Fission Cross Section Theory

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How to get the most out of these lectures

- See previous lectures from FIESTA2014, in particular J. E. Lynn's slides and notes on fission cross-section theory
- Difficult to absorb material during lecture
  - At your leisure, go through slides and pretend you're teaching
  - Work through the examples (especially the 1D problems)
  - Play with the codes (I will talk about a couple)
- Reaction theory and fission cross-section modeling is a <u>vast</u> topic
  - These slides will not cover everything!
  - Notes will contain references and suggestions for further reading

Outline

- Compound nucleus reaction theory
  - From resonances to Hauser-Feshbach cross-section theory
- Fission in the transition state model
  - A fission model for the Hauser-Feshbach formula
- Practical applications
  - A cross-section code, and some thoughts about evaluations and uncertainty quantification
- Future outlook
  - Cross sections starting from protons, neutrons, and their interactions

- Appendix (I will not have time to go through this)
  - Scattering theory

COMPOUND NUCLEUS REACTION THEORY

Reminder: scattering theory

- **From Schrödinger equation to resonances (see appendix)**
- **State with decay lifetime τ has an energy spectrum (instead of definite E)**

$$\mathrm{Prob}\,(E) = \frac{N_0}{(E - E_r)^2 + \frac{1}{4}\left(\frac{\hbar}{\tau}\right)^2}, \qquad \frac{\hbar}{\tau} \equiv \Gamma = \mathrm{width}$$

- **Absorption cross section for partial wave with angular momentum ℓ,**

$$\sigma_\ell = \frac{2\pi}{k^2}(2\ell + 1)\underbrace{\left(1 - \eta_\ell^2\right)}_{=T_\ell}$$

- **Transmission probability T_ℓ is related to width Γ and level spacing d,**

$$T_\ell = 2\pi\frac{\Gamma}{d}$$

Compound nucleus cross section

- For one resonance, we already showed:

$$\sigma_\ell = \frac{\pi}{k^2}(2\ell+1)\underbrace{\left(1-|\eta_\ell|^2\right)}_{=T_\ell}$$

- Cross section for making a compound state:

$$\sigma_{CN} = \sigma_\ell \times \mathrm{Prob}\,(E) = \sigma_\ell \frac{N_0}{(E-E_r)^2 + \left(\frac{\Gamma}{2}\right)^2}$$

- Get N_0 from normalization condition:

Level density

$$\int_{E_r-\Delta E/2}^{E_r+\Delta E/2} dE\, \frac{N_0}{(E-E_r)^2 + \frac{\Gamma^2}{4}} \rho(E) = 1, \quad \rho(E) \approx \frac{1}{d}$$

$$\sigma_{CN} = \frac{2\pi}{k^2}(2\ell+1)\frac{\Gamma_\alpha \Gamma}{(E-E_r)^2 + \left(\frac{\Gamma}{2}\right)^2}$$

Compound nucleus cross section: the Bohr hypothesis

- So far, for one open channel a + A → C (or C → a + A) with $\alpha \equiv$ a + A

$$\sigma_{CN} = \frac{\pi}{k^2}(2\ell+1)\frac{\Gamma_\alpha \Gamma}{(E-E_r)^2 + \left(\frac{\Gamma}{2}\right)^2}$$

- At higher E, more channels open up, then:

$$\text{total decay rate} \equiv \frac{1}{\tau} = \sum_\alpha \frac{1}{\tau_\alpha}$$
$$\Rightarrow \Gamma = \sum_\alpha \Gamma_\alpha$$

$$\frac{\Gamma_\beta}{\Gamma} = \text{Prob. decay into } \beta$$

- Bohr hypothesis: reaction proceeds in two independent steps:

$$\underbrace{a+A}_{\alpha} \to C \to \underbrace{b+B}_{\beta}$$

$$\sigma_{\alpha\beta} = \sigma_{CN} \times \frac{\Gamma_\beta}{\Gamma} = \frac{2\pi}{k^2}(2\ell+1)\frac{\Gamma_\alpha \Gamma_\beta}{(E-E_r)^2 + \left(\frac{\Gamma_\alpha+\Gamma_\beta}{2}\right)^2}$$

Hauser-Feshbach theory

- Caveat: Bohr hypothesis should not violate conservation laws (energy, angular momentum, parity)!
- More general form for a + A $\rightarrow$ C $\rightarrow$ b + B:
  - Include statistical spin factor to account for random orientation of beam and target nuclei

$$\sigma_{\alpha\beta}(E, J_C) = \frac{\pi}{k^2} \frac{(2J_C+1)}{(2j_a+1)(2J_A+1)} \sum_n \frac{\Gamma_\alpha^{(n)} \Gamma_\beta^{(n)}}{(E-E_n)^2 + \left(\frac{\Gamma^{(n)}}{2}\right)^2}$$

  - Note sum over compound states *n* with energy ≈ *E* and total spin J_C

Next: develop theory for energy-averaged cross sections (= Hauser-Feshbach theory)

Hauser-Feshbach theory

- **Average out individual resonances (integral over ΔE ≈ integral over ±∞):**

$$\int_{-\infty}^{+\infty} dE \, \frac{\Gamma_\alpha^{(n)}\Gamma_\beta^{(n)}}{(E-E_n)^2 + \left(\frac{\Gamma^{(n)}}{2}\right)^2} = 2\pi \frac{\Gamma_\alpha^{(n)}\Gamma_\beta^{(n)}}{\Gamma^{(n)}}$$

- **Average out the sum over resonances by going to continuous limit:**

$$\frac{1}{\Delta E}\sum_n \frac{\Gamma_\alpha^{(n)}\Gamma_\beta^{(n)}}{\Gamma^{(n)}} \approx \frac{1}{\Delta E}\frac{1}{d}\int_{E-\Delta E/2}^{E+\Delta E/2} dE \, \frac{\Gamma_\alpha(E)\,\Gamma_\beta(E)}{\Gamma(E)} = \frac{1}{d}\left\langle \frac{\Gamma_\alpha(E)\,\Gamma_\beta(E)}{\Gamma(E)} \right\rangle$$

- **Average cross section:**

$$\langle \sigma_{\alpha\beta}(E, J_C) \rangle = \frac{\pi}{k^2}\frac{(2J_C+1)}{(2j_a+1)(2J_A+1)}\frac{2\pi}{d}\left\langle \frac{\Gamma_\alpha(E)\,\Gamma_\beta(E)}{\Gamma(E)} \right\rangle$$

Width fluctuation correction

- Much more useful to write in terms of average widths:

$$\left\langle \frac{\Gamma_\alpha(E)\,\Gamma_\beta(E)}{\Gamma(E)} \right\rangle \equiv W_{\alpha\beta} \frac{\langle\Gamma_\alpha(E)\rangle\,\langle\Gamma_\beta(E)\rangle}{\langle\Gamma(E)\rangle}$$

  - $W_{\alpha\beta}$ = width fluctuation correction factor
  - If we can describe widths by probability distributions, then we can calculate $W_{\alpha\beta}$ explicitly

- Remember that

$$T_\mu = 2\pi \frac{\langle\Gamma_\mu\rangle}{d}$$

- Therefore:

$$\langle\sigma_{\alpha\beta}(E, J_C)\rangle = \frac{\pi}{k^2} \frac{(2J_C+1)}{(2j_a+1)(2J_A+1)} W_{\alpha\beta} \frac{T_\alpha T_\beta}{\sum_\mu T_\mu}$$

One more step: in practice we don't observe J_C (or the parity Π_C)

The Hauser-Feshbach cross section

- The full formula (Hauser-Feshbach with width fluctuation):

$$\sigma_{\alpha\beta}^{\mathrm{HF}}(E) = \frac{\pi}{k^2} \sum_{J_C \Pi_C} \frac{2J_C+1}{(2j_a+1)(2J_A+1)} \sum_{j_\alpha} \sum_{n_\beta} \sum_{j_\beta} W_{\alpha\beta} \frac{T_\alpha T_\beta}{\sum_\mu \sum_{n_\mu} \sum_{j_\mu} T_\mu}$$

Sum over spin couplings in entrance channel

Sum over energetically allowed exit channels

Sum over spin couplings in exit channel

- For simplicity, we will assume $W_{\alpha\beta} = 1$
  - Then we can sum over entrance (α) and exit (β) channels separately!

All that's left to do is calculate the transmission coefficients!

The neutron channel

Sums over all spin and parity couplings

Parity selection rule

$$\sum_{n_\beta}\sum_{j_\beta} T_\beta = \sum_{\ell=0}^{\infty}\ \sum_{j=\left|\ell-\frac{1}{2}\right|}^{\ell+\frac{1}{2}}\ \sum_{I=|J_C-j|}^{J_C+j}\ \sum_{\pi_j} \delta_{\Pi_C\pi_I,(-1)^\ell} \times \int_0^{E_x-S_n} d\varepsilon\, T_{\ell j}\left(E_x-S_n-\varepsilon\right)\rho\left(\varepsilon, I, \pi_I\right)$$

Integral over neutron kinetic energies

From optical model

Level density

The gamma channel

Sums over radiation character + all spin and parity couplings

Parity selection rule

$$\sum_{n_\beta}\sum_{j_\beta} T_\beta = \sum_{X=E,M}\sum_{L=0}^{\infty}\sum_{J'=|J_C-L|}^{J_C+L}\sum_{\pi'}\delta_{\Pi_C\pi',\pi_{XL}} \times \int_0^{E_x} d\varepsilon_\gamma\, f_{XL}(\varepsilon_\gamma)\,\rho\left(E_x-\varepsilon_\gamma, J', \pi'\right)$$

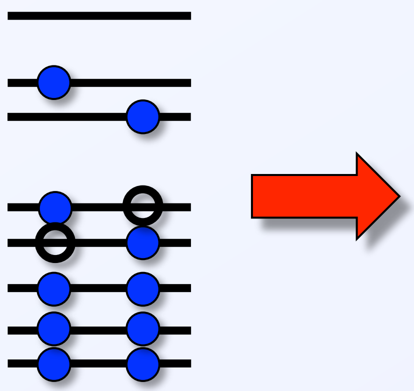
Integral over photon energies

Strength function, from model

Level density

The elephant in the room: level densities

- We have used $\rho(E) \sim 1/d$
  - Ok over small energy range, but not realistic otherwise
  - Dependence on E, J, π?
- Fundamentally, this is a counting problem:



$$E = \sum_i \left(\varepsilon_p^{(i)} - \varepsilon_h^{(i)} \right)$$

  - Loop through all proton and neutron multi-particle-multi-hole configs
  - Calculate E, J, π and store
  - Count levels in each energy bin with given J and $\pi \Rightarrow \rho(E,J,\pi)$

Hard to do without truncations and/or approximations (also ignores residual interactions, like pairing)

Counting energy states: Laplace transform trick

- We want density of states of given particle number A and energy E:

$$\rho(A,E) = \sum_n \sum_i \delta(A-n)\,\delta(E-E_{n,i})$$

$$A = \sum_\nu n_\nu, \quad E_{n,i} = \sum_\nu n_\nu \varepsilon_\nu$$

Huge number of terms!

Energy of mp-mh state

Sums over s.p. states

- Take Laplace transform → partition function

$$Z(\alpha,\beta) = \mathcal{L}\{\rho(A,E)\} = \sum_n \sum_i e^{\alpha A - \beta E_{n,i}}$$

Still a huge number of terms!

- Factorize sum into product over s.p. states

$$Z(\alpha,\beta) = \prod_{\nu=1}^{s} \left(1 + e^{\alpha - \beta\varepsilon_\nu}\right)$$

few terms!

- Invert Laplace transform (numerically or by saddle-point approximation)
- Can also include pairing by redefining *n* and $E_{n,i}$ sums over quasiparticles

Counting states: try this at home

- **Alternate counting method: using Fourier transform**

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Combinatorial level densities by the real-time method☆

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- **Short python code at end of paper, or:**
  - http://www.int.washington.edu/users/bertsch/computer.html
  - **Click on "Real-time method for level densities"**

Level density phenomenological models

- Gilbert and Cameron formulation (1965)
  - At low E, finite temperature model

$$\rho(E) = e^{(E-E_0)/T}$$

  - At high E, backshifted Fermi gas model

$$\rho(E) = \frac{1}{\sqrt{2\pi}\sigma(E)} \frac{\sqrt{\pi}}{12} \frac{\exp\left[2\sqrt{a(E-\Delta)}\right]}{a(E-\Delta)^{3/2}}$$

  - Level density parameter *a* can be given E dependence

Shell correction

$$a(U) = \tilde{a}\left[1 + \frac{\delta W}{U}\left(1 - e^{-\gamma U}\right)\right], \quad U = E - \Delta$$

Asymptotic value

Damping factor

Constrainted by matching the two parts, low-lying levels, and level spacing at neutron separation energy

Level density: angular momentum and parity dependence

- Typically, we assume

$$\rho(E, J, \pi) = \rho(E) P(E, J) P(E, \pi) K(E)$$

- Using statistical arguments:

$$P(E, J) = \frac{2J+1}{2\sqrt{2\pi}\sigma^3(U)} \exp\left[-\frac{(J+1/2)^2}{2\sigma^2(U)}\right]$$

$$U = E - \Delta$$
$$\Delta = \text{pairing gap parameter}$$

- Often, we make the simple assumption

$$P(E, \pi) = \frac{1}{2}$$

- *K*(*E*) = collective enhancement factor
  - Additional levels from collective vibrations and rotations of nucleus

Angular momentum distribution of levels

Random orientations of nucleon spins + central limit theorem:

$$\rho(E,K) = \rho(E) \times \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{K^2}{2\sigma^2}\right)$$

Pairing + temperature occupation probabilities for levels:

$$f_k = \frac{1}{1+e^{\beta E_k}}, \quad \beta = \frac{1}{T}, \; E_k = \sqrt{(\varepsilon_k - \lambda)^2 + \Delta^2}$$

