

Transition-state dynamics in complex quantum systems

Kouichi Hagino (Kyoto U.)

George F. Bertsch (U. of Washington)



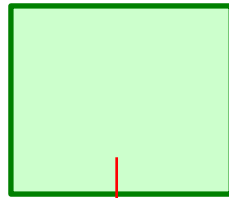
1. Introduction
2. 2-GOE model for a decay problem
3. Transition-state theory and the insensitive properties
4. Fluctuations: a deviation from the PT distribution
5. Summary

G.F. Bertsch and K. Hagino, arXiv:2105.12073 [quant-ph]

K. Hagino and G.F. Bertsch, arXiv:2106.152501 [quant-ph]

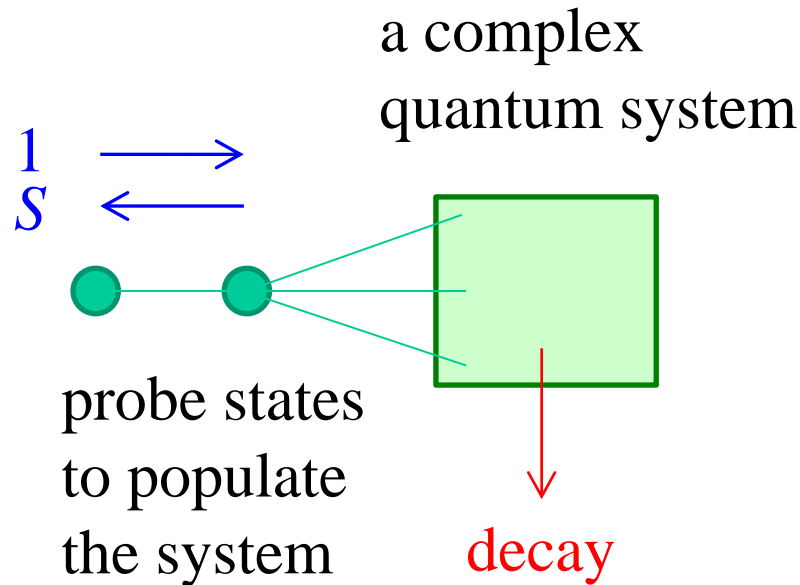
Introduction: decay of a complex quantum system

a complex
quantum system



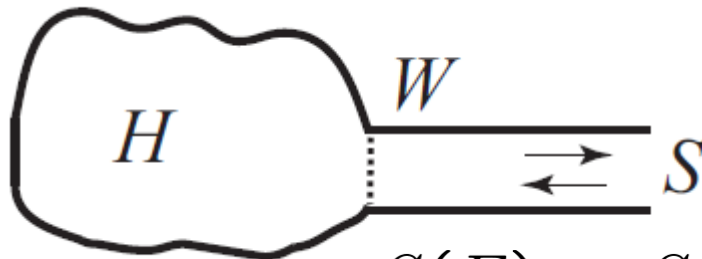
decay

Introduction: decay of a complex quantum system



$$T(E) = 1 - |S(E)|^2$$

Fyodorov's talk on Wednesday

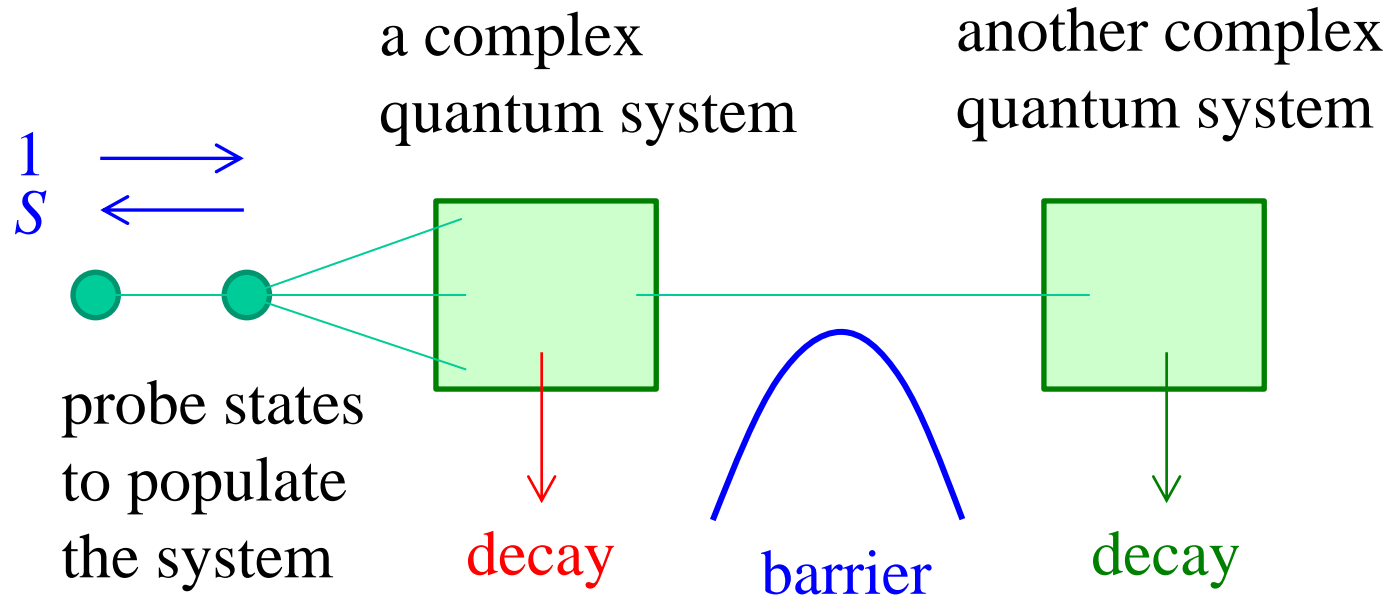


$$S(E) \rightarrow S(E + i\eta)$$

also:

Y.V. Fyodorov, D.V. Savin,
and H.-J. Sommers,
J. Phys. A38, 10731 (2005)

