Remarks on Reaction Theory

G.F. Bertsch
University of Washington

FRIB-TA meeting, April 19, 2023

0.
1. Compound-nucleus reactions
2. S-matrix in the configuration-interaction (CI) framework
3. DFT or Hamiltonians or both?
4. The most challenging problem in reaction theory
(for nonrelativistic fermions).

1. Compound-nucleus reactions

—All you need are optical potentials—when it works.

—We saw the need for reliable CN predictions in this workshop (Eg. Grzywacs).

—CN connection to (1+2)-body Hamiltonians is weak.

Rule of thumb: require $\rho\overline{|\langle i|v|j\rangle|} > 1$

See also Phys. Lett. **148B** 5 (1984):

GAUSSIAN DISTRIBUTIONS OF SHELL-MODEL EIGENVECTOR COMPONENTS

B.A. BROWN
Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824, USA

and

G. BERTSCH
Cyclotron Laboratory and Physics Department, Michigan State University, East Lansing, MI 48824, USA

Received 28 June 1984

The distribution of basis-vector amplitudes in realistic sd shell-model eigenfunctions has been calculated and compared with the gaussian distribution expected from the theory of random matrices. The states in the region of high level density show the expected behavior. The largest deviations from gaussian are found for the states at the ends of the spectrum where the level density is low compared to the off-diagonal hamiltonian matrix elements. It is essential to use basis vectors with good J and T rather than M-scheme vectors in order to obtain a gaussian distribution.

—Goal: a global theory of $\rho\overline{|\langle i|v|j\rangle}$ at (A,E,J) based on realistic 2B interactions.

2. Reaction theory in the configuration-interaction (CI) framework.

—The S-matrix is more fundamental than the R-matrix.

—The S-matrix may be calculated by linear algebra from the Hamiltonian matrix of the internal states together with the matrices of reduced widths of those states coupled to the external channels. The formulas (omitting direction reactions):

$$|S_{a,b}|^2 = \mathrm{tr}(\Gamma_a G \Gamma_b G^*)$$

$$G = \left(H - i \sum_k \Gamma_k/2 - E \right)^{-1}$$

—The formalism might be applied to large-amplitude shapes by making use of reference configurations calculated in DFT and in the presence of constraining fields (GCM). The resulting non-orthogonal CI bases is a minor complication.

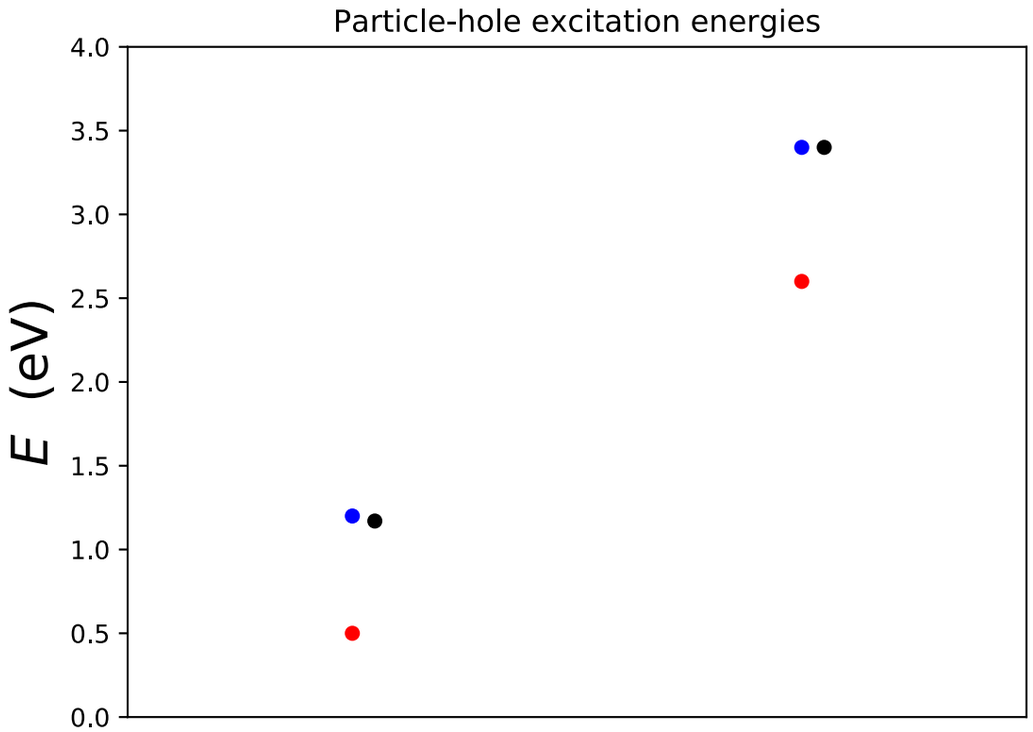
—E-dependent fluctuations are easy to extract in this formulation.