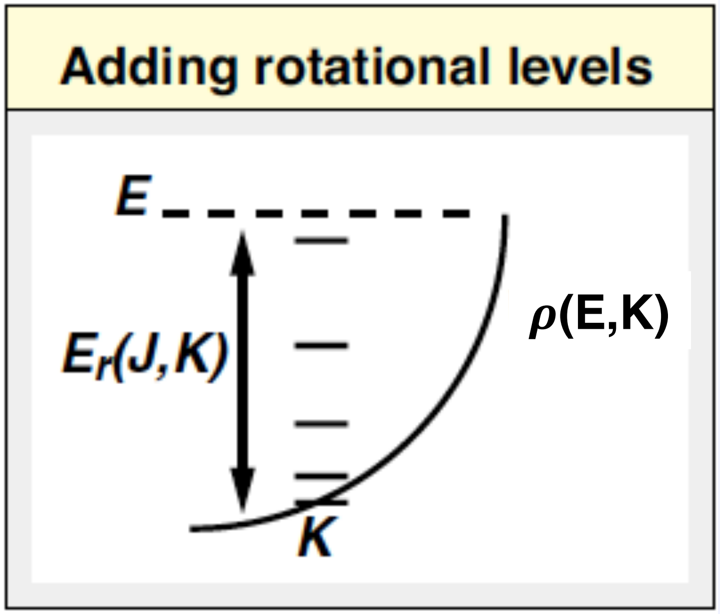
Energy dependence of spin cutoff parameter σ^2:

$$\sigma^2 = 2\sum_{k>0} \sigma_k^2$$

$$\sigma_k^2 = \langle m_k^2 \rangle - \langle m_k \rangle^2 = m_k^2 f_k - (m_k f_k)^2$$

$$\sigma^2 = \frac{1}{2} \sum_{q=n,p} \sum_{k>0} \left(m_k^{(q)}\right)^2 \operatorname{sech}^2\left(\frac{\beta E_k}{2}\right)$$

Rotational enhancement



$$\rho_{\rm rot}\left(E,J\right)=\sum_{K=-J}^{J}\rho\left(E-E_{\rm rot}\left(J,K\right),K\right)$$

$$\rho\left(E,K\right)=\rho\left(E\right)\times\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{K^2}{2\sigma^2}\right)$$

$$E_{\rm rot}\left(J,K\right)=\frac{\hbar^2}{2\mathfrak{J}_\perp}\left[J\left(J+1\right)-K^2\right]$$

Making Taylor expansion in energy

$$\rho\left(E+\delta E\right)\approx\rho\left(E\right)\exp\left(\beta\delta E\right)$$

$$\beta=\frac{1}{T}\equiv\frac{d}{dx}\ln\rho\left(x\right)\Big|_{x=E}$$

Rotational enhancement (continued)

$$\rho_{\mathrm{rot}}(E,J) = \frac{\rho(E)}{\sqrt{2\pi}\sigma} \exp\left[-\frac{J(J+1)}{2\sigma_\perp^2}\right] \sum_{K=-J}^{J} \exp\left(-\frac{K^2}{2\sigma_{\mathrm{eff}}^2}\right)$$

$$\sigma_\perp^2 = \frac{\mathfrak{I}_\perp}{\hbar^2\beta}, \quad \sigma_{\mathrm{eff}}^2 = \left(\frac{1}{\sigma^2} - \frac{1}{\sigma_\perp^2}\right)^{-1}$$

Energy dependence of spin cutoff parameter $\sigma_\perp{}^2$:

B&M vol 2, Eq. (4.128)

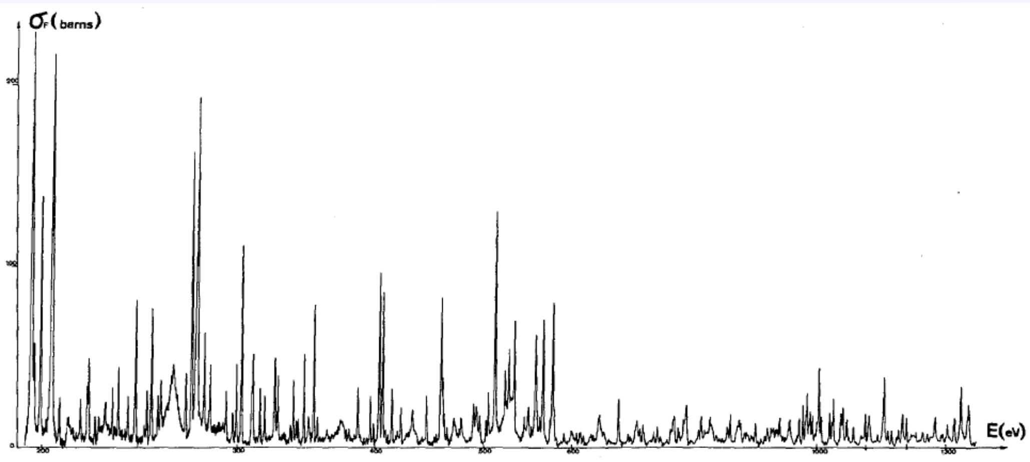
$$\mathfrak{I}_\perp = \mathfrak{I}_{\mathrm{rigid}}\left[1 - g\left(\frac{\hbar\omega_{\mathrm{sh}}\delta}{2\Delta}\right)\right]$$

$$g(x) = \frac{\ln\left(x + \sqrt{1+x^2}\right)}{x\sqrt{1+x^2}}$$

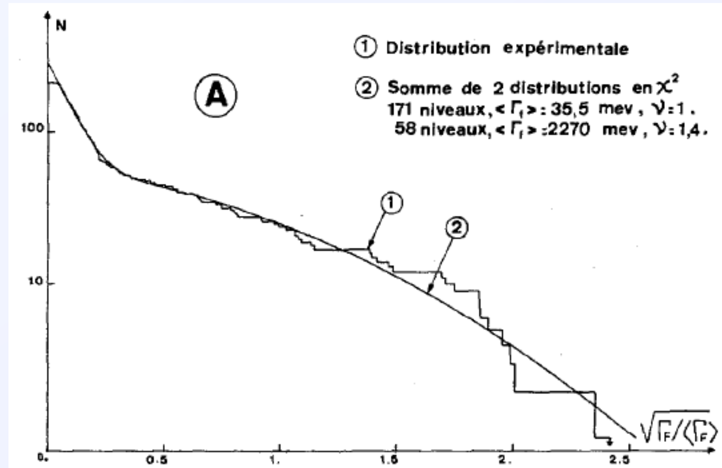
$$\mathfrak{I}_{\mathrm{rigid}} = \frac{2}{3}AMR^2\left(1 + \frac{\delta}{3}\right)$$

FISSION IN THE TRANSITION STATE MODEL

Fluctuations of fission widths



Blons et al. (1970): ^{239}Pu(n,f) from 200 to 1500 eV



Broad distribution of fission widths

- **Fission widths vary greatly from resonance to resonance**
- **Can we learn something from this?**

Width fluctuation statistics

Partial width: decay to one channel $\Gamma_{i\to f} \propto |\langle f|H|i\rangle|^2$

Transition matrix elements have Gaussian distribution about zero, therefore:

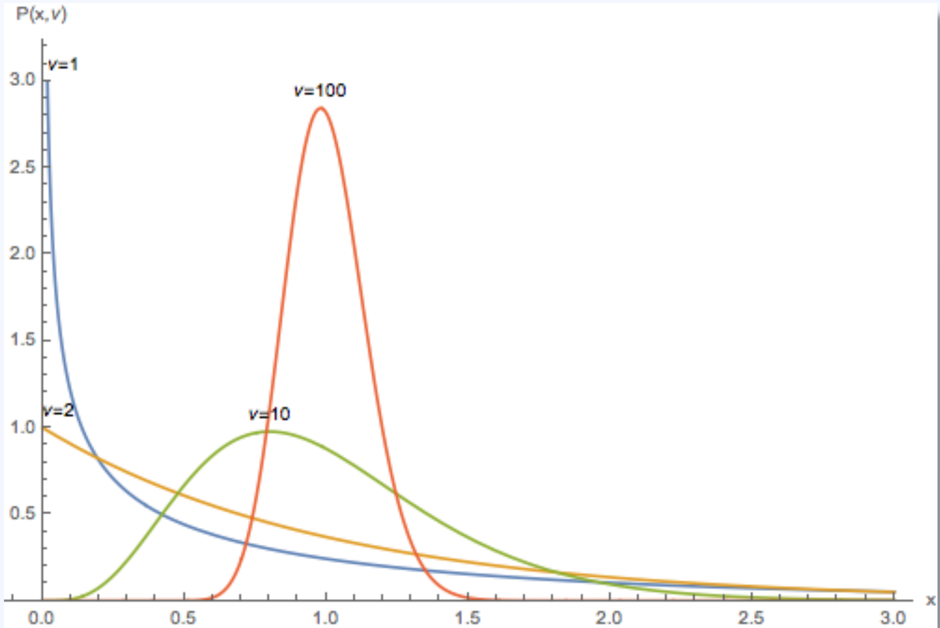
$$P_1(x) = \frac{1}{\sqrt{2\pi x}} \exp\left(-\frac{x}{2}\right), \quad x = \frac{\Gamma_{i\to f}}{\langle \Gamma_{i\to f}\rangle}$$

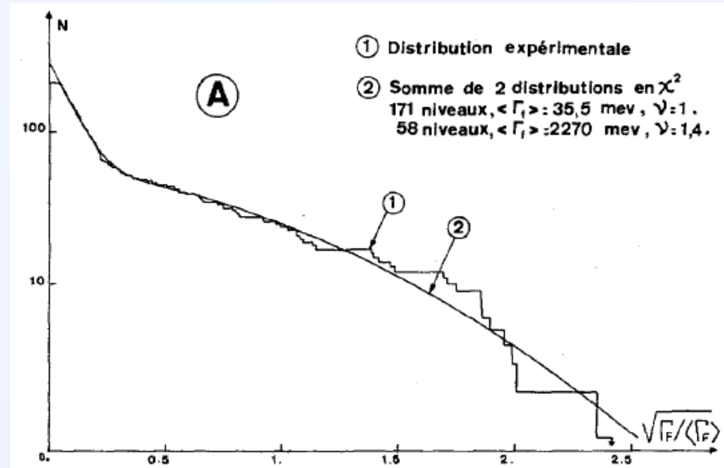
Decay width for many open channels: $\Gamma_i = \sum_{f=1}^{\nu} \Gamma_{i\to f}$

$$P_\nu(x) = \frac{\nu/2}{\Gamma(\nu/2)} \left(\frac{\nu x}{2}\right)^{\nu/2-1} \exp\left(-\frac{\nu x}{2}\right), \quad x = \frac{\Gamma_i}{\langle \Gamma_i\rangle}$$

Porter & Thomas (1956): width fluctuations related to number of open channels

Distribution of fission widths



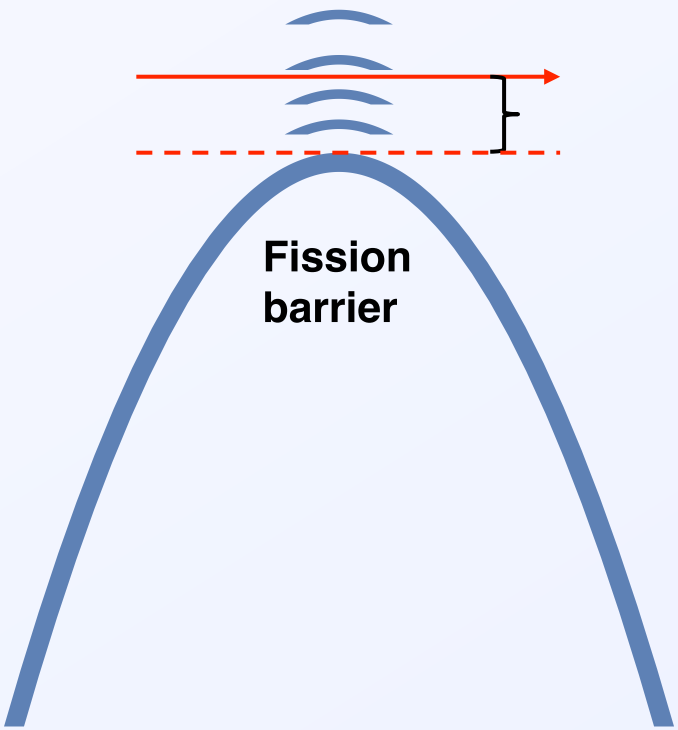


Broad distribution of fission widths: consistent with few open channels

- **Fission width distribution suggests few open channels**
- **But there are many exit channels: many divisions, many excited states**
  - **Estimated 10^{10} exit channels (Wilets, 1964)**

Paradox solved by A. Bohr's fission channel theory

Bohr's fission channel theory (1955)

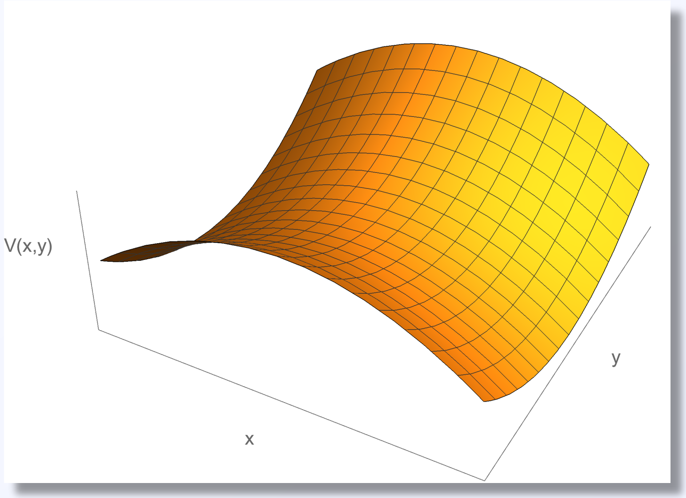


- For low-E fission:
  - Nucleus transits close to barrier top
  - Nucleus is cold at the barrier
  - Few <u>transition states</u> at such low energy
  - Many fission properties determined by few transition states at barrier, before scission!