Introduction: decay of a complex quantum system



$$T(E) = 1 - |S(E)|^2$$

Fyodorov's talk on Wednesday

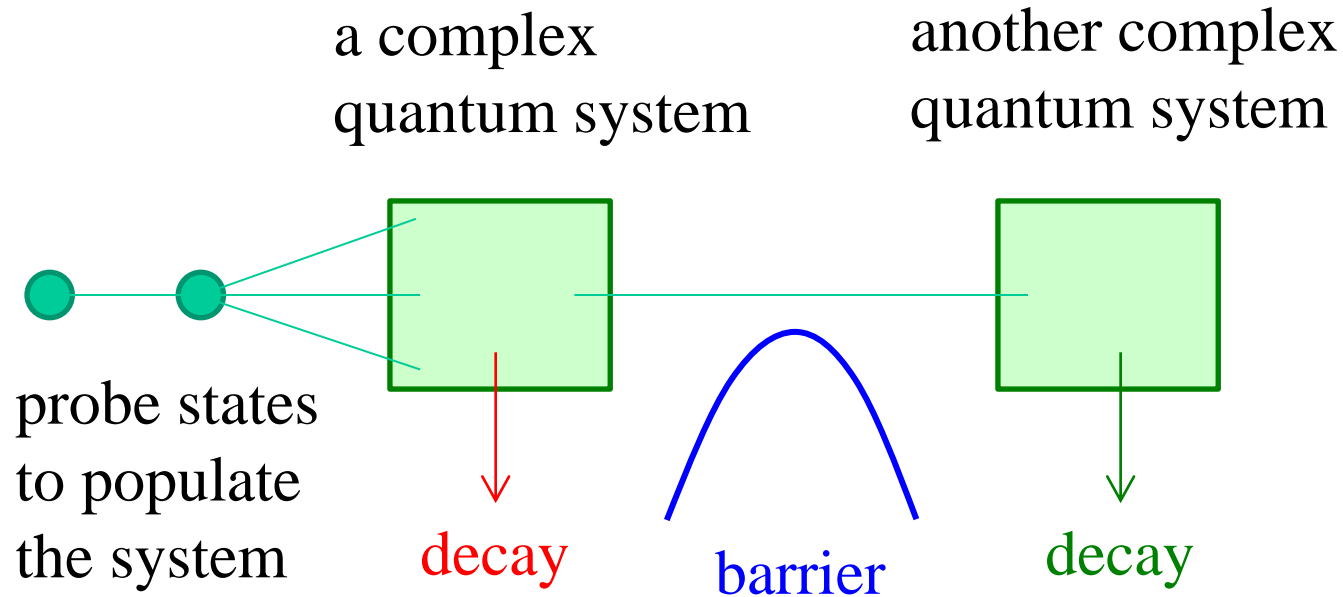


$$S(E) \rightarrow S(E + i\eta)$$

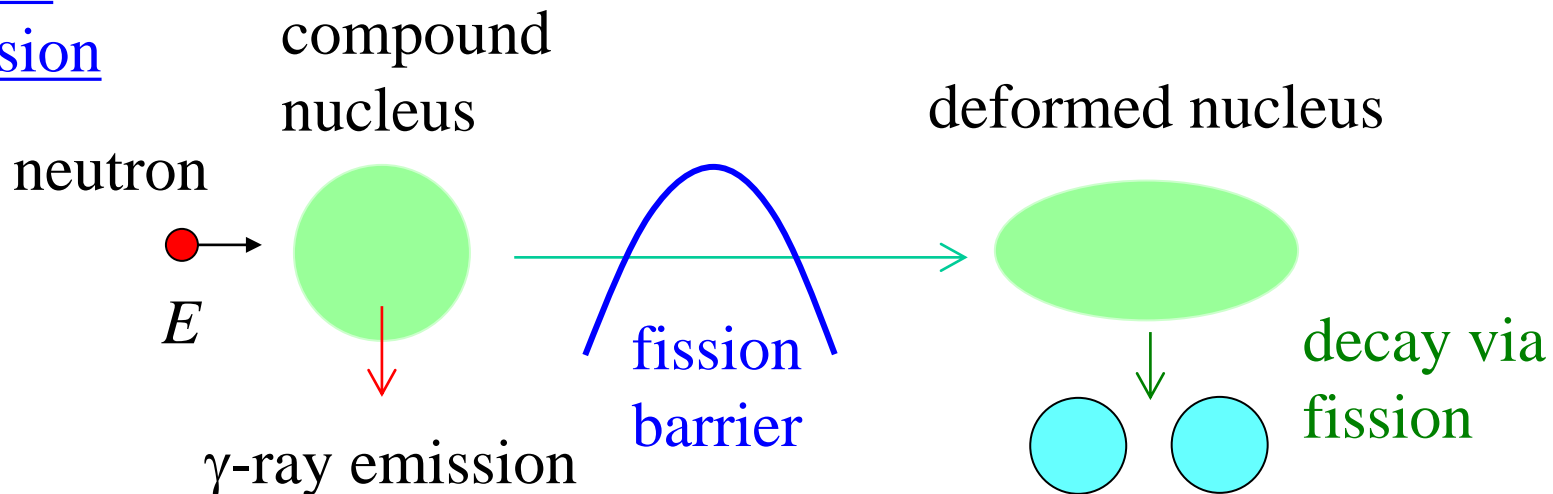
also:

Y.V. Fyodorov, D.V. Savin,
and H.-J. Sommers,
J. Phys. A38, 10731 (2005)