3. DFT or Hamiltonians or both?

—For computational reasons DFT is the method of choice for global surveys.

—The CI methodology requires a Hamiltonian.

—A compromise: use DFT to construct a space of orbitals and calculate the matrix elements with a Hamiltonian. Seems promising from the experience in condensed matter physics (D. Sangelli et al., Phys. Rev. B **94** 195205 (2016).



4. The challenging problem: nuclear fission at barrier-top energies

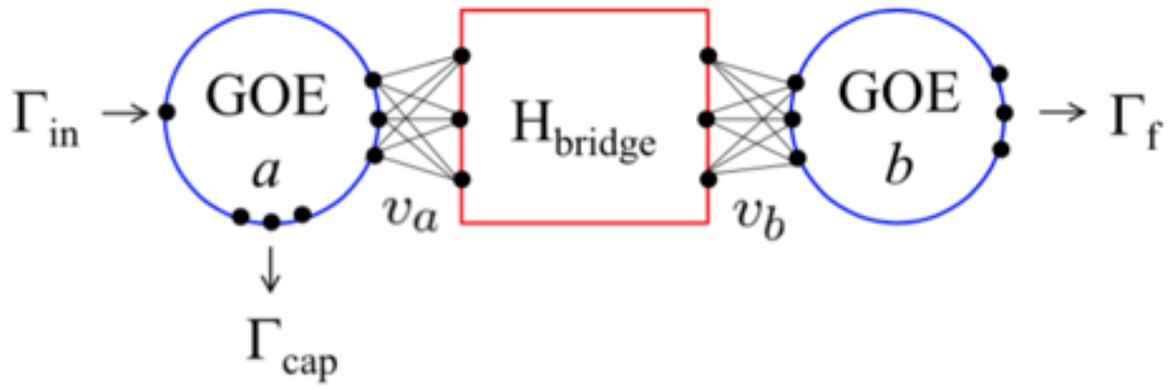
—TDDFT doesn't allow barrier penetration

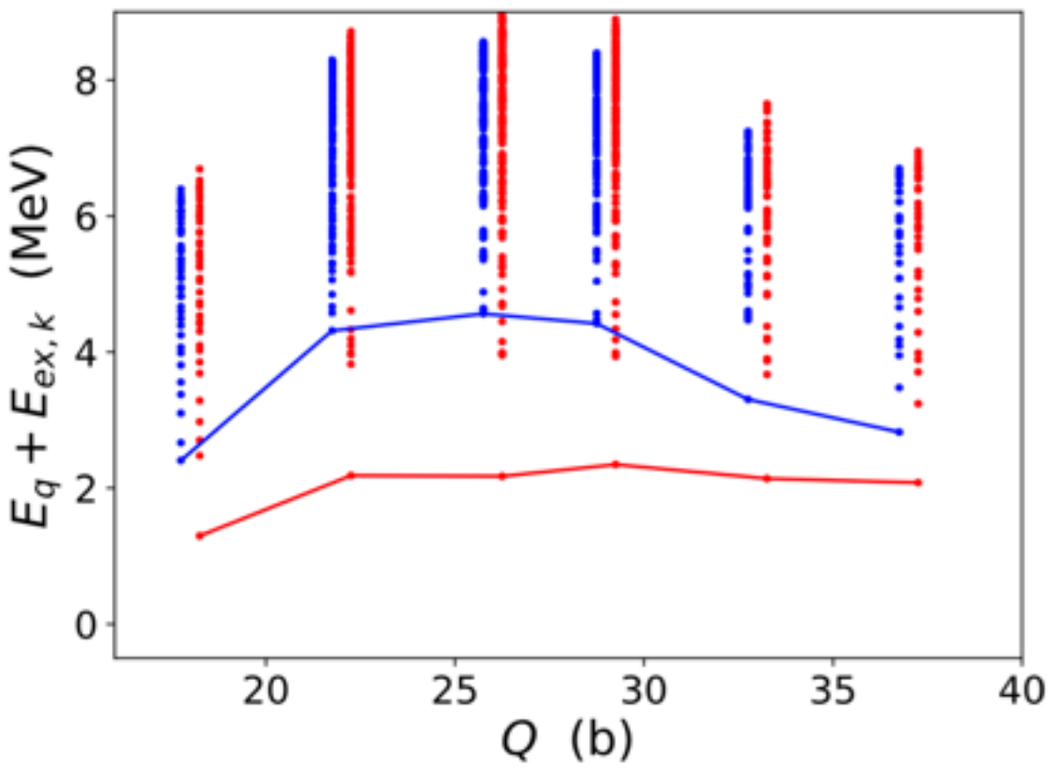
—GCM mapping to Schroedinger eq. doesn't allow diffusive dynamics.