Fission channels ≠ exit channels

What are the transition states?

Solution of Schrödinger equation for saddle-shaped potential



$$V\left(x,y\right) = V_0 - \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2$$

Motion in *x* and *y* can be separated:

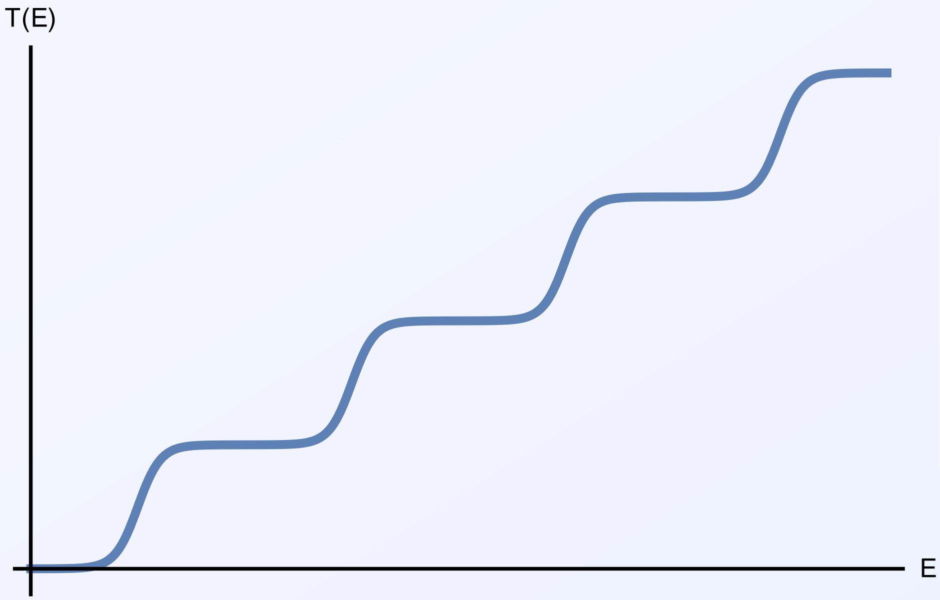
Transverse eigenstates → $$E_n = V_0 + \hbar\omega_y\left(n + \frac{1}{2}\right)$$

Effective potential in direction of motion (*x*) → $$V_0 + \hbar\omega_y\left(n + \frac{1}{2}\right) - \frac{1}{2}m\omega_x^2 x^2$$

Solution of Schrödinger equation for saddle-shaped potential

Transmission probabilities (Bütticker, 1990):

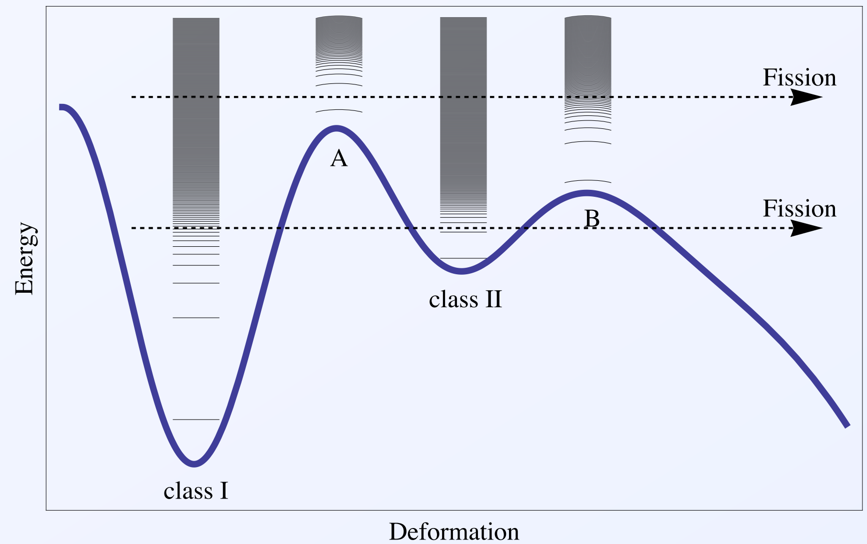
$$T_n(E) = \frac{1}{1+\exp\left[-\frac{2\pi}{\hbar\omega_x}\left(E-\hbar\omega_y\left(n+\frac{1}{2}\right)-V_0\right)\right]}, \qquad T(E) = \sum_n T_n(E)$$



- **In experiments we don't see this directly**
  - **Competition with other channels (e.g., neutron emission)**
  - **Entrance channel effects**
- **Can *x* and *y* be separated for realistic potential energy surfaces?**

The transition state model

- Originally used to calculate chemical reaction rates (Eyring, 1935)
- Adapted to fission rates by Bohr and Wheeler (1939)



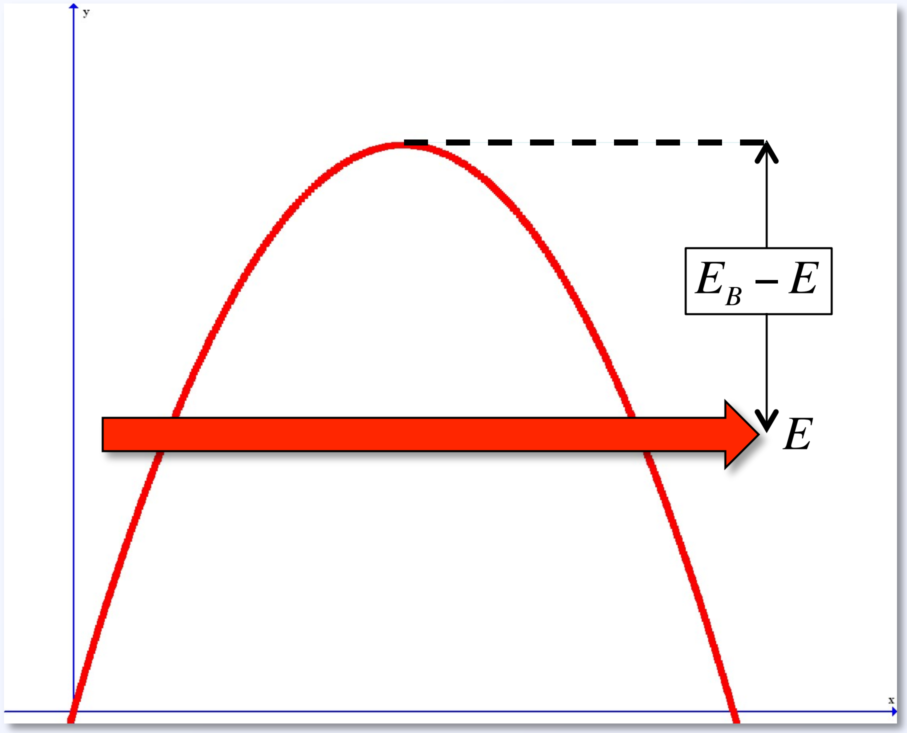
- Transmission across a barrier

$$T_f\left(E_x, J, \pi\right) = \int_0^\infty d\varepsilon\, T\left(E_x - E_b - \varepsilon\right) \rho\left(\varepsilon, J, \pi\right)$$

Transmission through one transition state

Density of transition states

Transmission through an inverted parabolic barrier

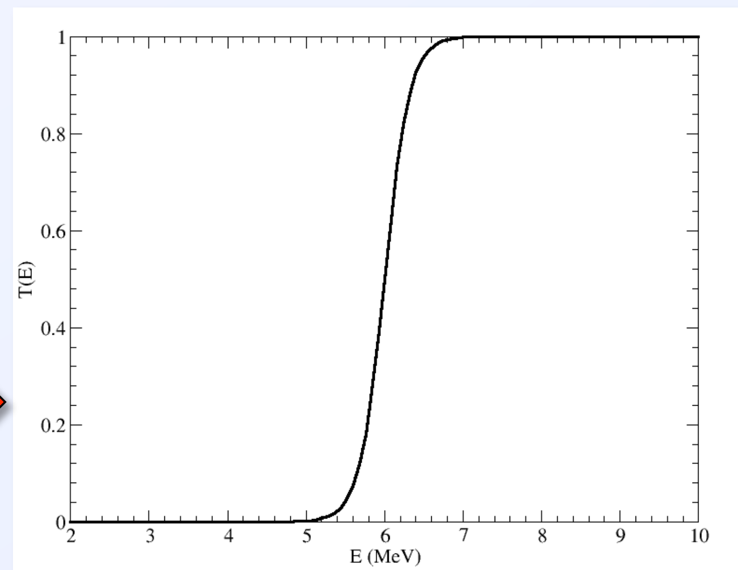


Solving the Schrodinger equation:

$$V(x) = E_B - \frac{1}{2}\mu\omega^2 (x - x_B)^2$$

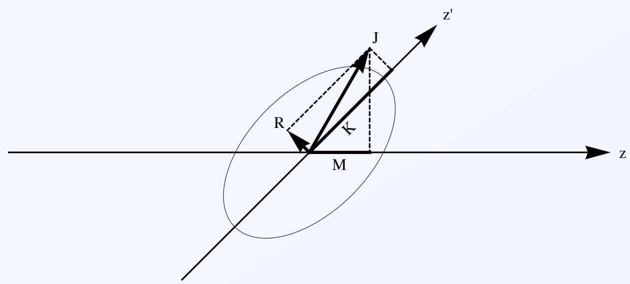
$$T(E) = \frac{1}{1 + \exp\left(\frac{2\pi}{\hbar\omega}(E_B - E)\right)}$$

Example for $\hbar\omega$ = 1 MeV and E_B = 6 MeV



The transition states

- **At low E above barrier, states are labeled by *J*, *K*, π:**



Angular distribution from Wigner "little d" function

$$W^J_{MK}(\theta) \propto \left|d^J_{MK}(\theta)\right|^2$$

- **At higher E, use level density**

$$\rho_{\rm rot}(E,J) = \frac{\rho(E)}{\sqrt{2\pi}\sigma}\exp\left[-\frac{J(J+1)}{2\sigma_\perp^2}\right]\sum_{K=-J}^{J}\exp\left(-\frac{K^2}{2\sigma_{\rm eff}^2}\right)$$

$$W(\theta,J,M) \propto \frac{2J+1}{2}\sum_{K=-J}^{J}\left|d^J_{MK}(\theta)\right|^2\exp\left(-\frac{K^2}{2\sigma_{\rm eff}^2}\right)$$

The discrete transition states

- Inner barrier (even nucleus):
- $K^{\pi} = 0^+$ - "ground"

  + rotational band ($J^{\pi} = 2^+, 4^+ \ldots$)

  $$\hbar^2 / 2\Im \approx 3.5 keV$$
- Gamma vibration, $K^{\pi} = 2^+$ - ~ 200keV

  + rotational band ($3^+, 4^+ \ldots$)
- Gamma vibrations, $K^{\pi} = 0^+$, 4^+ - ~400 to 500 keV

  + rotational band ($2^+, 4^+ \ldots; 5^+, 6^+$ resp.)
- Mass asymmetry vibration, $K^{\pi} = 0^-$ - ~700keV

  + rotational band ($1^-, 3^- \ldots$)
- Bending vibration, $K^{\pi} = 1^-$ - ~ 800keV

  + rotational band ($2^-, 3^- \ldots$)
- Combinations of above

- Outer barrier:
- $K^{\pi} = 0^+$ - "ground"

  + rotational band ($J^{\pi} = 2^+, 4^+ \ldots$)

  $$\hbar^2 / 2\Im \approx 2.5 keV$$
- Mass asymmetry vibration, $K^{\pi} = 0^-$ - ~100keV

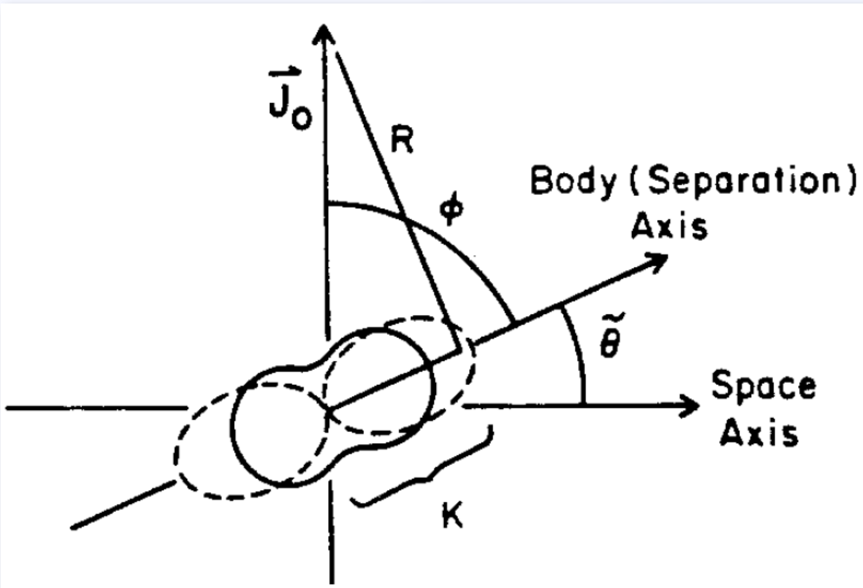
  + rotational band ($1^-, 3^- \ldots$)
- Gamma vibration, $K^{\pi} = 2^+$ - ~ 800keV

  + rotational band ($3^+, 4^+ \ldots$)
- Gamma vibrations, $K^{\pi} = 0^+$, 4^+ - ~1.5MeV + rotational band ($2^+, 4^+ \ldots; 5^+, 6^+$ resp.)
- Bending vibration, $K^{\pi} = 1^-$ - ~ 800keV