Introduction: decay of a complex quantum system

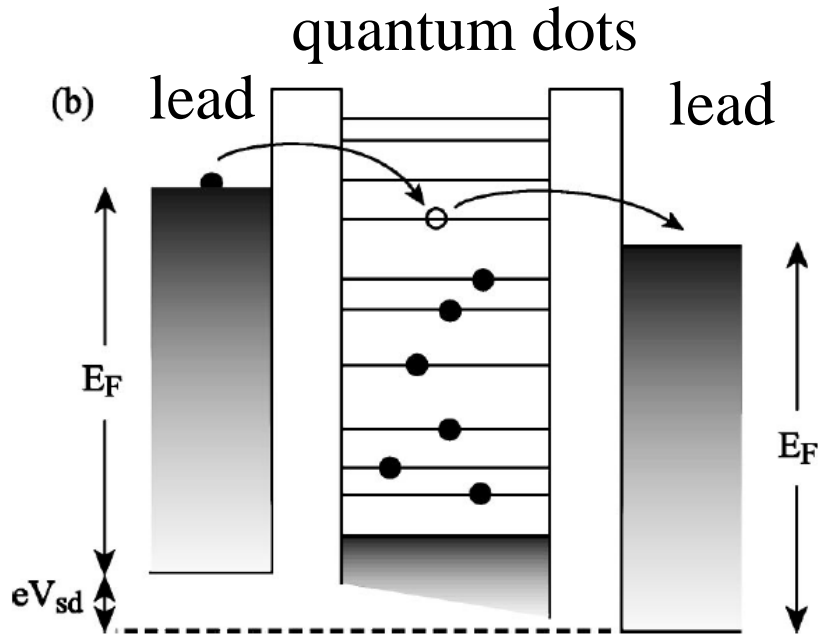


an example:
nuclear fission

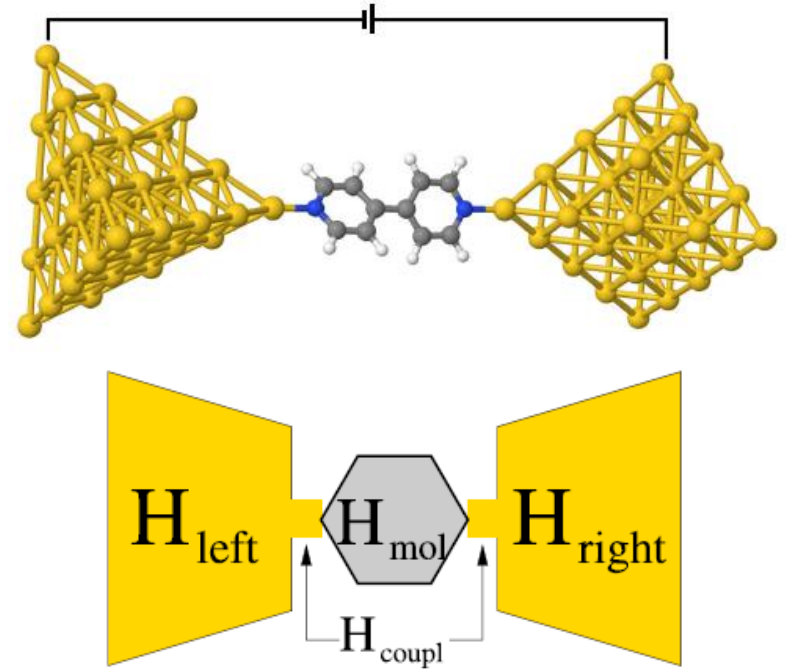


other examples: the problem of electron transport

tunnel junction



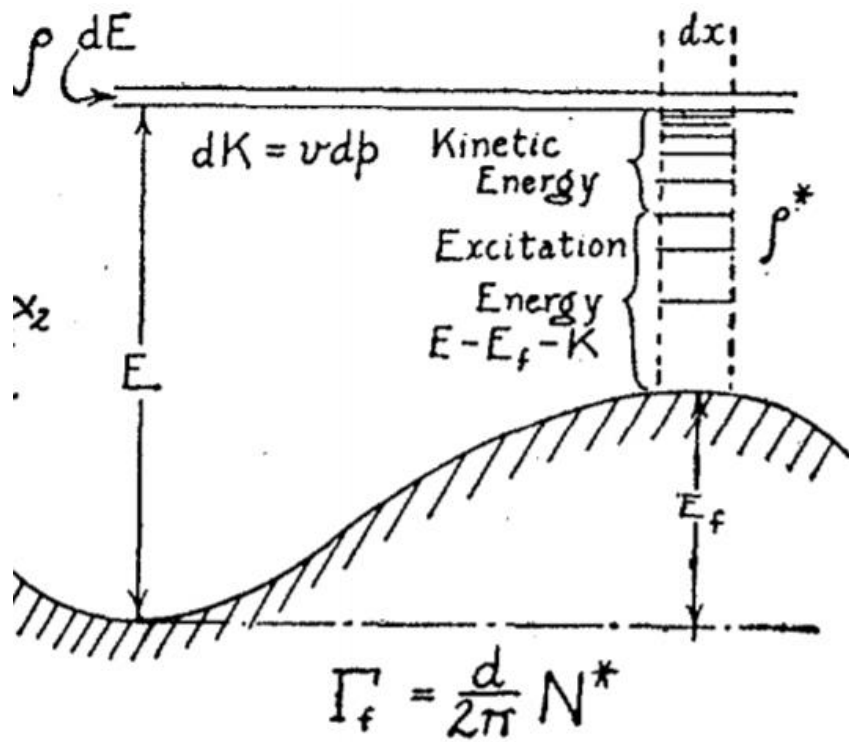
molecular bridge



Y. Alhassid,
Rev. Mod. Phys. 72, 895 (2000)

M. Thoss and F. Evers,
JCP148, 030901 (2018)

the transition state theory



N. Bohr and J.A. Wheeler,
Phys. Rev. 56, 426 (1939)

cf. RKKM theory
in chemistry

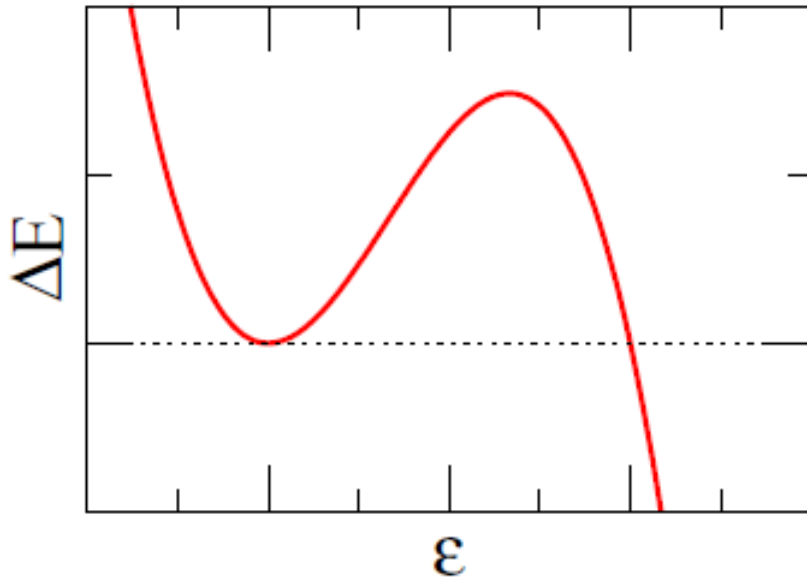
tunneling probability

cf. D.M. Brink and U. Smilansky,
Nucl. Phys. A405 ('83) 301

$$\Gamma_f = \frac{1}{2\pi \rho_{gs}(E^*)} \int_0^{E^* - B_f} \rho_{sd}(E^* - B_f - K) dK \rightarrow \frac{1}{2\pi \rho_{gs}(E^*)} \sum_c T_c$$

- ✓ decay dynamics: entirely determined at the saddle
- ✓ does not depend on what will happen after the barrier

