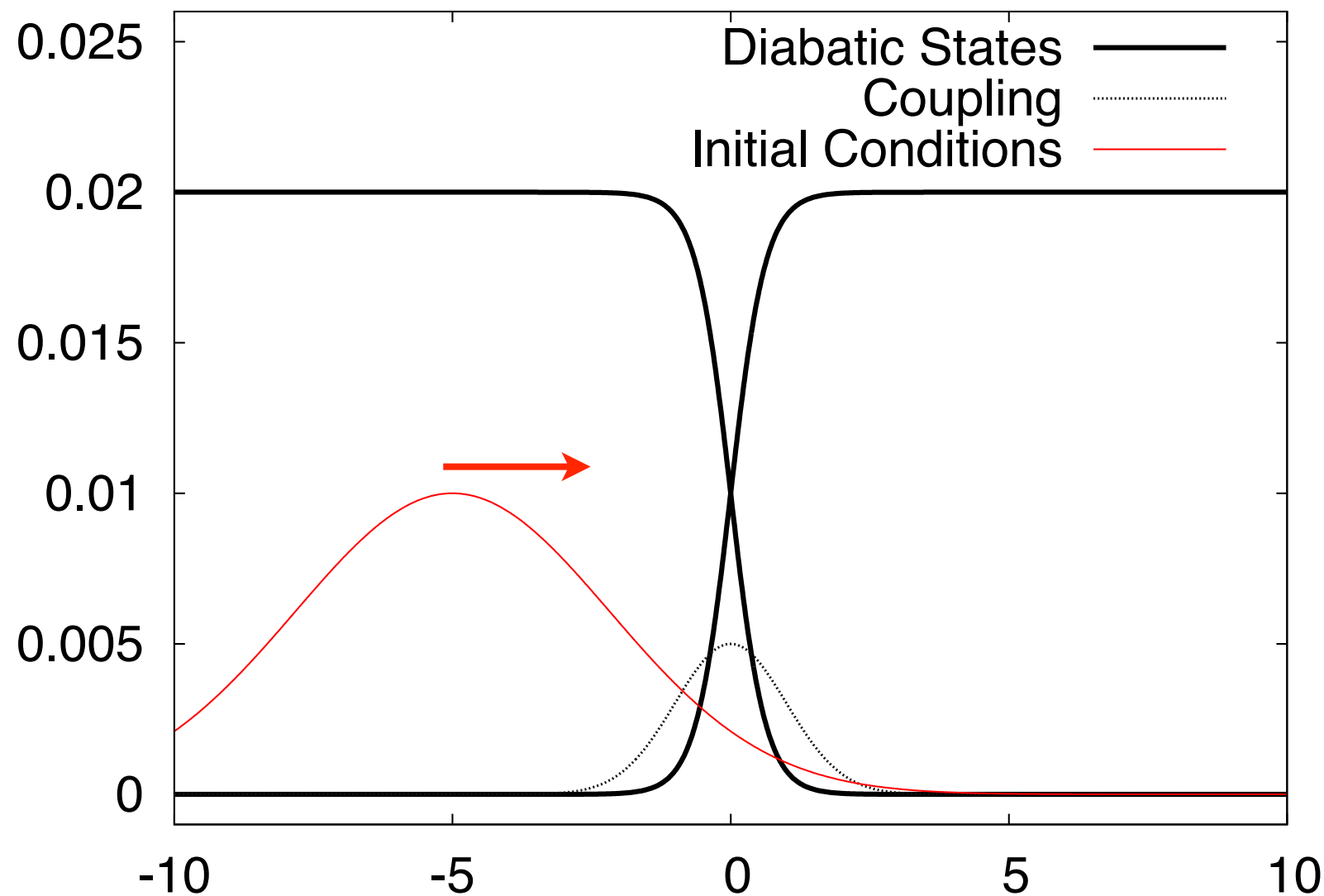
$E = 0.1$

$\hat{A} = |\Psi\rangle\langle\Psi|$

$\hat{B} = |\Phi_1\rangle\langle\Phi_1|$
or
$\hat{B} = \delta(\hat{P} - P_f)$

MMST maps electronic states to classical dofs

$$H_{\mathrm{MMST}} = \frac{P^2}{2m} + \frac{1}{2}\sum_{i,j} V_{ij}(R)\left(x_i x_j + p_i p_j - \delta_{ij}\right)$$

Tully Model: Tully. JCP **93** 1061 (1990).   MMST: Meyer, Miller. JCP **70** 3214 (1979).
Stock, Thoss. PRL **78** 578 (1997).