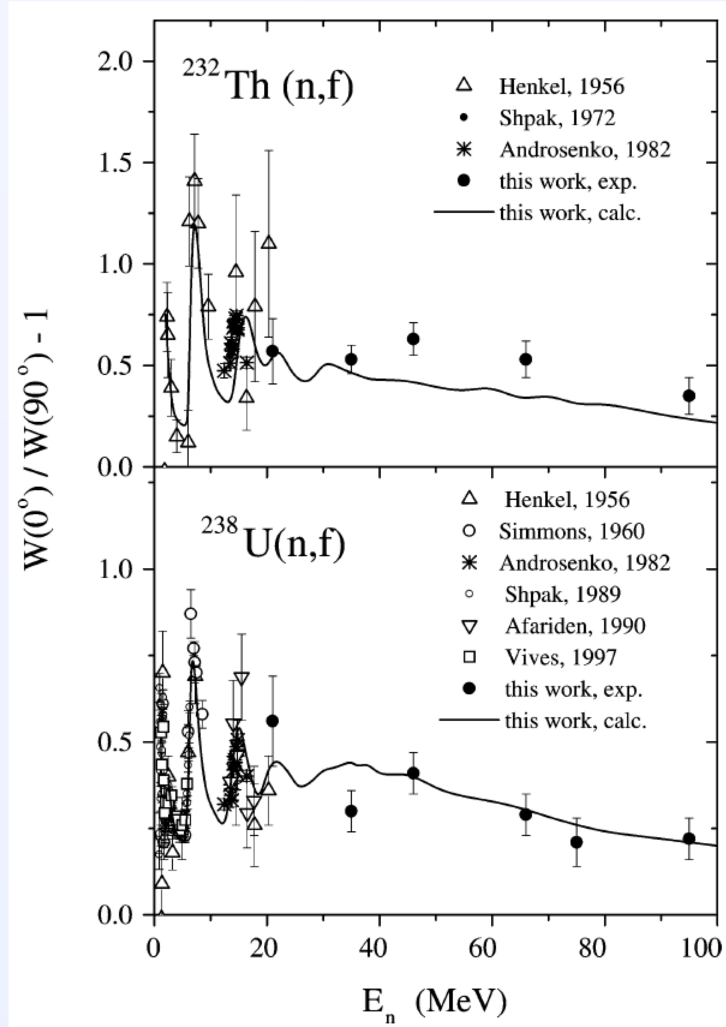
  + rotational band ($2^-, 3^- \ldots$)
- Combinations of above

From Lynn, FIESTA2014

Application: angular distributions, measured and calculated



$$W(\theta) \propto \frac{1}{\sigma_{(n,f)}(E)} \sum_{A,Z,J,M} \int dE\, W(\theta, A, Z, J, M, E) \times \sigma_{(n,f)}(A, Z, J, M, E)$$



Ryzhov et al., NPA 760, 19 (2005)

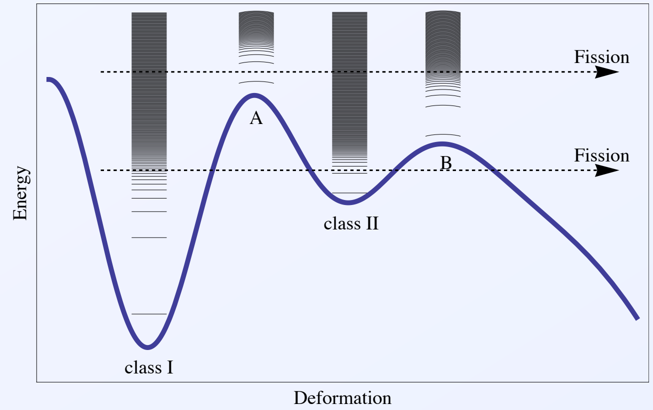
Transmission through two weakly coupled barriers

- **Fission rate from 2-step process**

$$R_f = R_{I\to II} \times P_{II\to f}$$

$$R_{I\to II} = \frac{\Gamma_{I\to II}}{\hbar}$$

$$P_{II\to f} = \frac{\Gamma_{II\to f}}{\Gamma_{II\to I} + \Gamma_{II\to f}}$$



- **Remember the all-important formula:** $T_{\alpha\to\beta} = \frac{2\pi}{d_\alpha}\Gamma_{\alpha\to\beta}$

- **Fission transmission coefficient:**

$$\Gamma_f = \hbar R_f = \frac{d_I}{2\pi} \times \frac{T_A T_B}{T_A + T_B} \quad \Rightarrow \quad T_f = \frac{T_A T_B}{T_A + T_B}$$

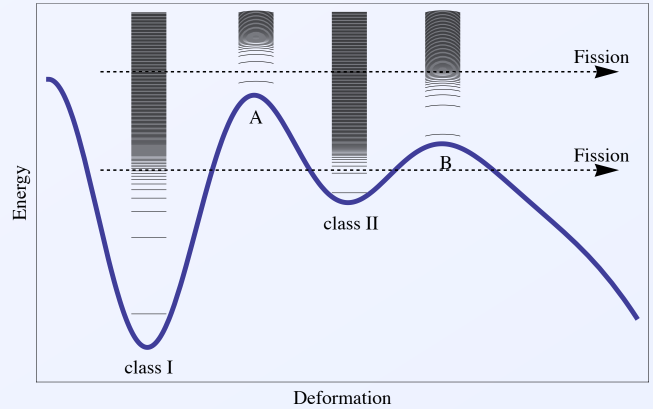
Appropriate above barrier tops

Transmission through two strongly coupled barriers

- **Assume equidistant-level model for class-II states**

$$E_{II} = E_0 + n d_{II}$$

$$T_f(E) = \sum_{n=-\infty}^{\infty} \frac{\Gamma_{II\to I}\Gamma_{II\to f}}{\left[E-(E_0+nd_{II})\right]^2 + \left(\frac{\Gamma_{II\to I}+\Gamma_{II\to f}}{2}\right)^2}$$



- **Fission probability from competition with other channels:**

$$P_f(E) = \frac{T_f(E)}{T_f(E)+T'}$$

Other channels (e.g, n and γ)

- **Energy average**

$$\bar{P}_f = \frac{1}{d_{II}}\int_{E_0-d_{II}/2}^{E_0+d_{II}/2} dE\, P_f(E) = \left[1+\left(\frac{T'}{\bar{T}_f}\right)+2\left(\frac{T'}{\bar{T}_f}\right)\coth\left(\frac{T_A+T_B}{2}\right)\right]^{-1/2}$$

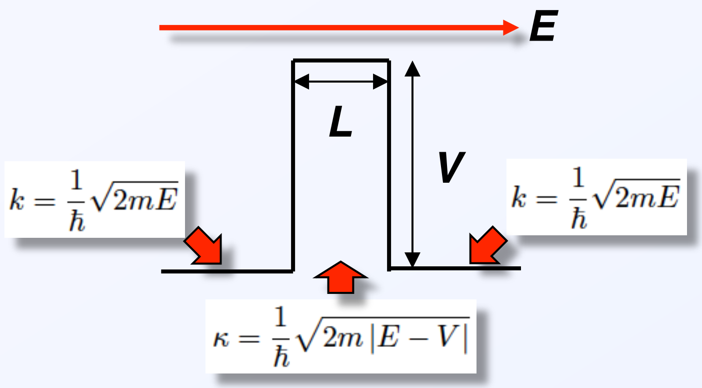
Where:

$$\bar{T}_f = \frac{T_A T_B}{T_A+T_B}$$

Appropriate below barrier tops

Calculating transmission probabilities for any 1D potential

Gilmore (2004):



1) Calculate 2×2 matrix depending on *E* and *V*:

$$M = \begin{pmatrix} \cos(\kappa L) & -\frac{1}{\kappa}\sin(\kappa L) \\ +\kappa\sin(\kappa L) & \cos(\kappa L) \end{pmatrix}, \quad E > V$$

$$M = \begin{pmatrix} \cosh(\kappa L) & -\frac{1}{\kappa}\sinh(\kappa L) \\ -\kappa\sinh(\kappa L) & \cosh(\kappa L) \end{pmatrix}, \quad E < V$$

$$M = \begin{pmatrix} 1 & -L \\ 0 & 1 \end{pmatrix}, \quad E = V$$

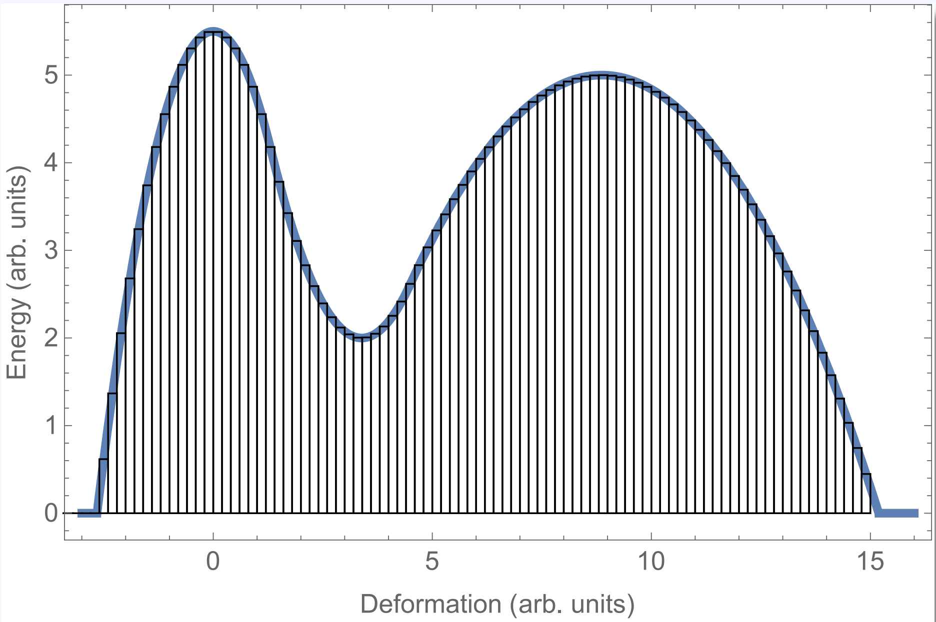
2) Calculate transmission probability:

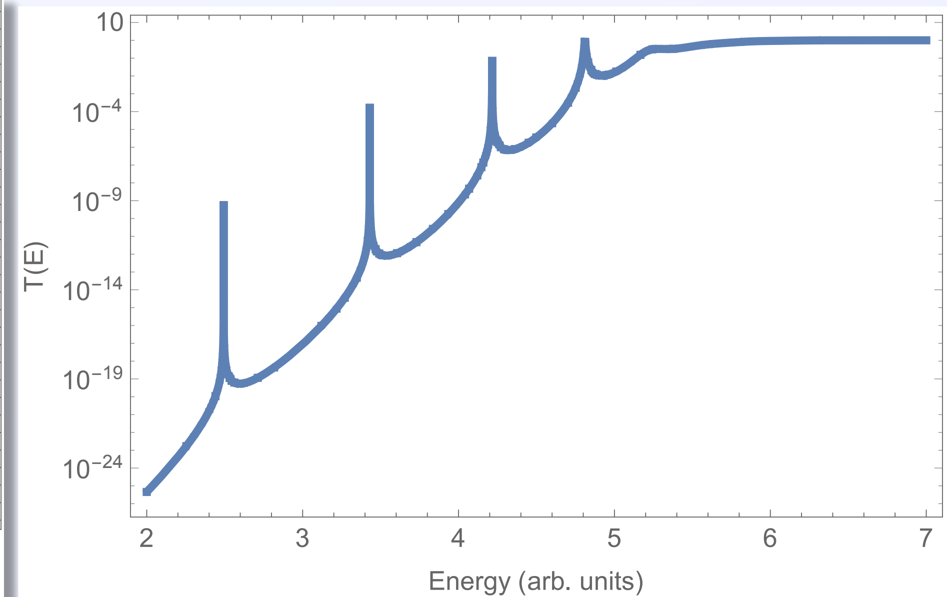
$$T(E) = \frac{4}{(M_{11} + M_{22})^2 + (kM_{12} - M_{21}/k)^2}$$

For a general potential:

1. **Break up into sequential rectangular barriers**
2. **Calculate matrix M for each, Multiply them into single M matrix**
3. **Calculate T(E) as in the 1-barrier case**

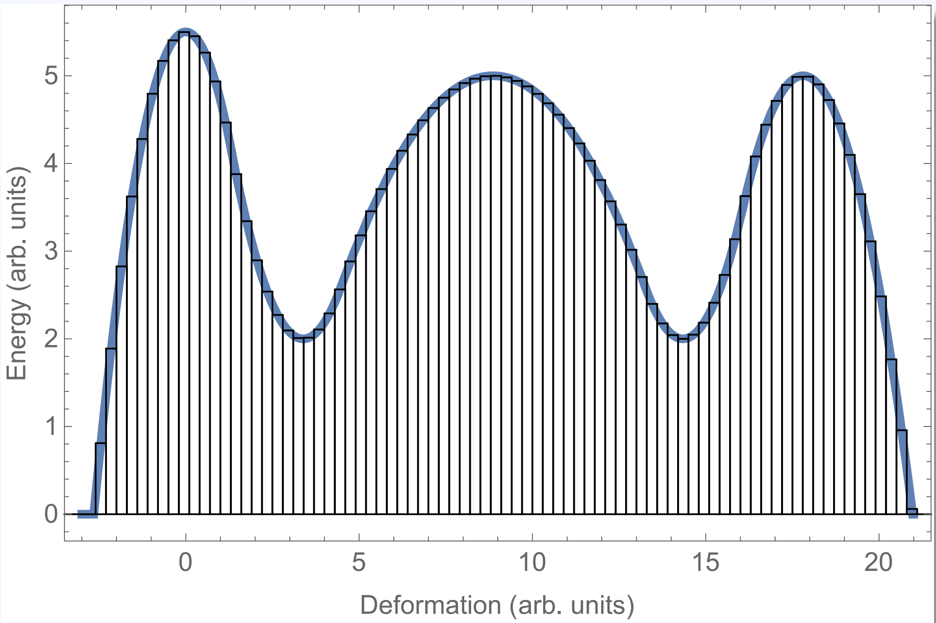
Application: transmission through double-humped barrier