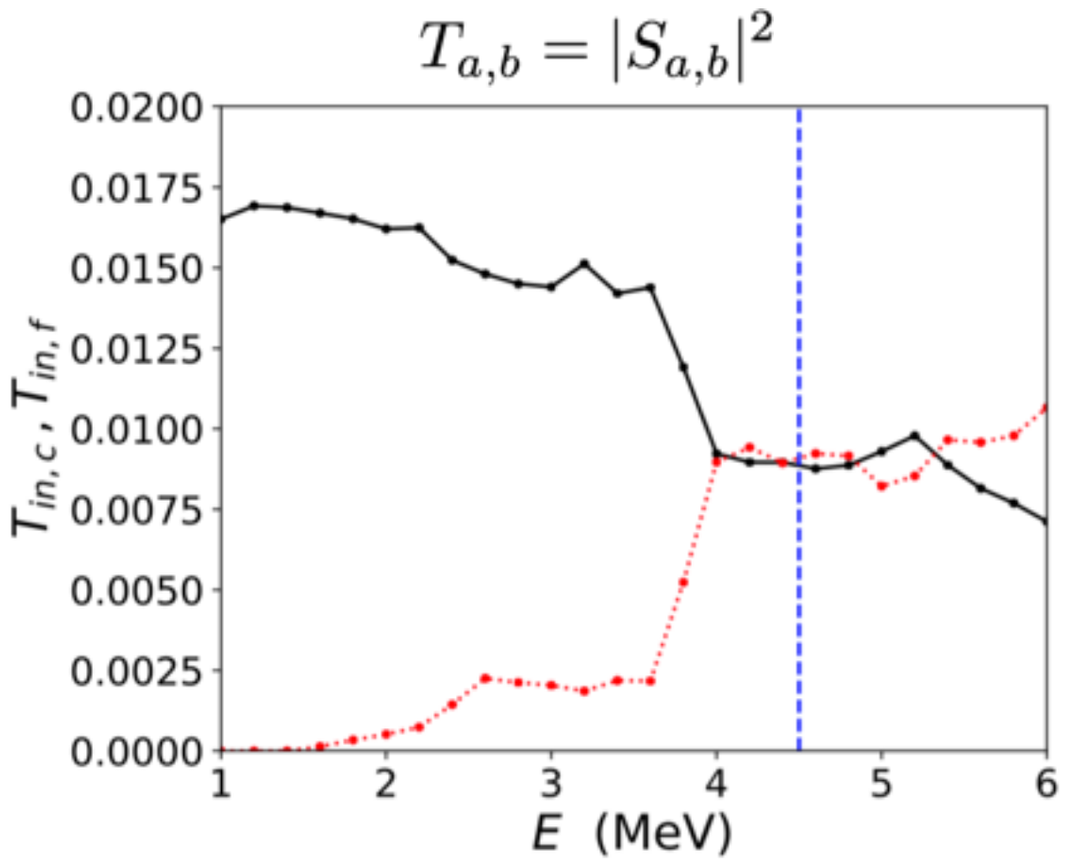
—What can one learn from the S-matrix/CI approach with limited computational resources?