the transition state theory



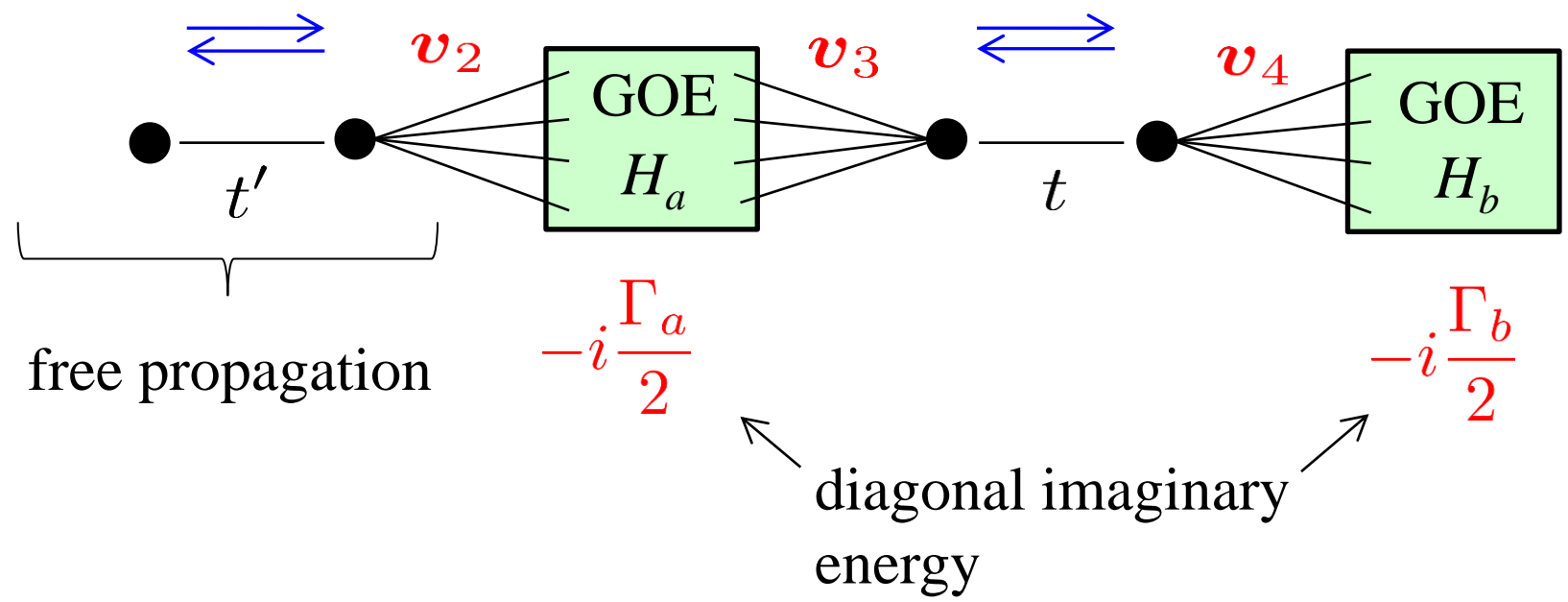
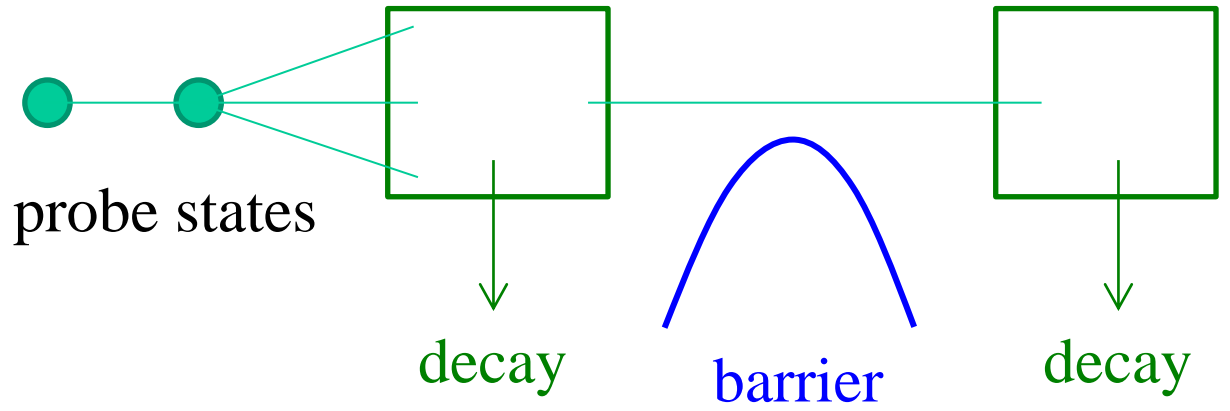
$$\Gamma_f = \frac{1}{2\pi\rho_{\text{gs}}(E^*)} \sum_c T_c$$

- ✓ decay dynamics: the saddle only
- ✓ the insensitivity property

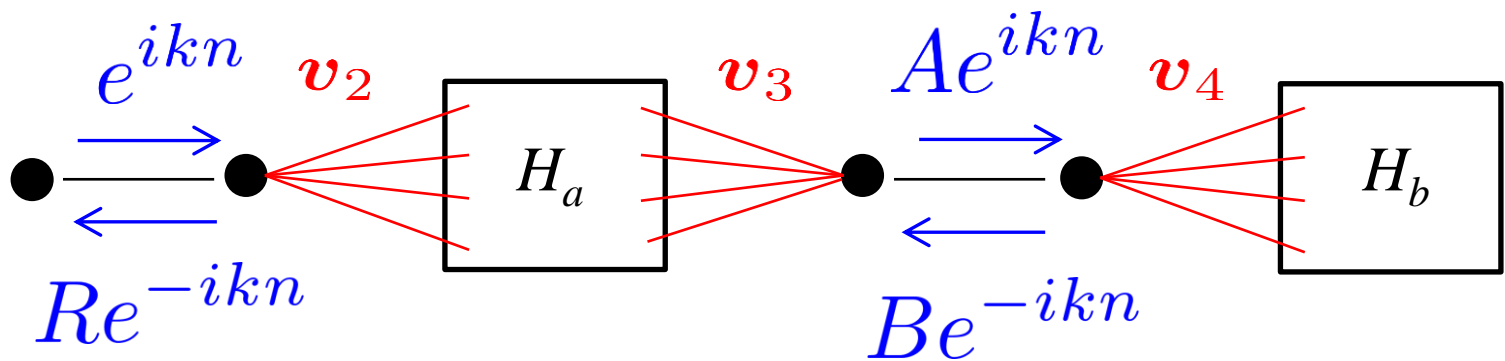
a question which we ask:

Can one derive the properties of the transition state theory based on a *microscopic* many-body Hamiltonian?

2 GOE Model



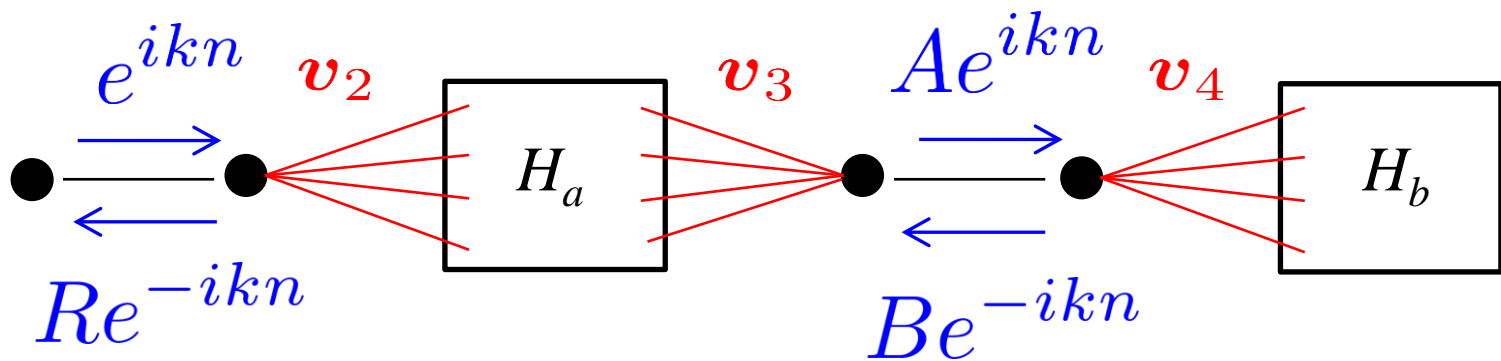
v_k ($k = 2, 3, 4$): random interactions