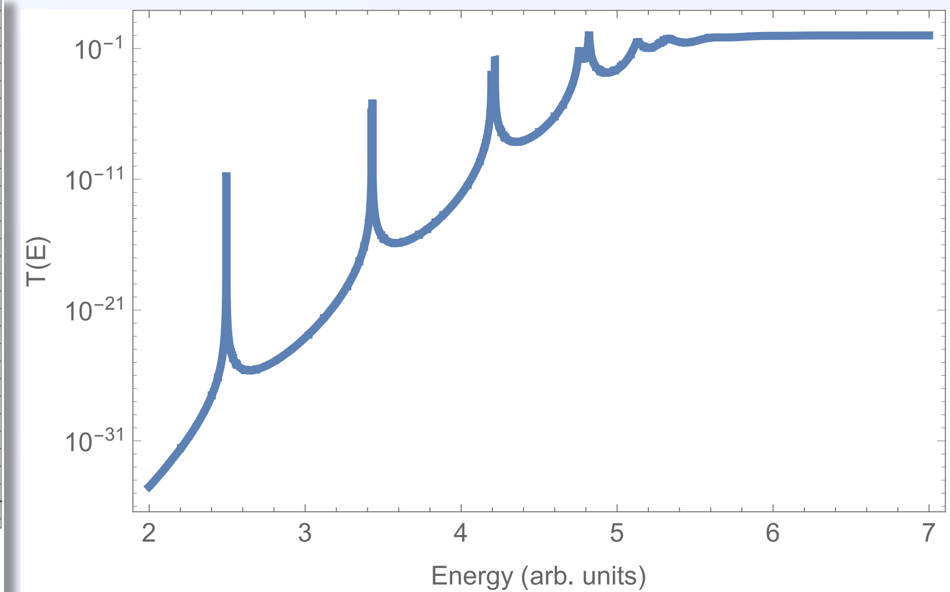




- **Resonances below barriers**
- **Above barriers: T(E) tends to 1**

Application: transmission through triple-humped barrier





- More complex resonance structure below barriers
- Above barriers: T(E) tends to 1

PRACTICAL APPLICATIONS

Cross section evaluations: what's involved?

- Measurements are inherently incomplete, and sometimes impossible
  - Evaluation completes and complements measurements
- Fit measured data with physics models (e.g., as coded in TALYS)
  - To fill in gaps in data for interpolation (and extrapolation, with caution)
  - To tighten experimental uncertainties by imposing physical constraints
- Combine with other data, or merge with existing evaluation
- Quantify uncertainties (e.g., generate a covariance matrix)
  - Points with error bars are often not sufficient
  - Behavior at different energies is correlated through physics
  - Covariance matrix accounts for correlations (to 1^{st} order)

Application: evaluations using the TALYS code

- Remember: ”All models are wrong but some are useful” – G. Box
- TALYS is one of many other reaction codes (EMPIRE, GNASH, YAHFC, STAPRE,…)
- Easy to get, easy to use
  - Download from: http://www.talys.eu/
  - Simplest input file:

```
projectile n
element U
mass 235
energy 14
```

or

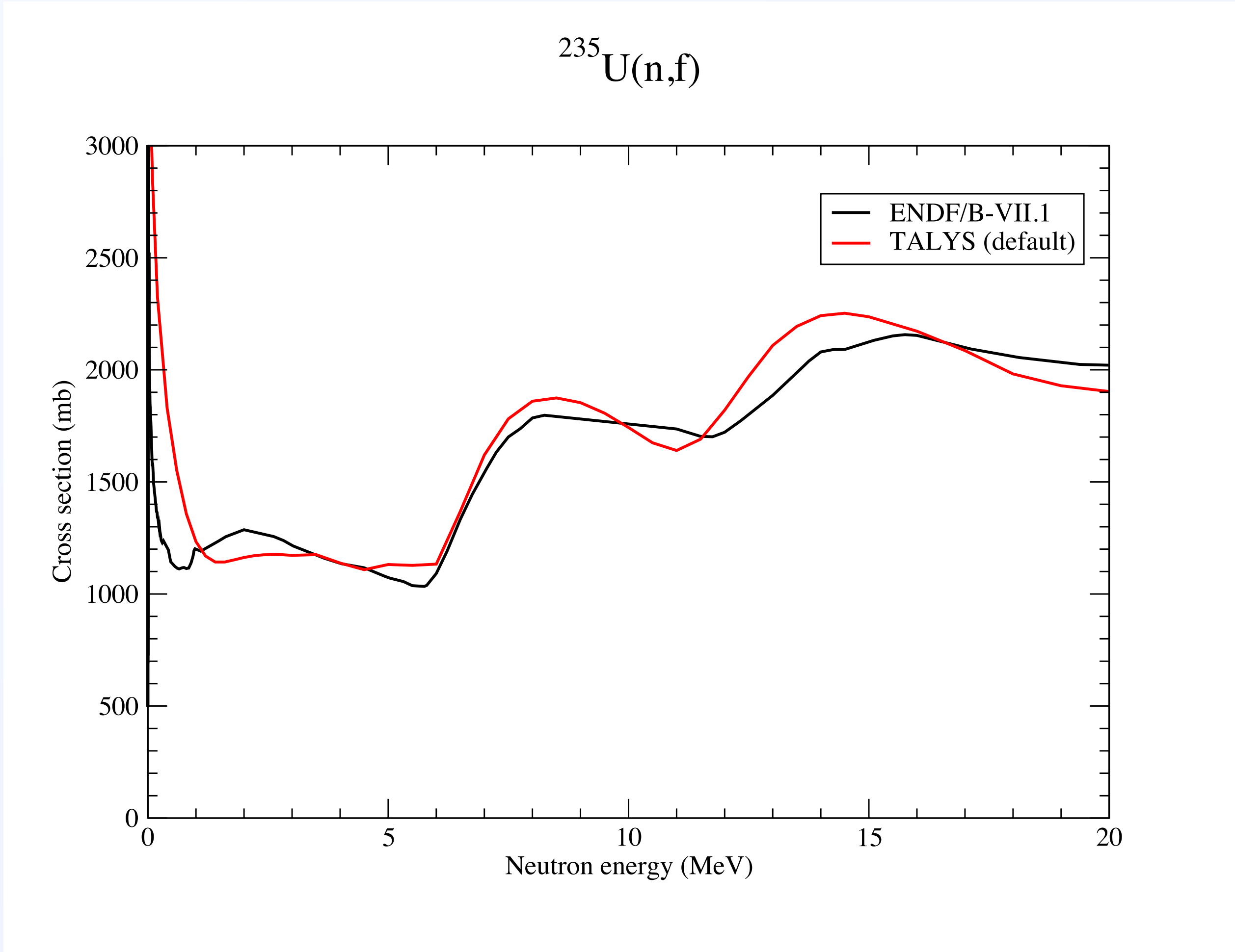
```
projectile n
element U
mass 235
energy energies
```

  - Running it:

```
talys < input > output
```

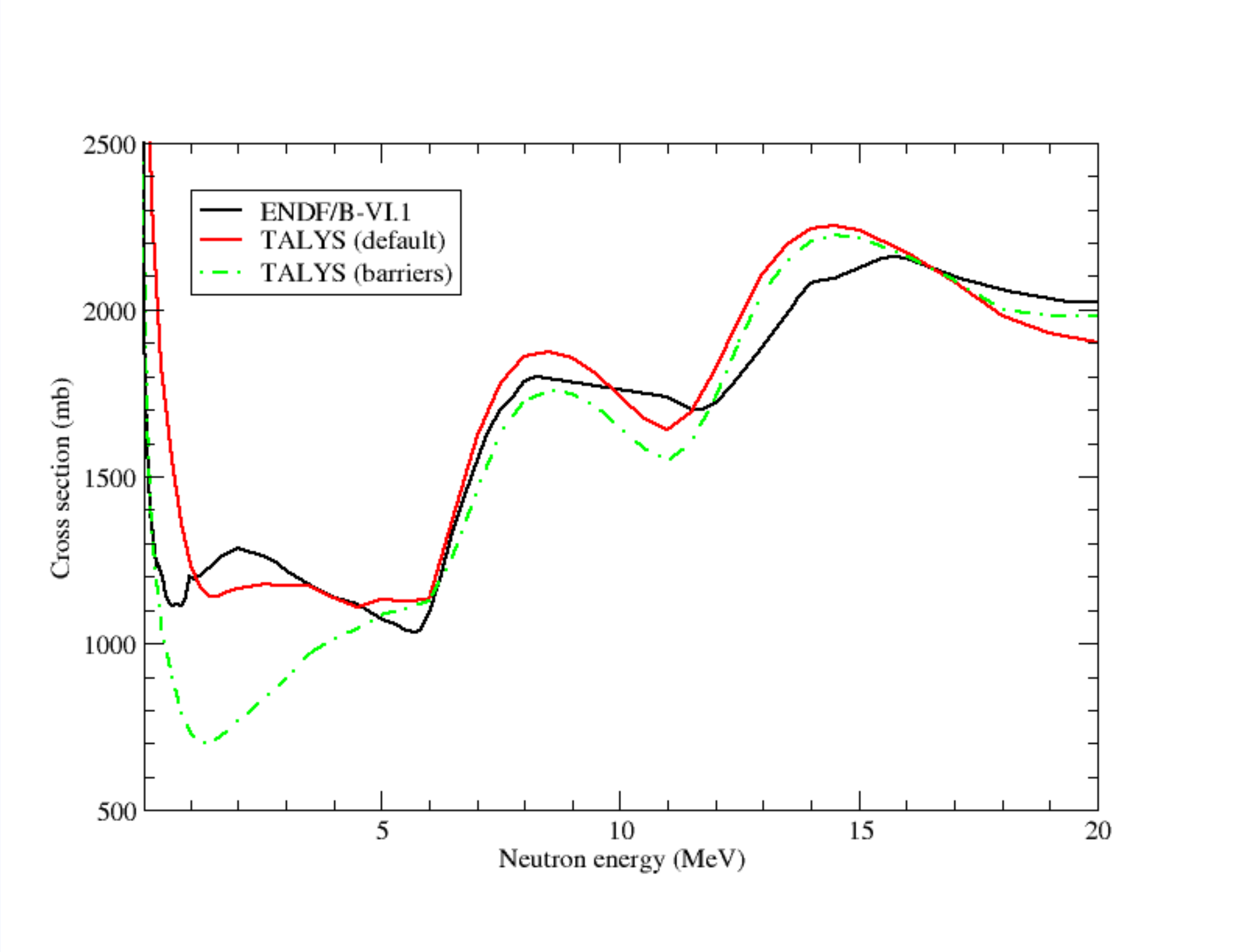
  - Output
    - Lots, but we'll focus on “fission.tot” for now

TALYS example: ^{235}U(n,f)



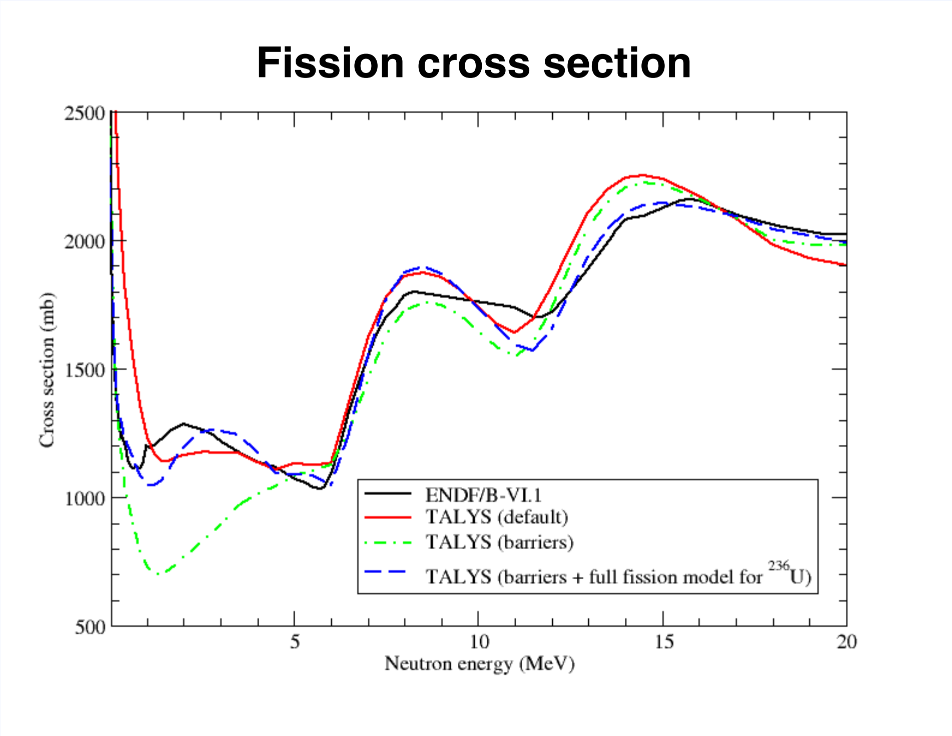
Parameter defaults (usually) get you pretty close

