Generator coordinate method for transition-state dynamics in nuclear fission

George F. Bertsch and
Kouichi Hagino

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Transition-state theory from Bohr&Wheeler

$$W = \frac{1}{2\pi\hbar\rho}\sum_c T_c$$

$$0 < T_c < 1$$

Current theory of transmission coefficient
RIPL-3:

$$T_i^{HW}(U) = \frac{1}{1+\exp\left[-(2\pi/\hbar\omega_i)(U-B_{fi})\right]} \qquad i = 1, N, \tag{194}$$

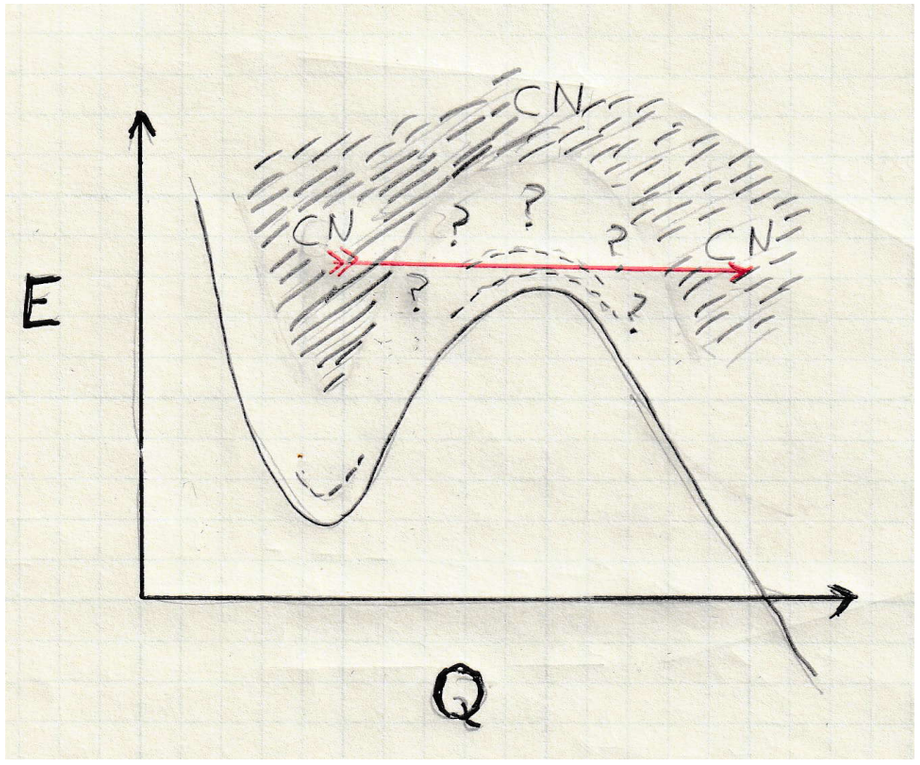
Many-body formalism to calculate the transmission coefficient—start with GCM construction of configuration space.

$$\boldsymbol{G} = (\boldsymbol{H} - i\boldsymbol{\Gamma}/2 - E\boldsymbol{N})^{-1}$$

$$T_{ab} = \mathsf{Tr}\,(\boldsymbol{\Gamma}_a \boldsymbol{G} \boldsymbol{\Gamma}_b \boldsymbol{G}^*)$$

Datta (2001);
see also Alhassid (2020)

The fission landscape: PES, CN, transition states.

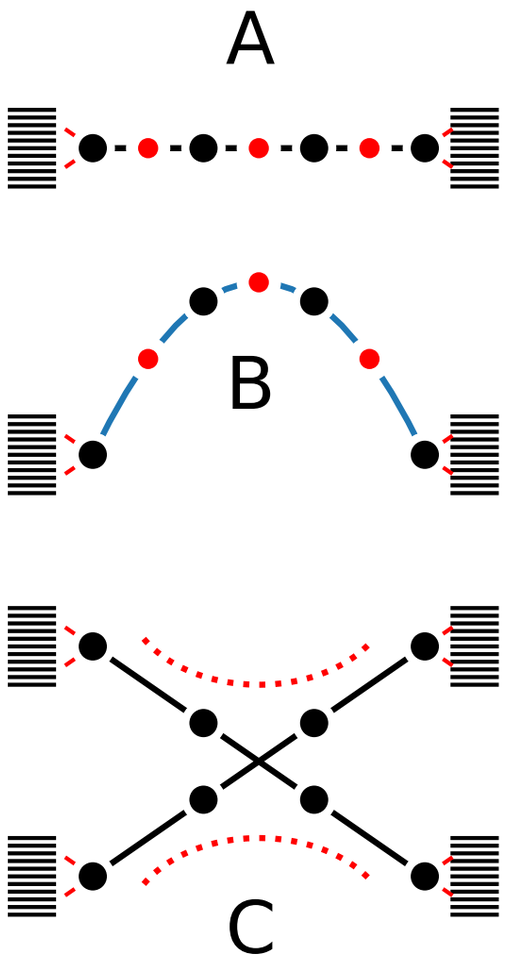


A working criterion for the compound nucleus:

$$\rho\overline{\langle i|v|j\rangle} > 1$$

Zirnbauer (1983)

Schematic models for transition state dynamics



We compare 4- and 7-state models to examine the dependence on the spacing of the reference states.

Hamiltonian matrix elements are parameterized with the factorization hypothesis.

Gaussian overlap hypothesis gives exact free-particle kinetic energy (Flocard and Vautherin, (1976).

$$|k\rangle = \int_{-\infty}^{\infty} dx\, e^{ikx} |\Psi(x)\rangle$$

$$\langle \Psi(0)|H|k\rangle = \langle \Psi(0)|k\rangle \left(\frac{k^2}{2Nm} - E_{zp} + E_0 \right)$$

With a discrete mesh of points

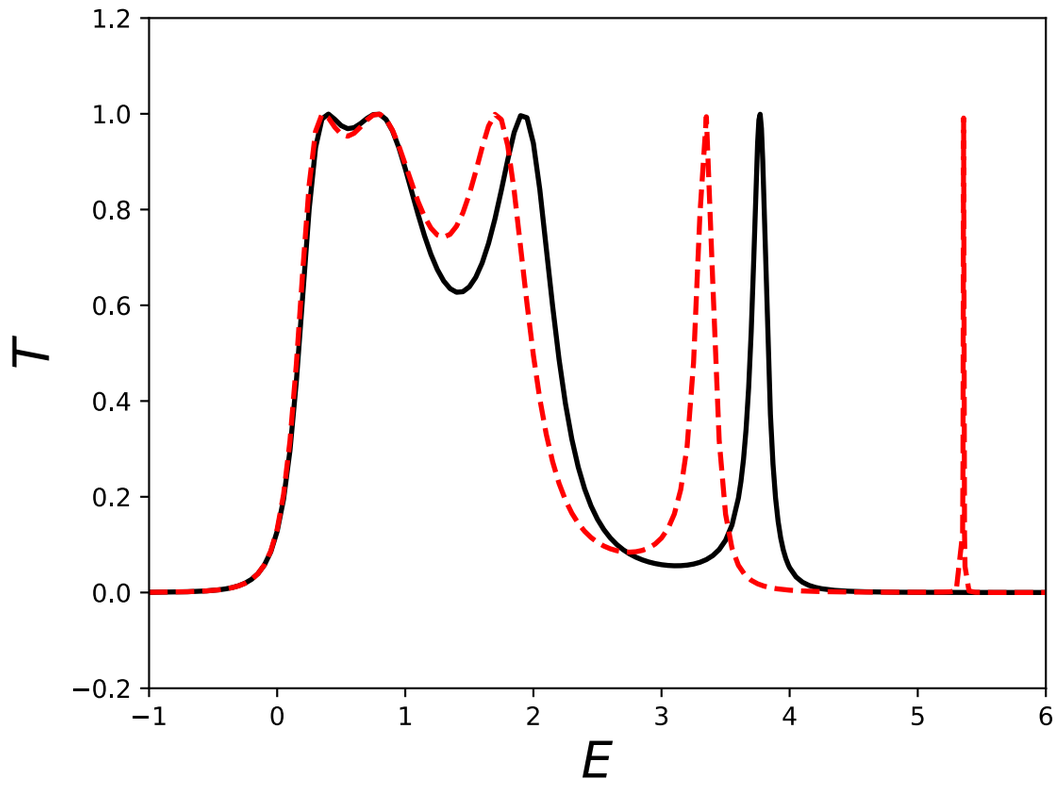
$$|k\rangle = \sum_n e^{ikn\Delta x} |\Psi(n\Delta x)\rangle$$