$$T(E) = T_a(E) + T_b(E) = 1 - |R(E)|^2$$

$$T_a(E) = 1 - |R(E)|^2 - |A(E)|^2 + |B(E)|^2$$

$$T_b(E) = |A(E)|^2 - |B(E)|^2$$



$$T(E) = T_a(E) + T_b(E) = 1 - |R(E)|^2$$

$$T_a(E) = 1 - |R(E)|^2 - |A(E)|^2 + |B(E)|^2$$

$$T_b(E) = |A(E)|^2 - |B(E)|^2$$

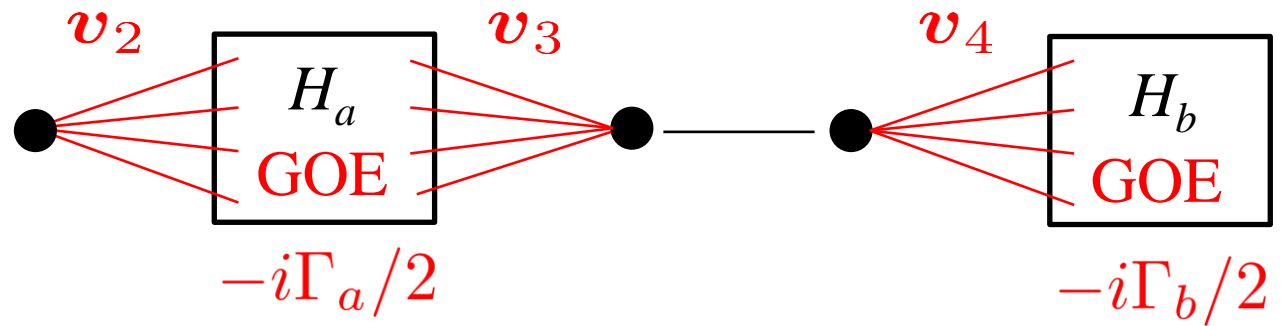
branching ratio:

$$Br = \frac{\int dE T_b(E)}{\int dE T_a(E)}$$

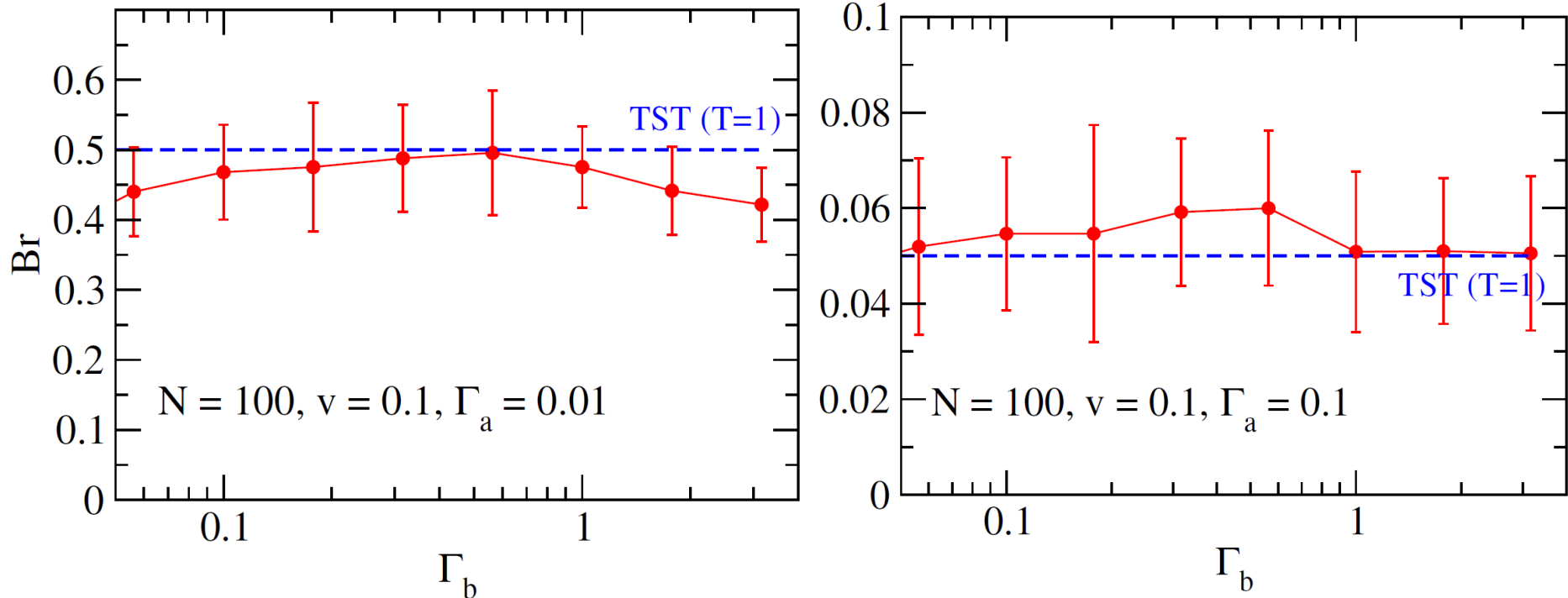
the relative decay probability from b:

$$P_b(E) = \frac{T_b(E)}{T(E)}$$

branching ratios



the average and the variance with 20 ensembles



Branching ratios: **insensitive** to Γ_b ← the main assumption of the TST

*also with analytical study with Stieltjes transform

fluctuations of decay rates

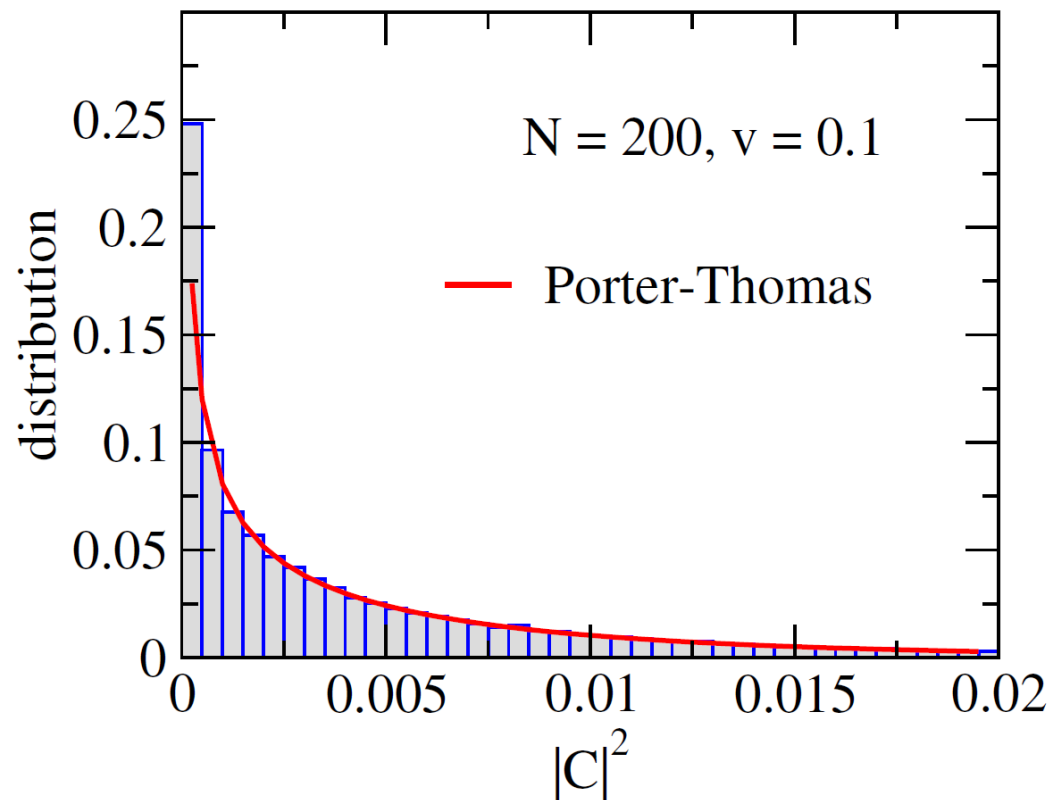
a common *belief*: a fluctuation of decay rates follows the Porter-Thomas distribution

$$\psi_i = \sum_k C_k^{(i)} |k\rangle$$

$$P(y) = \frac{1}{\sqrt{2\pi y}} e^{-y/2}$$

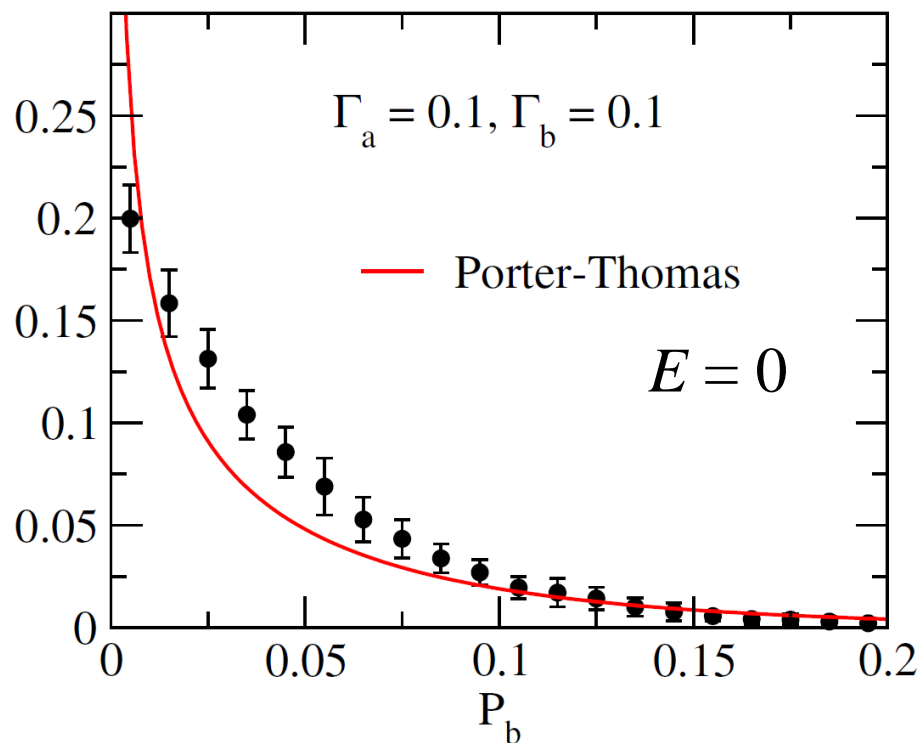
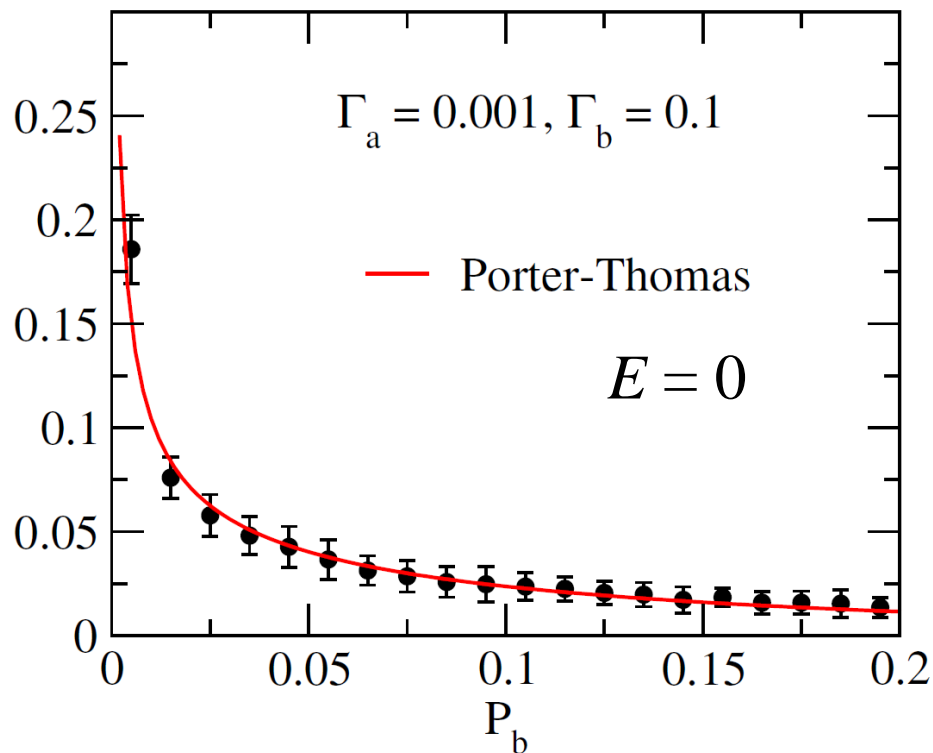
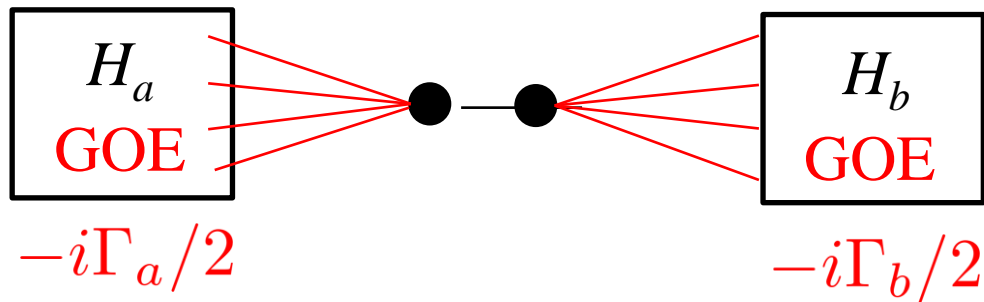
$$y = |C_k^{(i)}|^2 / \langle |C_k^{(i)}|^2 \rangle$$