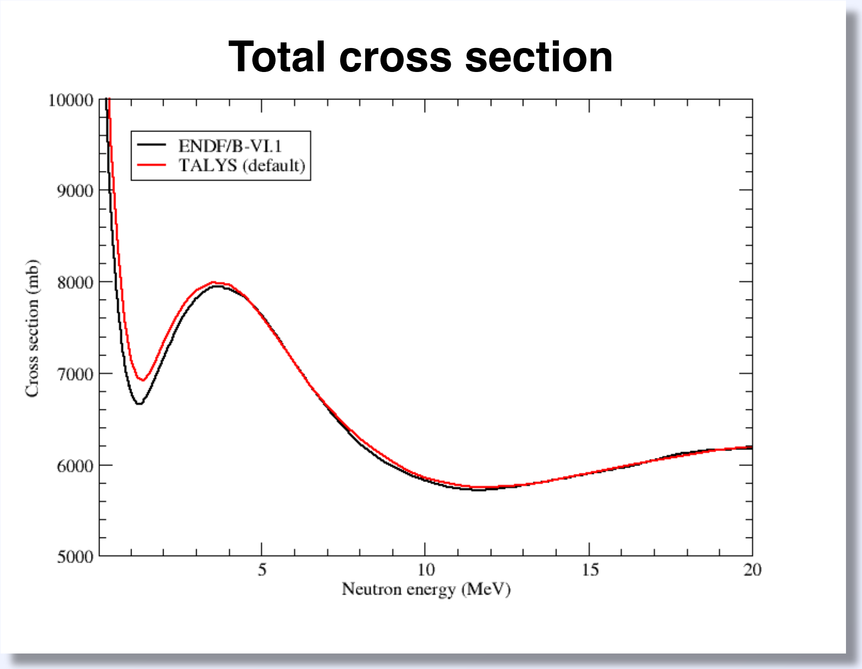
TALYS example: ^{235}U(n,f)



Adjusted barrier heights and curvatures for all U isotopes using Monte-Carlo parameter search

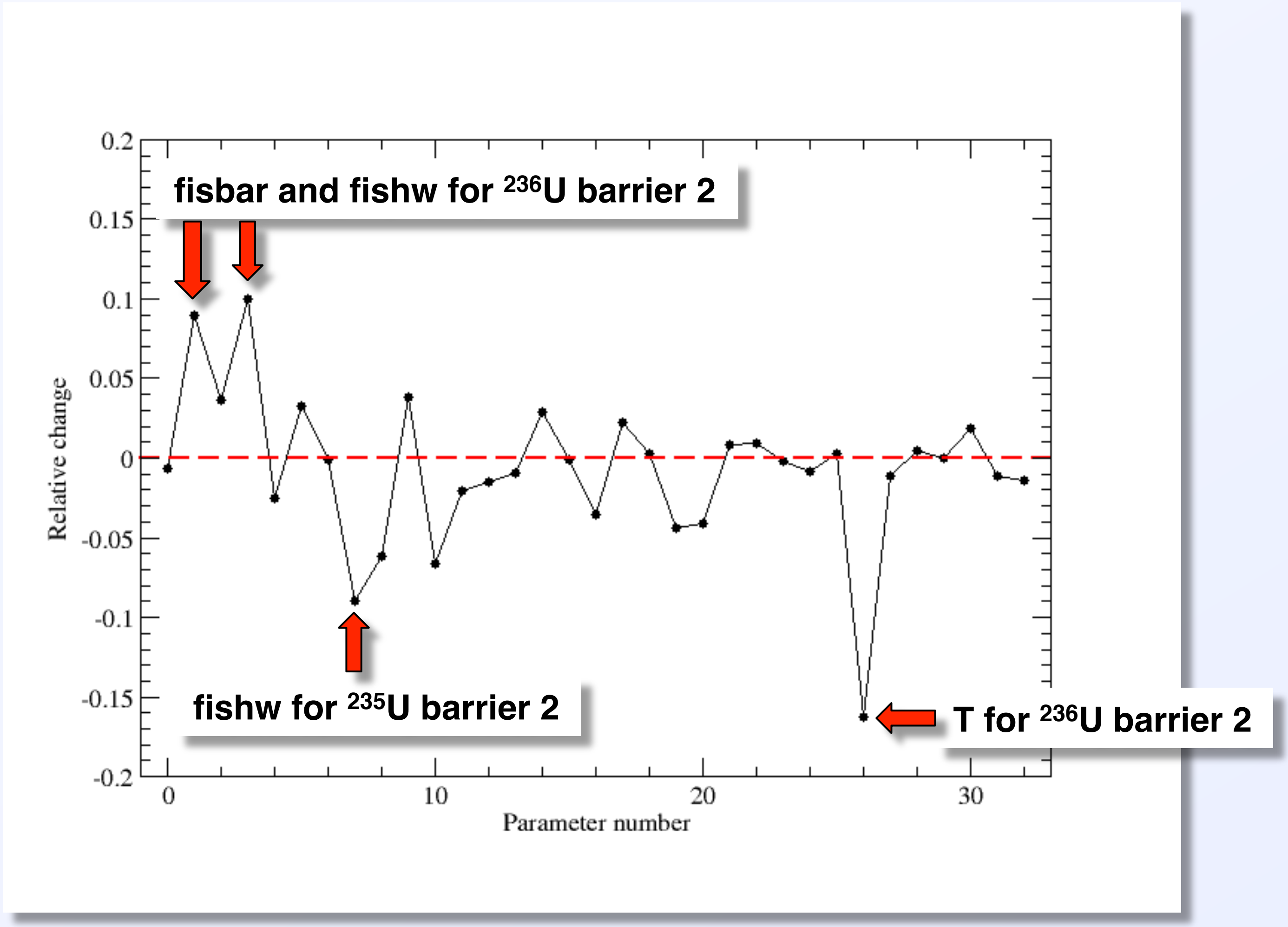
TALYS example: ^{235}U(n,f)





- **Adjusted barrier heights and curvatures for all U isotopes and all fission-model parameters for ^{236}U (Monte-Carlo search)**
- **Total cross section is still well reproduced (could fit it along with fission xs if necessary)**

Change in fit parameters (compared to default)



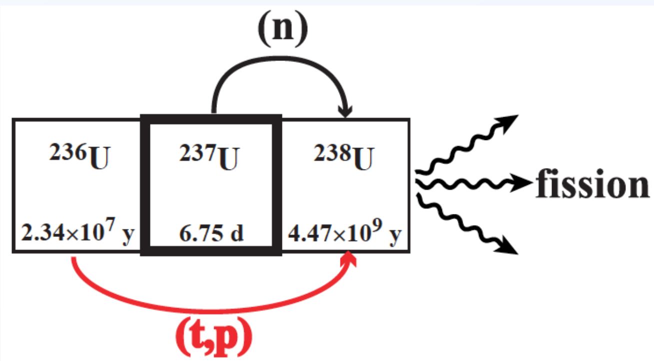
Adjusting model parameters and generating a covariance matrix

- **Deterministic methods: e.g., Kalman filter**
  - linearize cross-section model and calculate its sensitivity matrix

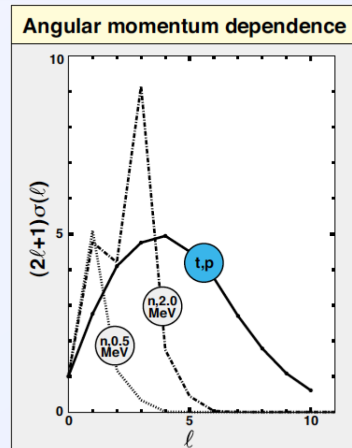
$$S_{ij} = \frac{\partial}{\partial p_j} \sigma \left(E_i, p_1, \ldots, p_j, \ldots \right)$$

  - Both data and model parameters have a covariance matrix
  - Linear equations derived from χ^2 minimization are used to update model parameter values and covariances for each new data set
- **Stochastic methods: e.g, Markov Chain Monte Carlo**
  - Take random walk in parameter space
    - Guided by likelihood function (measure of how likely the data are given a set of model parameter values)
  - Density of points visited gives probability distribution (and hence covariance matrix) in parameter space

Application to the surrogate reaction method



- Some reactions are too difficult to measure in the lab
  - Fission probabilities, $P_f(E)$, from the same CN can be measured using a different reaction
  - Theory used to compensate for different angular momentum distributions between reactions



Basic technique:

Measure — Calculate — Fit model

$$P_{(t,pf)}(E_x) = \sum_{J^\pi} P_{(t,p)}(J^\pi) \times P_f(E_x, J^\pi)$$

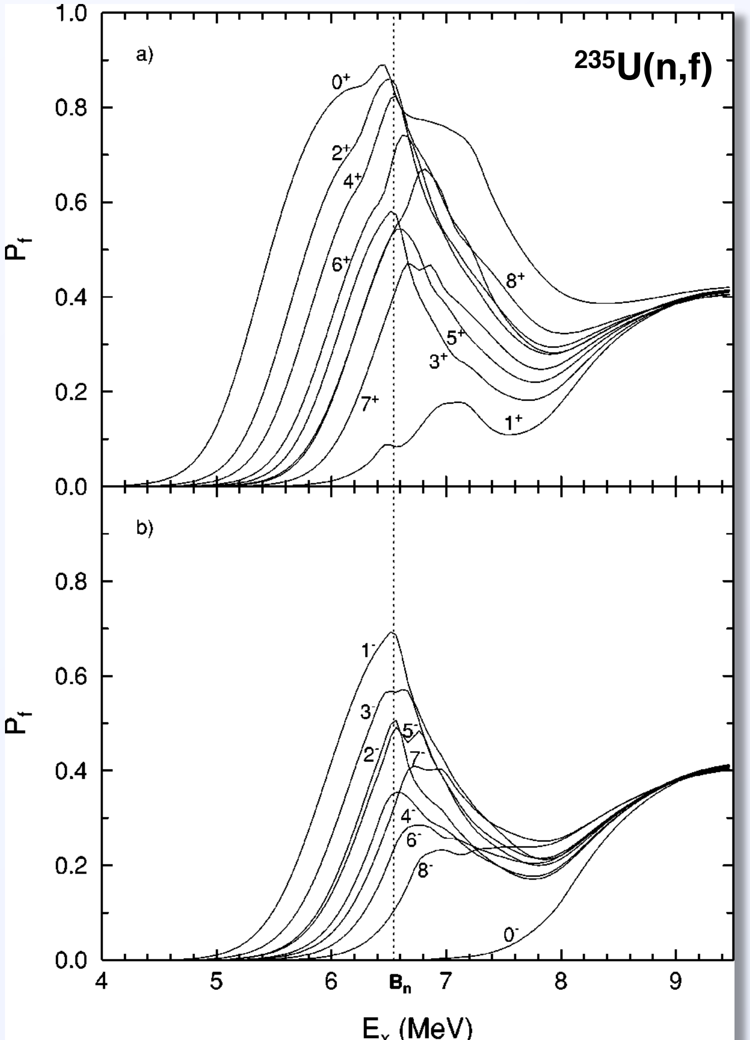
Reuse

$$\sigma_{(n,f)}(E_n) = \sum_{J^\pi} \sigma_{CN}(E_n, J^\pi) \times P_f(E_x, J^\pi)$$

Deduce — Calculate

Justification:
- We have a better understanding of the formation process than decay (fission)
- Use measured fission probabilities to constrain transition-state fission model

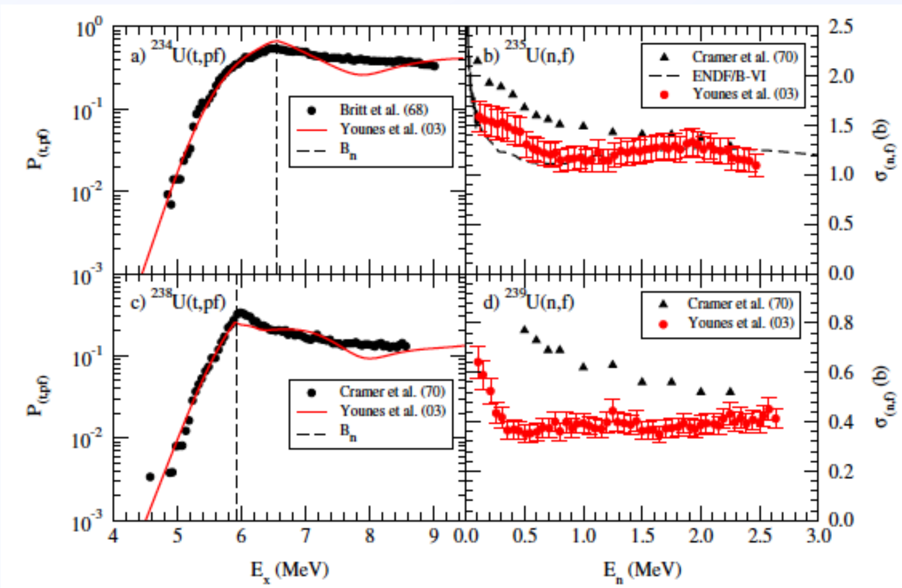
Dependence of fission probabilities on angular momentum



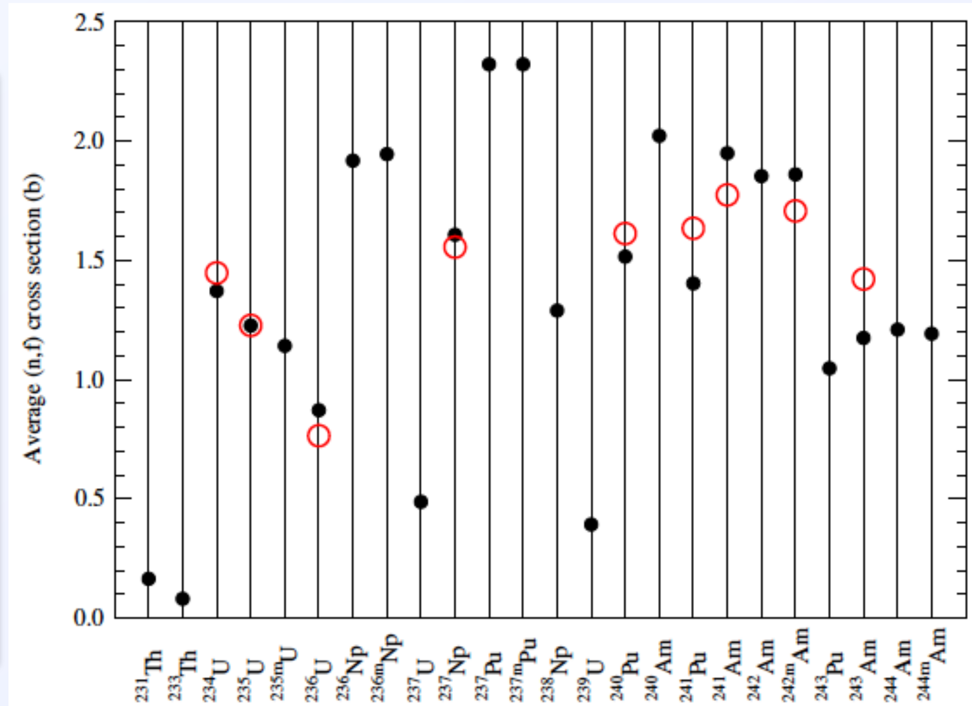
Younes & Britt (2003)