Works quite well if

$$\langle \Psi(0)|\Psi(\Delta x)\rangle > 0.25 \qquad \text{and} \qquad k\Delta x < \frac{\pi}{2}$$

$$\frac{k^2}{2Nm} < \frac{E_{zp}}{2}$$

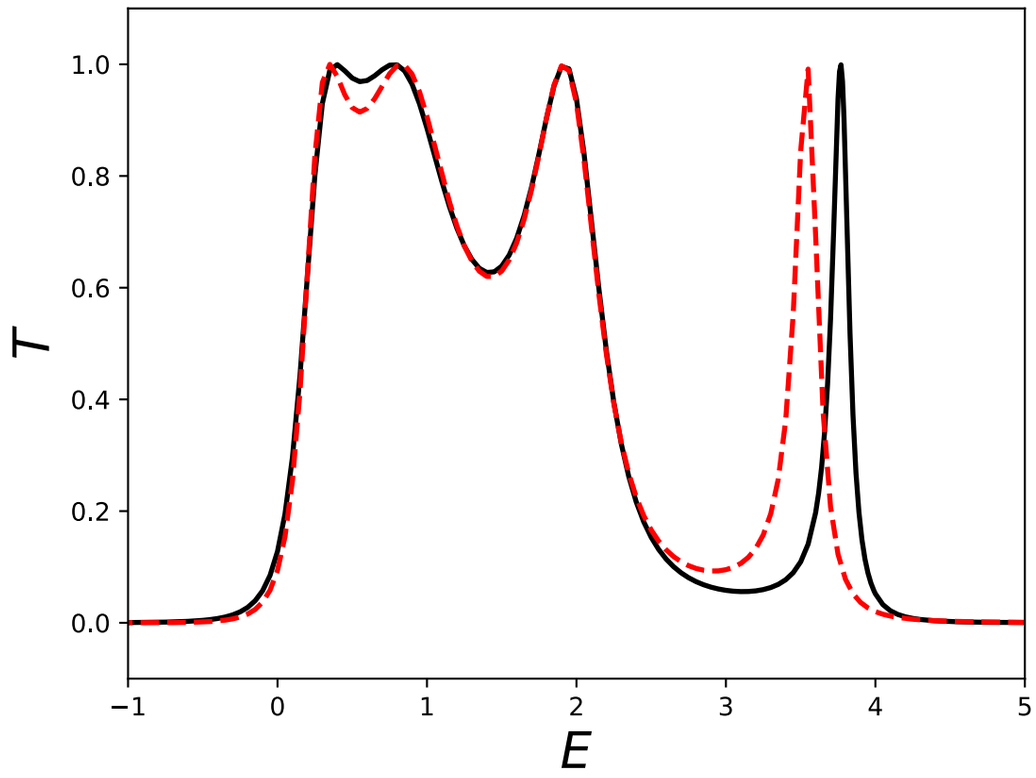
Model A



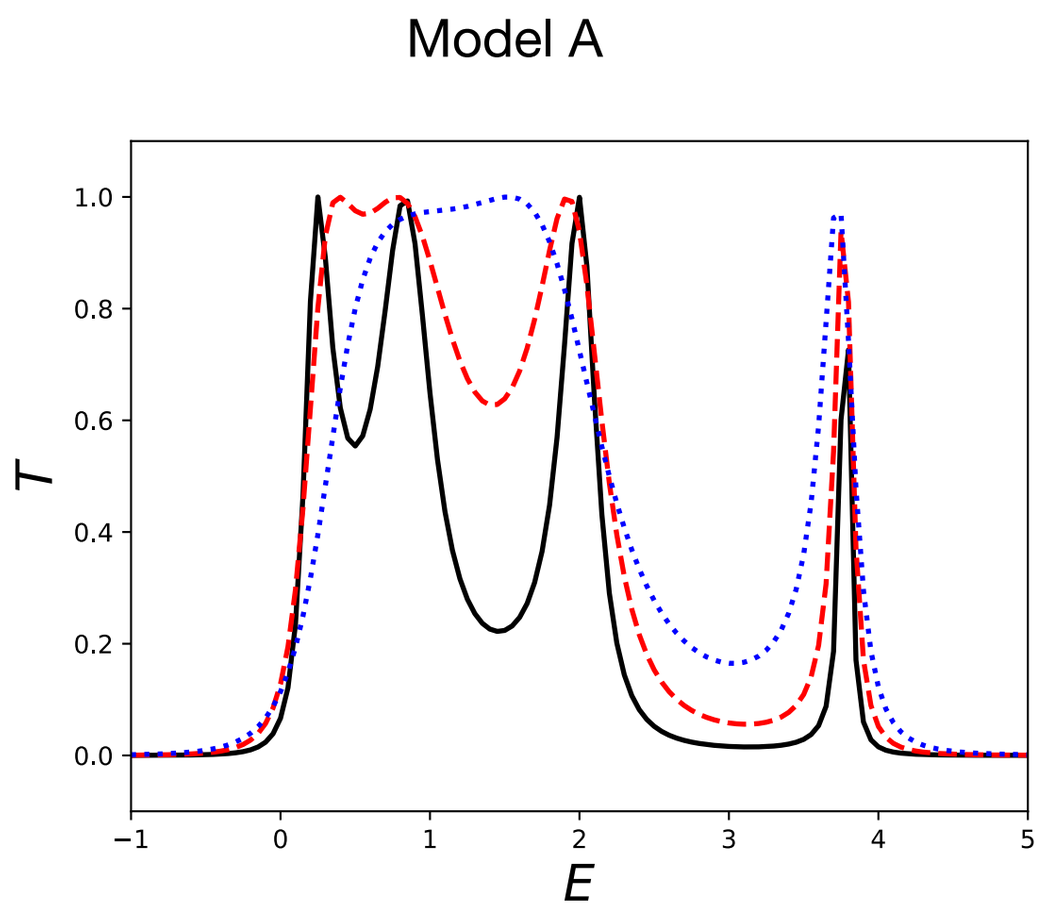
Black: 4-state model $\langle n|n+1\rangle = 0.29$