Modeling fission dynamics at the barrier in a discrete-basis formalism

G. F. Bertsch [1] and K. Hagino [2]







Preliminary findings

1. Transmission coefficients are insensitive to fission exit widths
2. No dominating transition states
3. Moderate sensitivity to pairing interaction strengths

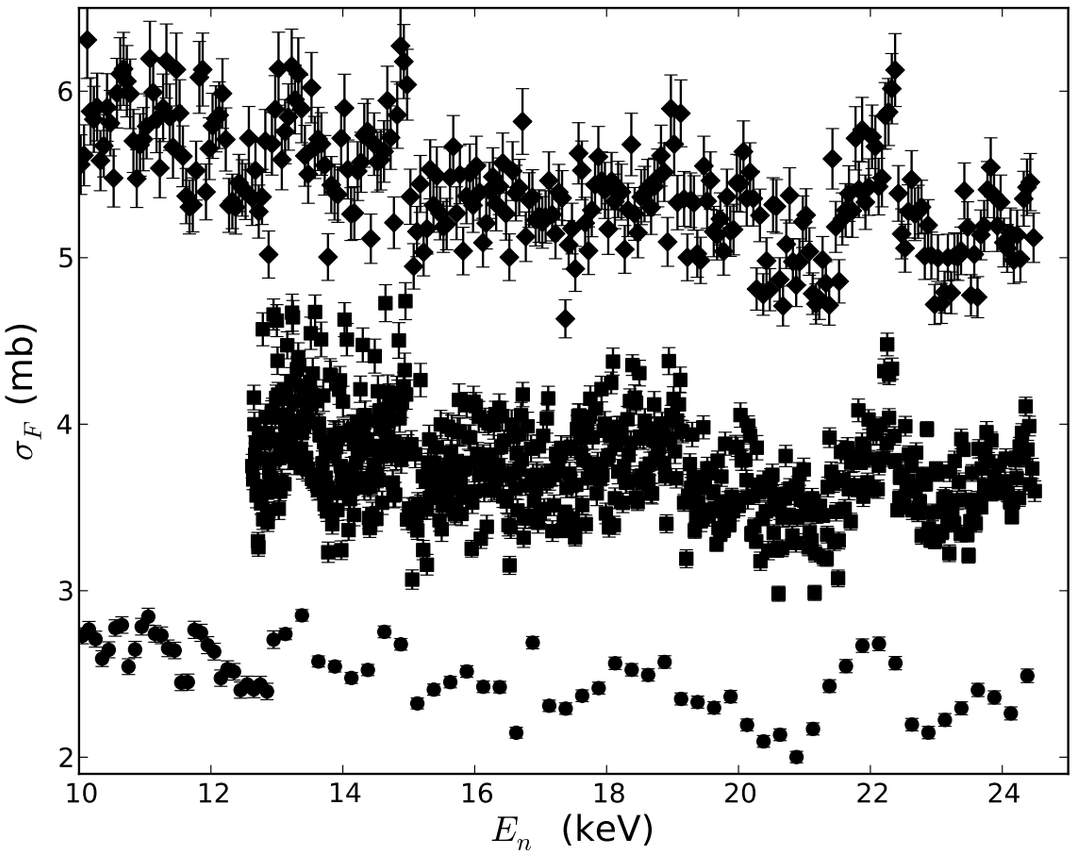
Caveats

1. Coupling of CN states to bridge states not yet anchored to a (1+2)-body Hamiltonian.
2. GCM requires a Gaussian overlap approximation.
3. Methodology needs to be validated with respect to other reaction theory methods.

My original motivation: are there fission-channel resonances above the barriers?

Some provocative data:

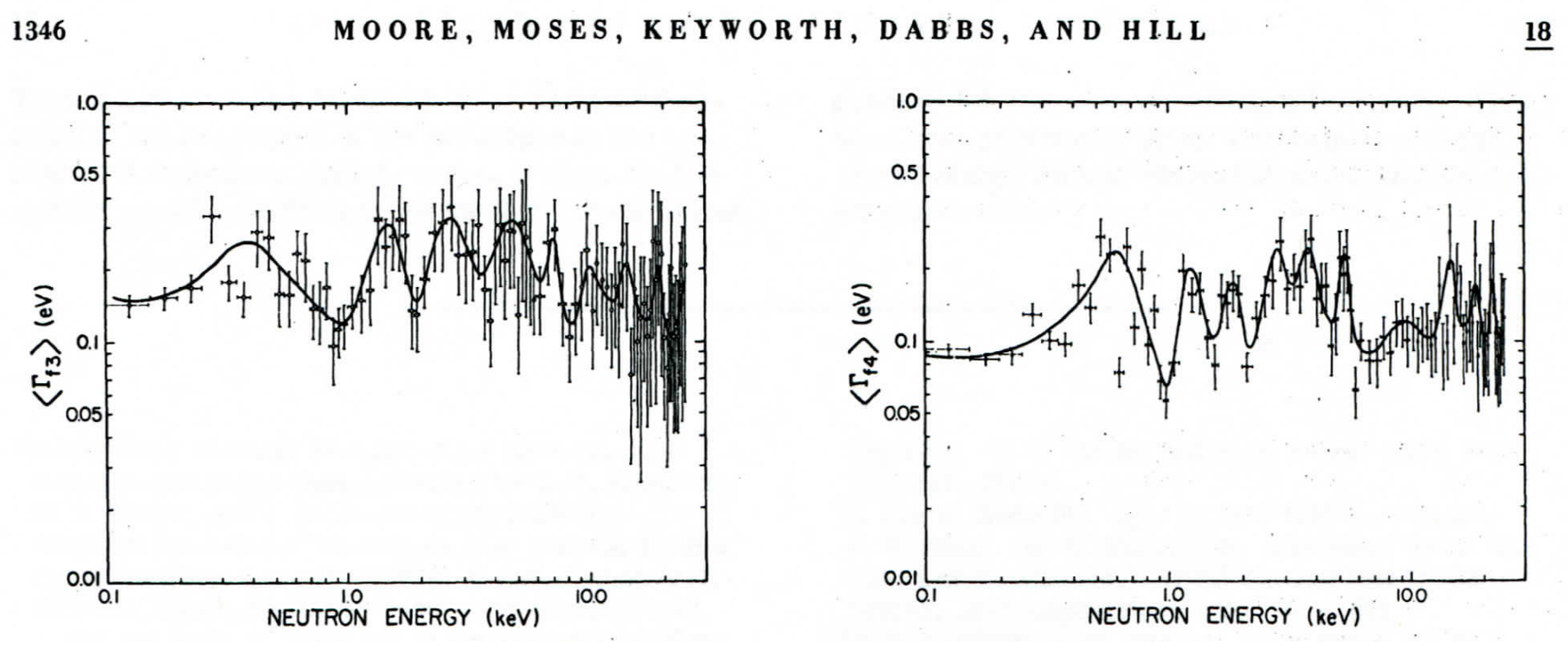
^{235}U(n,f)



Perez, et al. (1971)

Bowman, et al. (1971)

Moore, et al. (1971)



DFT in quantum chemistry and condensed matter

TABLE I: Atomization energies of selected molecules

	Li_2	C_2H_2	20 simple molecules (mean absolute error)
Experimental	1.04 eV	17.6 eV	-
Theoretical errors:			
Hartree-Fock	-0.94	-4.9	3.1
LDA	-0.05	2.4	1.4
GGA	-0.2	0.4	0.35
τ	-0.05	-0.2	0.13

Perdue, et al., PRL 77 (1996)