- **Probabilities due to angular momentum distribution at barriers**
- **Note low probabilities for 1^+ and 0^-**
  - **Few transition states with Jp = 1^+, 0^- close to barrier top**

Results: fission cross sections from surrogate measurements



Younes et al. (2003)



Younes et al. (2004)

FUTURE OUTLOOK

Limitations of the transition state model

- The good:
  - It works!
  - Physics-based model
- The bad:
  - Transition states are essentially free parameters (some evidence from experiment, but no stringent constraints)
    - Can hide missing physics
    - Solution may not be unique
  - Emphasis on critical points in the energy surface (minima, maxima), but there is more to fission

  ⇒ Descriptive, rather than predictive model

A better starting point: protons, neutrons, and an interaction between them ⇒ microscopic model

Different microscopic calculations of fission cross sections

- 1D Transition state model with microscopic ingredients
  - Fission barrier heights and curvatures
  - Level densities at barriers
- Dynamical treatment of fission
  - Configuration interaction: diagonalize H in space of orthogonal particle excitations
  - Generator coordinate method (see talk by Schunck): diagonalize H in space of constrained mean-field solutions
    - Discretize in deformation
    - Expand to 2nd order in deformation → Schrodinger-like equation
  - Diffusion models

Dynamical treatment can be in many dimensions, does not assume Hill-Wheeler transmission

From fission dynamics to cross sections

- Suppose you can solve TDSE to get $\Psi(t)$ describing fissioning nucleus
- Q: how do you calculate a cross section?
- A: calculate fission probability by coupling with particle & gamma emission at each time step

$$x \equiv \frac{\Delta t}{\tau_{\text{tot}}}, \quad \Delta t = \text{time step}$$

$$\tau_{\text{tot}} = \frac{\hbar}{\Gamma_{\text{tot}}}, \quad \Gamma_{\text{tot}} = \Gamma_n + \Gamma_\gamma$$

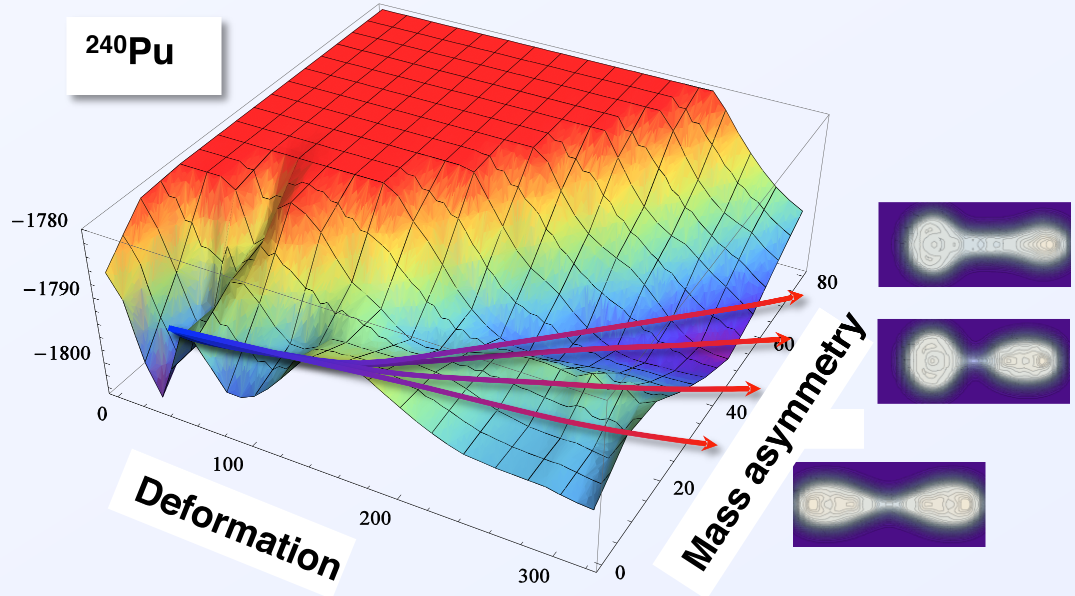
1. Choose random $0 \leq r \leq 1$: emit something if $x > r$
2. Choose random $0 \leq r \leq 1$: emit n if $r < \Gamma_n / \Gamma_{tot}$, otherwise γ
3. Sample random energy from emission spectrum
4. Remove appropriate amount of spin
5. Continue fission with remaining mass, energy, spin

After long time, obtain fraction of initial state that survives to fission

Fission dynamics in the Generator Coordinate Method

- Start from protons, neutrons, and their interactions
- Construct <u>all relevant configurations</u> of protons and neutrons and their <u>couplings</u> by constraining shape
- Evolve in time over these configurations according to the laws of quantum mechanics
- Measure the flow over time

See lecture by N. Schunck for more



- In the long term, this will provide a microscopic alternative to transition-state model
- In the short term, some challenges to overcome
  - Configs calculated by imposing "shape" ⇒ orthogonality issues
  - Currently, can only handle a limited number of degrees of fredom
    - Full calculation (5 collective + 10 intrinsic) ⇒ ~ 10^{15} times more couplings!

In the meantime, there is room for an intermediate approach that uses some of the same the main ingredients

Concept behind the configuration-interaction approach

- **Mean field and residual interaction**

$$H = \underbrace{T^{(1)}}_{\substack{\text{kinetic} \\ \text{(1-body)}}} + \underbrace{V^{(2)}}_{\substack{\text{interaction} \\ \text{(2-body)}}} + \underbrace{V^{(3)}}_{\substack{\text{interaction} \\ \text{(3-body)}}} + \ldots$$

  - Add and subtract mean-field potential $V^{(1)}$ (e.g., Hartree-Fock from protons + neutrons + effective interaction), and regroup terms

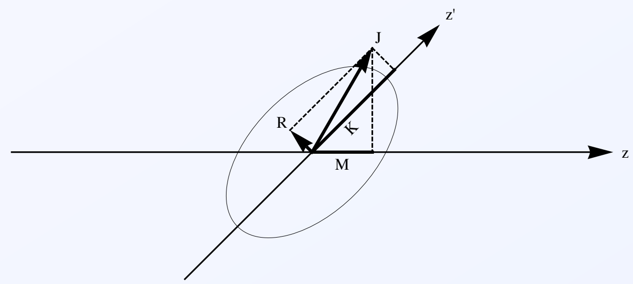
$$H = \underbrace{T^{(1)} + V^{(1)}}_{\text{mean-field Hamiltonian}} + \underbrace{V^{(2)} + V^{(3)} + \ldots - V^{(1)}}_{\text{residual interaction}}$$

  - Mean field $\longrightarrow$ single-particle (sp) states
  - Elementary excitations = multi-particle multi-hole (mp-mh) built on sp states
  - Residual interaction mixes mp-mh configurations

    $\Longrightarrow$ Dynamical evolution between mp-mh states

A discrete basis for fission

- **Axial symmetry ⇒ K and π are good quantum numbers**



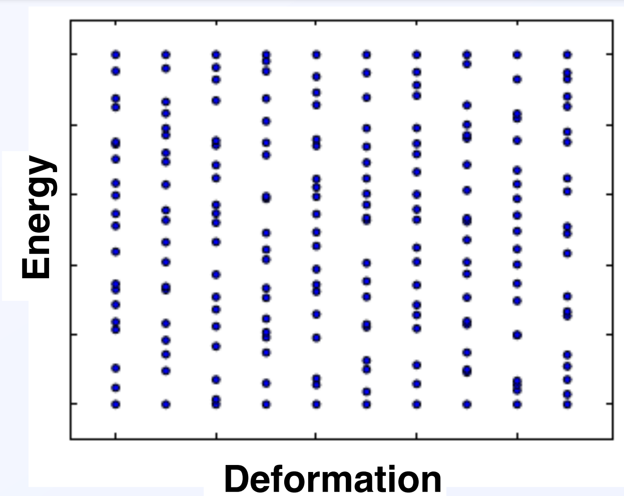
- **Hamiltonian matrix breaks up into K^π blocks along diagonal**

$$H = \begin{pmatrix} \boxed{K^\pi = \frac{1}{2}^+} & & & \\ & \boxed{K^\pi = \frac{1}{2}^-} & & \\ & & \boxed{K^\pi = \frac{3}{2}^+} & \\ & & & \ddots \end{pmatrix}$$

- **mp-mh excitations with differing populations of the K^π blocks are orthogonal**
  - **⇒ Useful, discrete state basis**
- **Time evolution dictated by matrix elements between mp-mh configs**
- **G. F. Bertsch, arXiv:1611.09484**

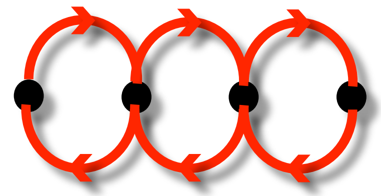
Fission dynamics in the discrete basis approach

Discrete basis of mp-mh excitations can be arranged in layers:



Bertsch & Mehlhaff, arXiv:1511.01936

- **Nucleus "hops" between discrete states**



- **Evolution by diffusion equation:**

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial q} D\left(q\right) \frac{\partial P}{\partial q}$$

$P =$ probability distribution

$q =$ shape variable

$$D\left(q\right) = \text{diffusion coefficient} = 2\pi\rho\left(E\right) \overline{\left(q_\alpha - q_\beta\right)^2 \left\langle \alpha \left| V_{res} \right| \beta \right\rangle^2}$$

- **Can also use average interaction from random matrix theory as a placeholder**

- **Diffusive approach to fission shows promise (e.g., Randrup & Moller, PRL 106, 132503 (2011))**
- **Obtain fission rate ⇒ fission width to use in Hauser-Feschbach formula**
- **Research on this approach in progress…**

Some final thoughts

- Hauser-Feshbach formalism
  - Simple but important formulas: $$T_{\alpha\to\beta} = \frac{2\pi}{d_\alpha}\Gamma_{\alpha\to\beta}$$
  - Bohr hypothesis
  - Level densities: combinatorial and phenomenological models
- Transition state model
  - States at barrier and in between (class-II) mediate transition
  - Hill-Wheeler formula gives transmission probability
- Microscopic approaches
  - Generator coordinate method (see talk by N. Schunk)
  - Discrete basis diffusion approach
- Some toys to play with
  - TALYS
  - Level density code by Bertsch & Robledo

APPENDIX: SCATTERING THEORY

1D Scattering theory: the Schrödinger equation

- Time-dependent Schrödinger equation (TDSE):

$$\hbar i \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t)$$

  - Assume continuously incident beam (e.g., plane wave):

$$\Psi_{\text{inc}}(x,t) = e^{i(kx-\omega t)}$$

- Can then use time-independent Schrödinger equation (TISE):

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) = \frac{\hbar^2 k^2}{2m}\Psi(x,t)$$

- Also, we'll assume V(x) = V(-x) and V(x) = 0 for x > a

Wave function in the exterior region

Outside range of potential: only plane waves

$$\Psi_{\text{ext}}(x) = \begin{cases} A_- e^{ikx} + B_- e^{-ikx} & x < -a \\ A_+ e^{ikx} + B_+ e^{-ikx} & x > +a \end{cases}$$

We can re-write this in a more suggestive form:

$$\Psi_{\text{ext}}(x) = e^{ikx} + \frac{i}{k} f_k(\epsilon)\, e^{ikr}$$

where

$$\epsilon \equiv \text{sign}(x), \quad r \equiv |x| = \epsilon x$$

- e^{ikx}: Incident wave
- $\frac{i}{k} f_k(\epsilon)$: Scattering amplitude
- e^{ikr}: Scattered wave

Note: in 1D only two possible scattering directions (forward or backward) ⇒ $\epsilon = \pm 1$ (in 3D we cover 4π sr)

A useful quantity: the probability current

$$j = \frac{\hbar i}{2m}\left[\frac{\partial \Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial \Psi}{\partial x}\right]$$

Particle flux

1D: $\Phi = |j|$

3D: $\Phi = \vec{j} \cdot d\vec{A}$

Let's use our generic external wave function:

$$\Psi_{\text{ext}}(x) = e^{ikx} + \frac{i}{k} f_k(\epsilon)\, e^{ikr}$$

to calculate the current:

$$j_{\text{ext}} = \underbrace{\frac{\hbar k}{m}}_{\text{incident}} + \underbrace{\frac{\hbar k}{m}\frac{\epsilon}{k^2}\left|f_k(\epsilon)\right|^2}_{\text{scattered}} \underbrace{-\frac{\hbar k}{m}\frac{1}{k}\text{Im}\left[(1+\epsilon)\, f_k(\epsilon)\, e^{i(\epsilon-1)kx}\right]}_{\text{interference}}$$

Now we have what we need to calculate cross sections

The absorption cross section

- Measures loss of current due to potential:

Backward current

Forward current

$$\sigma_{\text{abs}} \equiv \frac{j_{\text{ext}}(\epsilon = -1) - j_{\text{ext}}(\epsilon = +1)}{|j_{\text{inc}}|}$$

  - For V(x) = 0 or for pure scattering, σ_{abs} = 0
- Using j_{ext} from previous slide:

$$\sigma_{\text{abs}} = -\frac{1}{k^2}\left(|f_k(-1)|^2 + |f_k(+1)|^2\right) + \frac{2}{k}\text{Im}\left[f_k(+1)\right]$$