a distribution of wf amplitudes in GOE



fluctuations of decay rates

$$P_b(E) = \frac{T_b(E)}{T(E)}$$



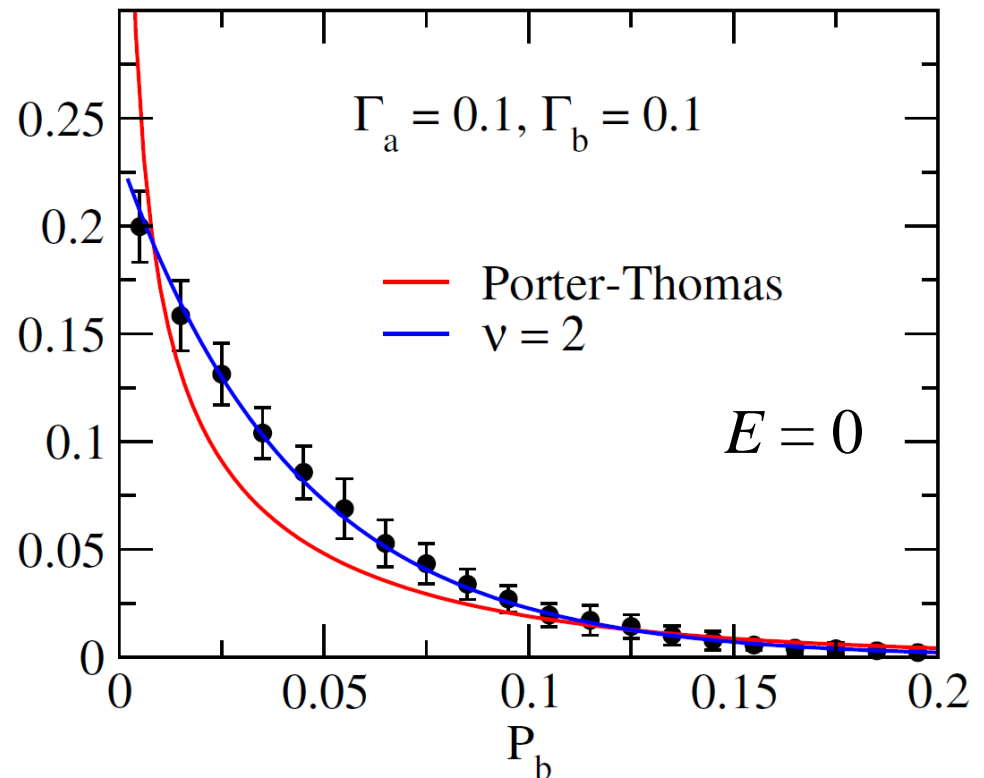
PT: reasonably good,
but with a significant deviation