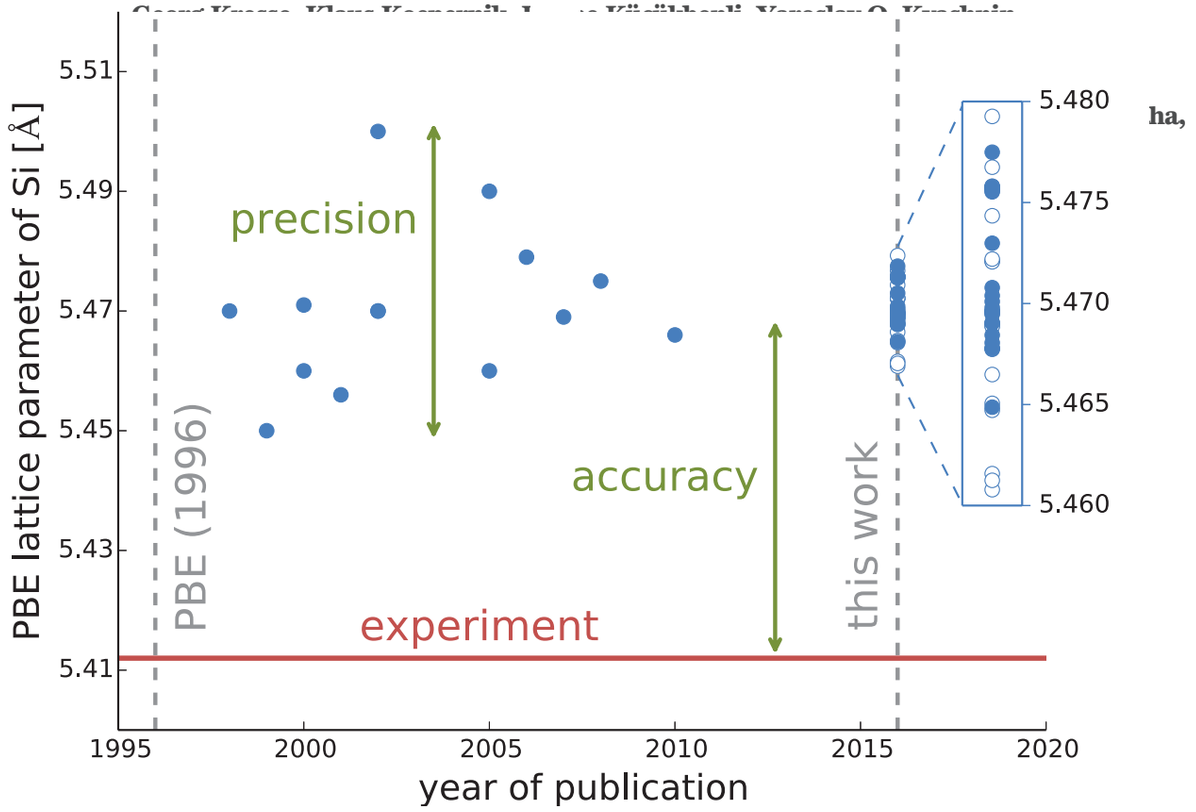
Science **351** 1415 (2016)

RESEARCH ARTICLE SUMMARY

DFT METHODS

Reproducibility in density functional theory calculations of solids

Kurt Lejaeghere,* Gustav Bihlmayer, Torbjörn Björkman, Peter Blaha, Stefan Blügel, Volker Blum, Damien Caliste, Ivano E. Castelli, Stewart J. Clark, Andrea Dal Corso, Stefano de Gironcoli, Thierry Deutsch, John Kay Dewhurst, Igor Di Marco, Claudia Draxl, Marcin Dułak, Olle Eriksson, José A. Flores-Livas, Kevin F. Garrity, Luigi Genovese, Paolo Giannozzi, Matteo Giantomassi, Stefan Goedecker, Xavier Gonze, Oscar Grånäs, E. K. U. Gross, Andris Gulans, François Gygi, D. R. Hamann, Phil J. Hasnip, N. A. W. Holzwarth, Diana Iuşan, Dominik B. Jochym, François Jollet, Daniel Jones,



Dynamics from scattering theory

Key concept is the channel and its transmission coefficient *T.*

In mesoscopic physics, the Landauer formula for quantized conductance:

$$G(E_f) = \frac{1}{R} = \frac{e^2}{2\pi\hbar} \sum_i T_i(E_f)$$

$$T(E) \approx \Theta(E - E_0)$$

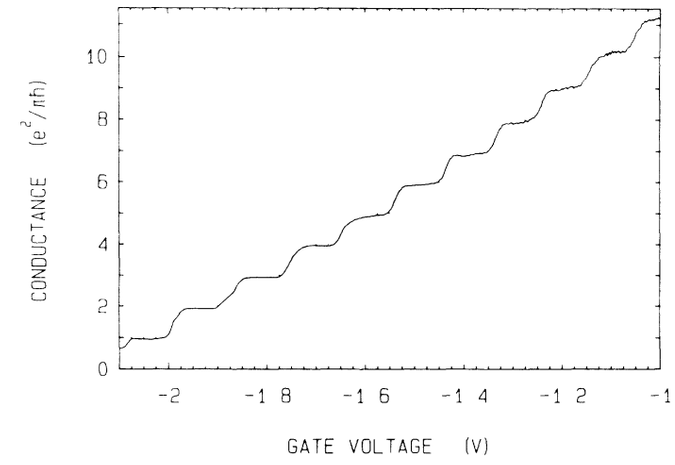


FIG. 2. Point-contact conductance as a function of gate voltage, obtained from the data of Fig. 1 after subtraction of the lead resistance. The conductance shows plateaus at multiples of $e^2/\pi\hbar$.

Same physics is in the original formula for fission decay rates:

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

Bohr and Wheeler (1939)