Red: 7-state model $\langle n|n+1\rangle = 0.73$

Model A

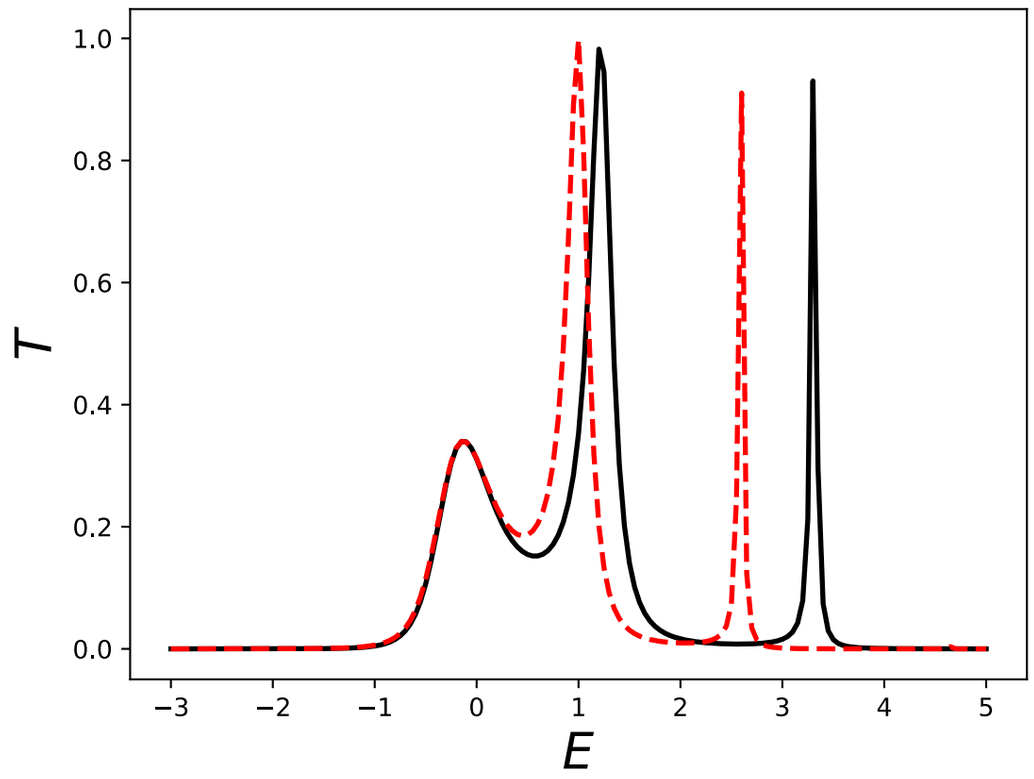


Here the 7-state model is reduced to 4 states by the usual singular value decomposition of the overlap matrix.