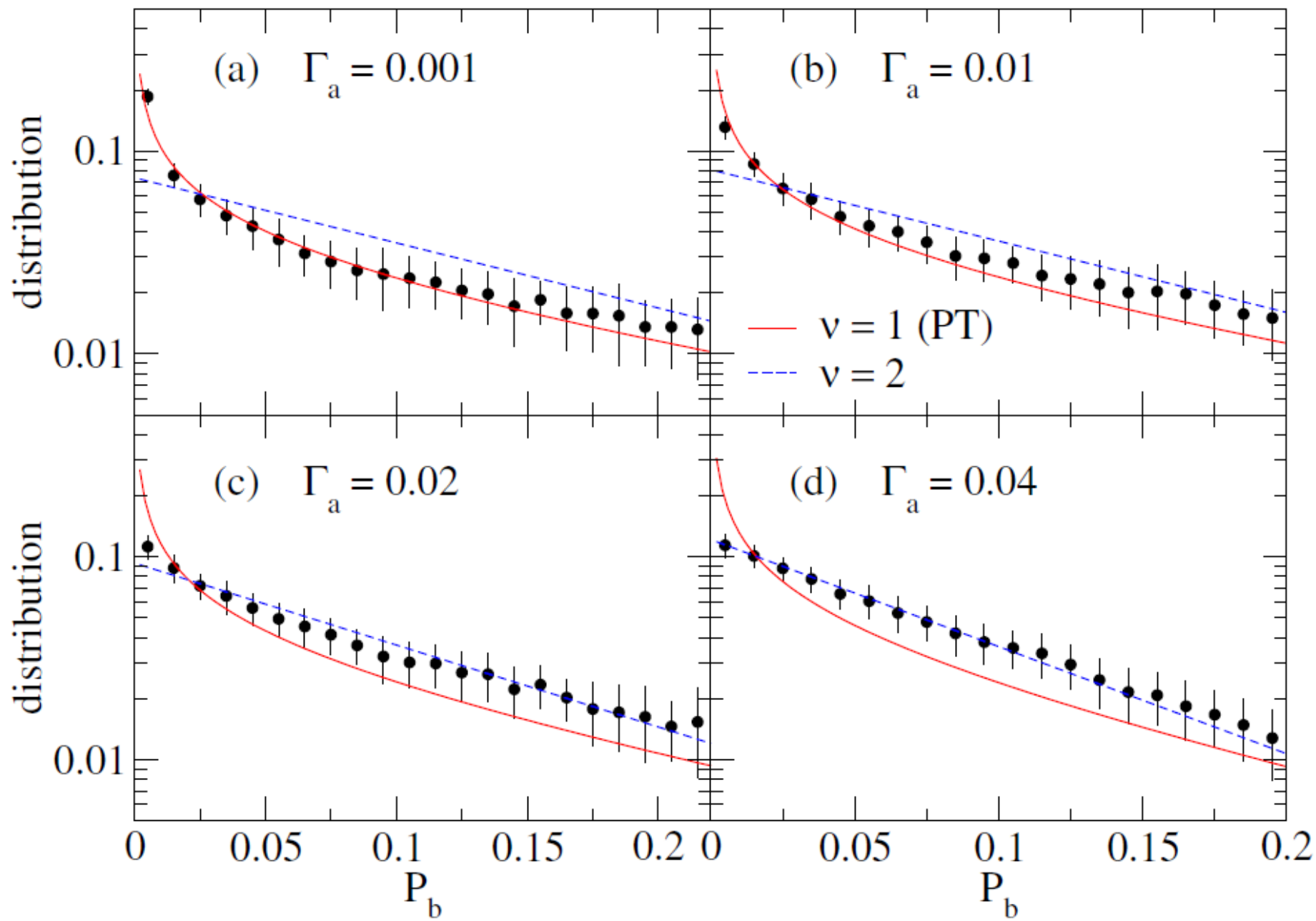
fluctuations of decay rates

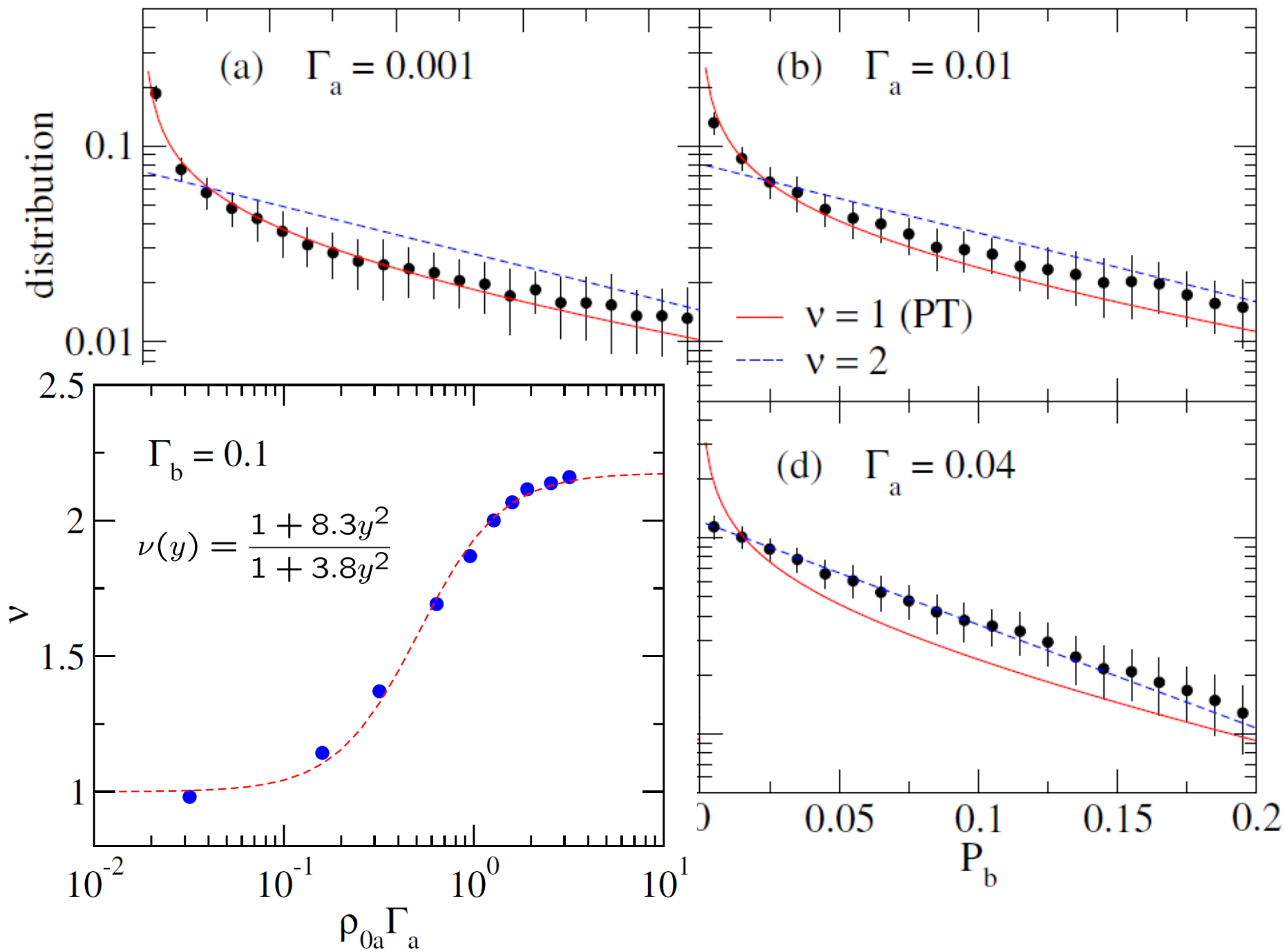
$$P_\nu(x) = \frac{\nu}{2x_0\Gamma(\nu/2)} \left(\frac{\nu x}{2x_0}\right)^{\nu/2-1} e^{-\nu x/2x_0}$$

ν = the number of d.o.f.
($\nu=1$ for PT)

cf. GUE: $\nu=2$

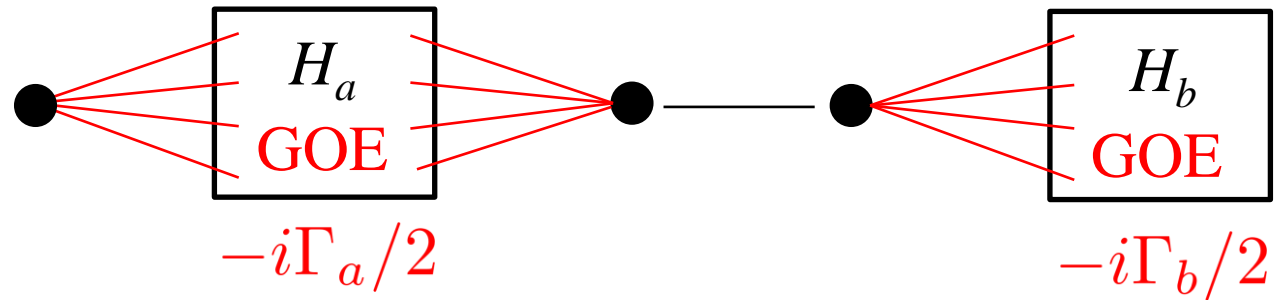






Summary

2-GOE model for a decay of quantum complex systems



✓ decay rates: insensitive to Γ_b
→ the first microscopic realization of the transition-state theory

✓ fluctuations of the decay rates:
a transition from the Porter-Thomas to the $\nu=2$ distribution

the boundary condition can make the distribution deviate from the PT

G.F. Bertsch and K. Hagino, arXiv:2105.12073, JPSJ in press.
K. Hagino and G.F. Bertsch, arXiv:2106.152501 [quant-ph]

➤ ongoing works

applications to nuclear fission: CI approach