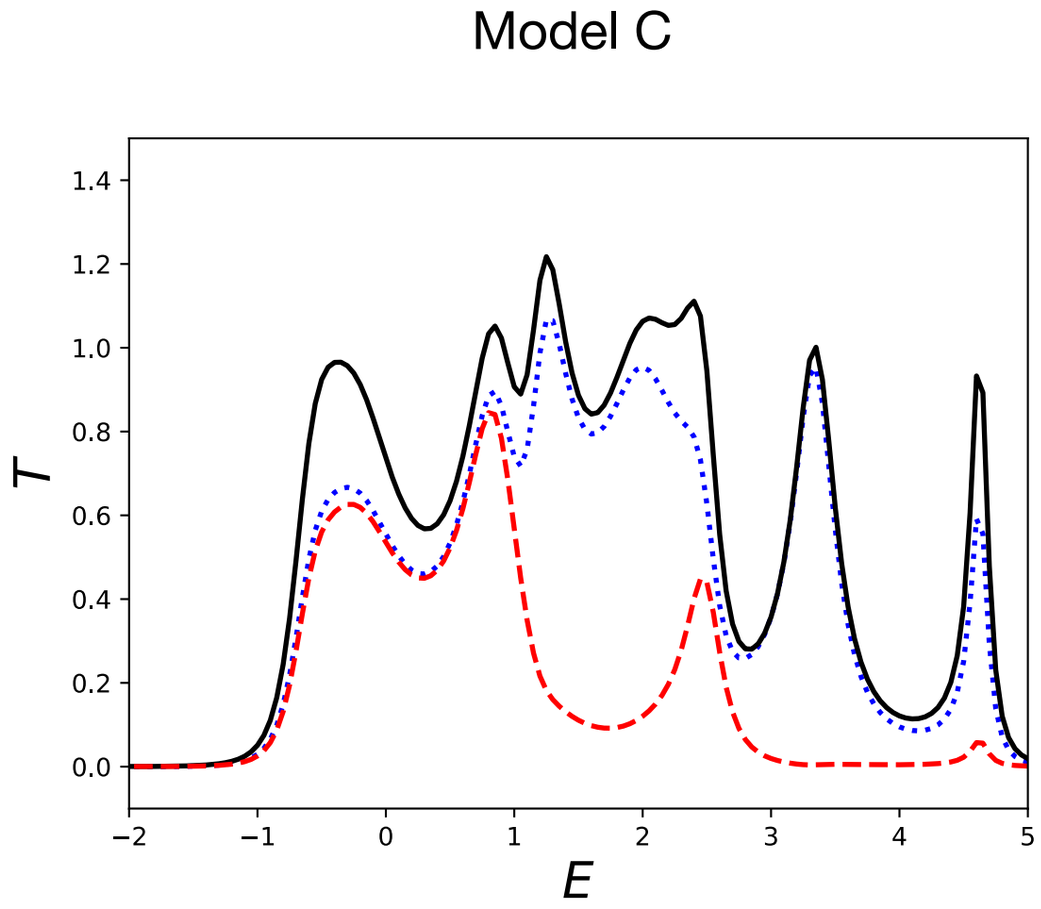


Variation with the strength of the absorptive potential

Model B



Parabolic barrier



Two coupled diabetic barriers—
red: lowest adiabatic barrier
blue: two adiabatic channels
black: all possible paths

TABLE I. Integrated channel properties of the models discussed in the text. The model labels refer to the subsections in Sec. IV where they were discussed. The subscript refers to the dimension of the GCM space. The average energy $\langle E \rangle$ is computed with respect to the Hamiltonian at the midpoint of the q interval omitting the zero-point energy E_K. In case C, the energy is the adiabatic one computed by diagonalizing the 2×2 matrix mixing the two GCM states. The row marked C_8^a ignores the coupling between the adiabatic channels.

Model	I_T	$\langle E \rangle / E_K$	$\sigma(E/E_K)$
A_4	1.69	1.17	0.81
A_7	1.65	1.11	0.77
B_4	0.61	0.80	0.84
B_7	0.56	0.60	0.67
C_8	3.12	1.28	1.15
C_8^a	2.54	1.31	1.09

Take-away messages

—No need for fine GCM meshes

—transition state channels have a limited bandwidth

—Bandwidth is controlled by the zero-point energy of the GCM configurations

Some questions

Do we want to understand mechanisms using schematic interactions or calculate numbers with realistic interactions?

How a large a configuration space do we need to calculate fission branching ratios?

Do the energy fluctuations in the cross sections carry useful information?

$$\frac{k^2}{2Nm} < \frac{E_{zp}}{2}$$