The scattering cross section

- Measures the current scattered in all directions (forward and back in 1D)

$$\sigma_{\mathrm{sca}} = \frac{j_{\mathrm{ext}}\left(\epsilon = -1\right) + j_{\mathrm{ext}}\left(\epsilon = +1\right)}{\left|j_{\mathrm{inc}}\right|}$$

- Using our explicit formulas for the currents:

$$\sigma_{\mathrm{sca}} = \frac{1}{k^2}\left(\left|f_k\left(-1\right)\right|^2 + \left|f_k\left(+1\right)\right|^2\right)$$

The total cross section

- Particles are either scattered or absorbed, so the total cross section is

$$\sigma_{\rm tot} = \sigma_{\rm sca} + \sigma_{\rm abs}$$

- Using the explicit formulas for the cross sections obtained so far, we get

$$\boxed{\sigma_{\rm tot} = \frac{2}{k}\,{\rm Im}\left[f_k\left(+1\right)\right]}$$

- Which is known as the optical theorem: it relates the total cross section to the forward scattering amplitude
- In 3D we get an almost identical formula:

$$\boxed{\sigma_{\rm tot} = \frac{4\pi}{k}\,{\rm Im}\left[f_k\left(\theta = 0^\circ\right)\right]}$$

Partial wave expansions

- In 3D it is convenient to write the reaction quantities (cross sections, scattering amplitudes, etc.) as a partial wave expansion, as function of orbital angular momentum ℓ
  - Usually only lowest ℓ values are needed ⇒ simplifies calculations
- In 1D can't define angular momentum, but we can use parity instead to illustrate the concept
- Any function can always be split into even and odd parts:

$$g(x) = \underbrace{\frac{1}{2}\left[g(x) + g(-x)\right]}_{\text{even} \equiv g_{\ell=0}(x)} + \underbrace{\frac{1}{2}\left[g(x) - g(-x)\right]}_{\text{odd} \equiv g_{\ell=1}(x)}$$

We will now write partial (parity) wave expansions for various quantities

Partial wave expansions: wave function

- External wave function (looks like plane wave, i.e. sin and cos, far away):

$$\Psi_{\text{ext}}(x) = \sum_{\ell=0}^{1} \epsilon^{\ell} A_{\ell} \cos\left(kr + \ell\frac{\pi}{2} + \delta_{\ell}\right)$$

  - A_{ℓ} = constant coefficient to be determined (can be complex)
  - δ_{ℓ} = phase shift
- Check that $\ell = 0$ term is even and $\ell = 1$ term is odd (remember: ϵ = sign(x), r = |x|)

Partial wave expansion: scattering amplitudes

- From the previous slide,

$$\Psi_{\text{ext}}\left(x\right) = \sum_{\ell=0}^{1} \epsilon^{\ell} A_{\ell} \cos\left(kr + \ell\frac{\pi}{2} + \delta_{\ell}\right)$$

- But we also have our old formula:

$$\Psi_{\text{ext}}\left(x\right) = e^{ikx} + \frac{i}{k} f_k\left(\epsilon\right) e^{ikr}$$

- Which we can split into even and odd parts (after a little math):

$$\Psi_{\text{ext}}\left(x\right) = \underbrace{\left[\cos kr + \frac{i}{k} f_k^{(0)} e^{ikr}\right]}_{\text{even}} + \epsilon \underbrace{\left[i \sin kr + \frac{i}{k} f_k^{(1)} e^{ikr}\right]}_{\text{odd}}$$

- Where we've also written: $f_k\left(\epsilon\right) = \underbrace{f_k^{(0)}}_{\text{even}} + \epsilon \underbrace{f_k^{(1)}}_{\text{odd}}$

Partial wave expansion: scattering amplitudes

- From the previous slide,

$$\Psi_{\text{ext}}(x) = \sum_{\ell=0}^{1} \epsilon^{\ell} A_{\ell} \cos\left(kr + \ell\frac{\pi}{2} + \delta_{\ell}\right)$$

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- Which we can split into even and odd parts (after a little math):

$$\Psi_{\text{ext}}(x) = \underbrace{\left[\cos kr + \frac{i}{k} f_k^{(0)} e^{ikr}\right]}_{\text{even}} + \epsilon \underbrace{\left[i \sin kr + \frac{i}{k} f_k^{(1)} e^{ikr}\right]}_{\text{odd}}$$

- Where we've also written: $f_k(\epsilon) = \underbrace{f_k^{(0)}}_{\text{even}} + \epsilon \underbrace{f_k^{(1)}}_{\text{odd}}$

Next: equate the 2 forms, deduce $f_k^{(0)}$ and $f_k^{(1)}$

Partial wave expansion: scattering amplitudes

- We get an the scattering amplitude components in terms of the phase shifts

$$f_k^{(\ell)} = \frac{k}{2i}\left(e^{2i\delta_\ell} - 1\right), \quad \ell = 0, 1$$

- However, with this formula we find σ_{abs} = 0, so we make a slight modification to allow for absorption:

$$f_k^{(\ell)} = \frac{k}{2i}\left(\eta_\ell e^{2i\delta_\ell} - 1\right), \quad \ell = 0, 1$$

$$\eta_\ell < 1 \Rightarrow \text{absorption}$$

- And the partial wave expansion for the 1D scattering amplitude is then

$$f_k(\epsilon) = \frac{k}{2i}\sum_{\ell=0}^{1} \epsilon^\ell \left(\eta_\ell e^{2i\delta_\ell} - 1\right)$$

Partial wave expansion: absorption cross section

- Using the partial wave expansion for the scattering amplitude, we get for 1D

$$\sigma_{\rm abs} = \frac{1}{2}\sum_{\ell=0}^{1}\left(1-\eta_\ell^2\right)$$

- Compare with the 3D result:

$$\sigma_{\rm abs} = \frac{\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\left(1-\eta_\ell^2\right)$$

Note one difference between 1D and 3D cross-section formulas:

- **In 1D cross sections are dimensionless**
- **In 3D cross sections have units of surface area**

Partial wave expansion: scattering cross section

- Using the partial wave expansion for the scattering amplitude, we get for 1D

$$\sigma_{\text{sca}} = \sum_{\ell=0}^{1} \left[2\eta_\ell \sin^2 \delta_\ell + \frac{1}{2} (1 - \eta_\ell)^2 \right]$$

- Compare with the 3D result:

$$\sigma_{\text{sca}} = \frac{2\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \left[2\eta_\ell \sin^2 \delta_\ell + \frac{1}{2} (1 - \eta_\ell)^2 \right]$$

Partial wave expansion: total cross section

- Using either $\sigma_{tot} = \sigma_{abs} + \sigma_{sca}$ or the optical theorem, we get for 1D

$$\sigma_{\rm tot} = \sum_{\ell=0}^{1} \left[2\eta_\ell \sin^2\delta_\ell + (1-\eta_\ell)\right]$$

- Compare with the 3D result

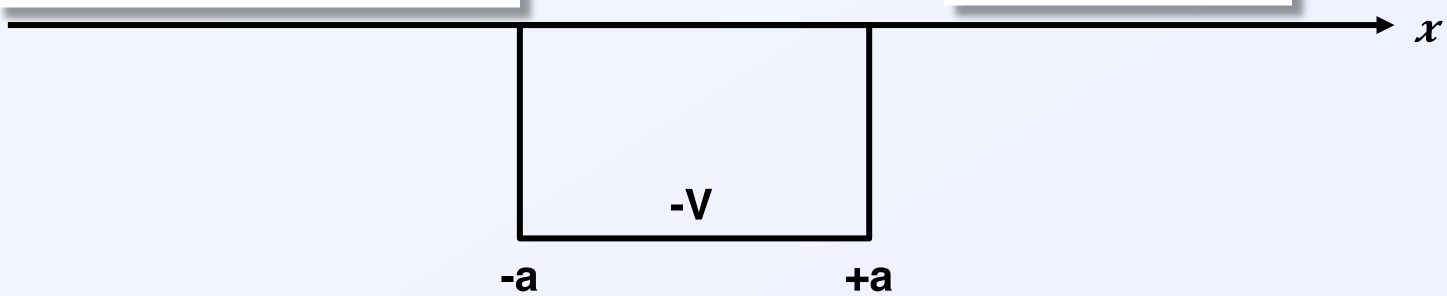
$$\sigma_{\rm tot} = \frac{2\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\left[2\eta_\ell \sin^2\delta_\ell + (1-\eta_\ell)\right]$$

Example: 1D square well with coupled channels

One incident wave, two outgoing:

$$\Psi_1(x) = e^{ikx} + R_1 e^{-ikx}$$
$$\Psi_2(x) = R_2 e^{-ikx}$$

$$\Psi_1(x) = T_1 e^{ikx}$$
$$\Psi_2(x) = T_2 e^{ikx}$$



Waves Ψ_1 and Ψ_2 are coupled through a potential V_c, i.e. we must solve the following TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\begin{pmatrix}\Psi_1(x)\\ \Psi_2(x)\end{pmatrix} - \begin{pmatrix}V & V_c\\ V_c & V\end{pmatrix}\begin{pmatrix}\Psi_1(x)\\ \Psi_2(x)\end{pmatrix} = E\begin{pmatrix}\Psi_1(x)\\ \Psi_2(x)\end{pmatrix}$$

Example: 1D square well with coupled channels

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\begin{pmatrix}\Psi_1(x)\\ \Psi_2(x)\end{pmatrix}-\begin{pmatrix}V & V_c\\ V_c & V\end{pmatrix}\begin{pmatrix}\Psi_1(x)\\ \Psi_2(x)\end{pmatrix}=E\begin{pmatrix}\Psi_1(x)\\ \Psi_2(x)\end{pmatrix}$$

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\begin{pmatrix}\Phi_+(x)\\ \Phi_-(x)\end{pmatrix}-\begin{pmatrix}V_+ & 0\\ 0 & V_-\end{pmatrix}\begin{pmatrix}\Phi_+(x)\\ \Phi_-(x)\end{pmatrix}=E\begin{pmatrix}\Phi_+(x)\\ \Phi_-(x)\end{pmatrix}$$

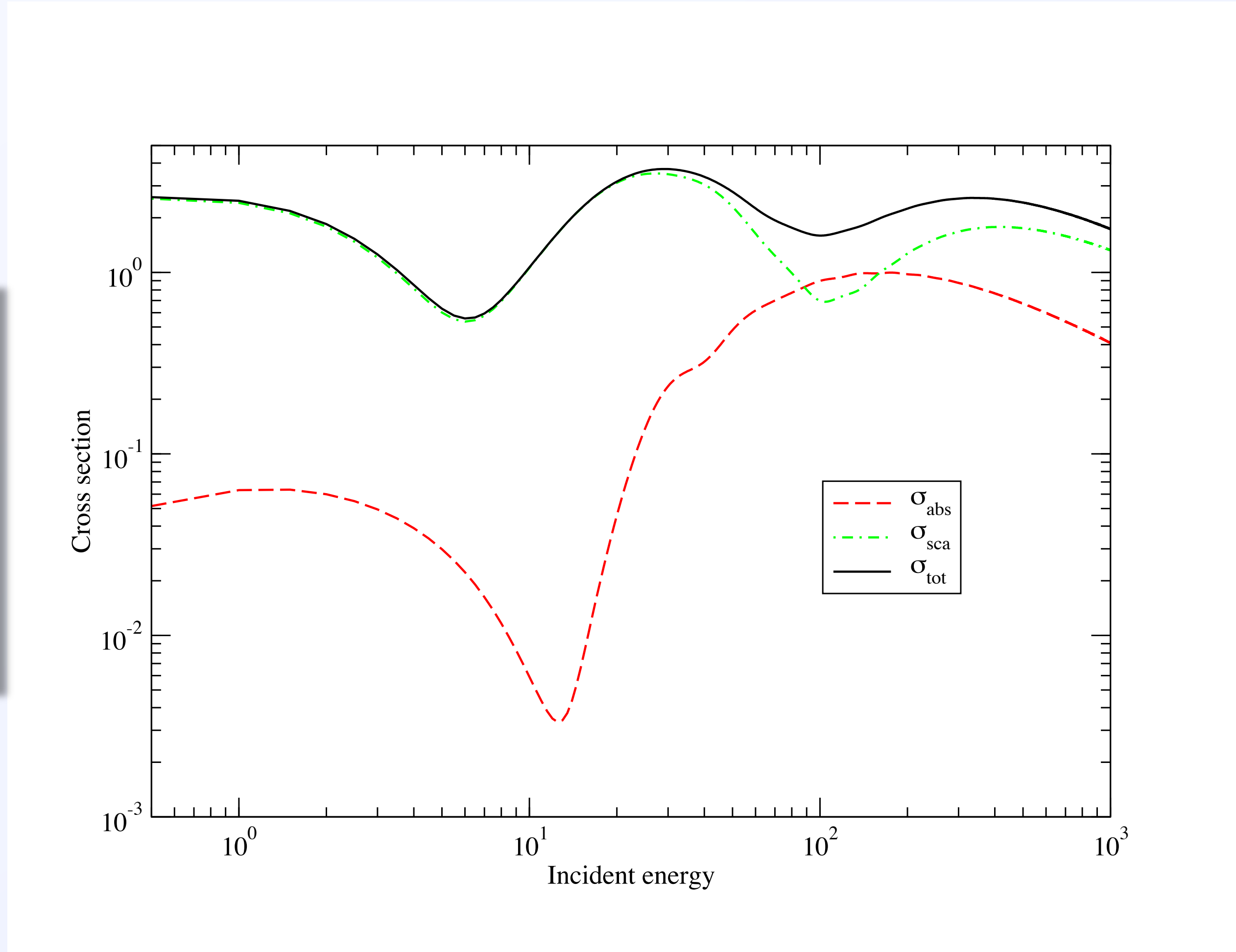
Transformation decouples the TISE

- **Solve two independent equations for Φ_+ and Φ_-**
- **Transform back to Ψ_1 and Ψ_2**
- **Calculate scattering amplitude**
- **Calculate cross sections**

Goal: calculate cross sections associated with channel 1

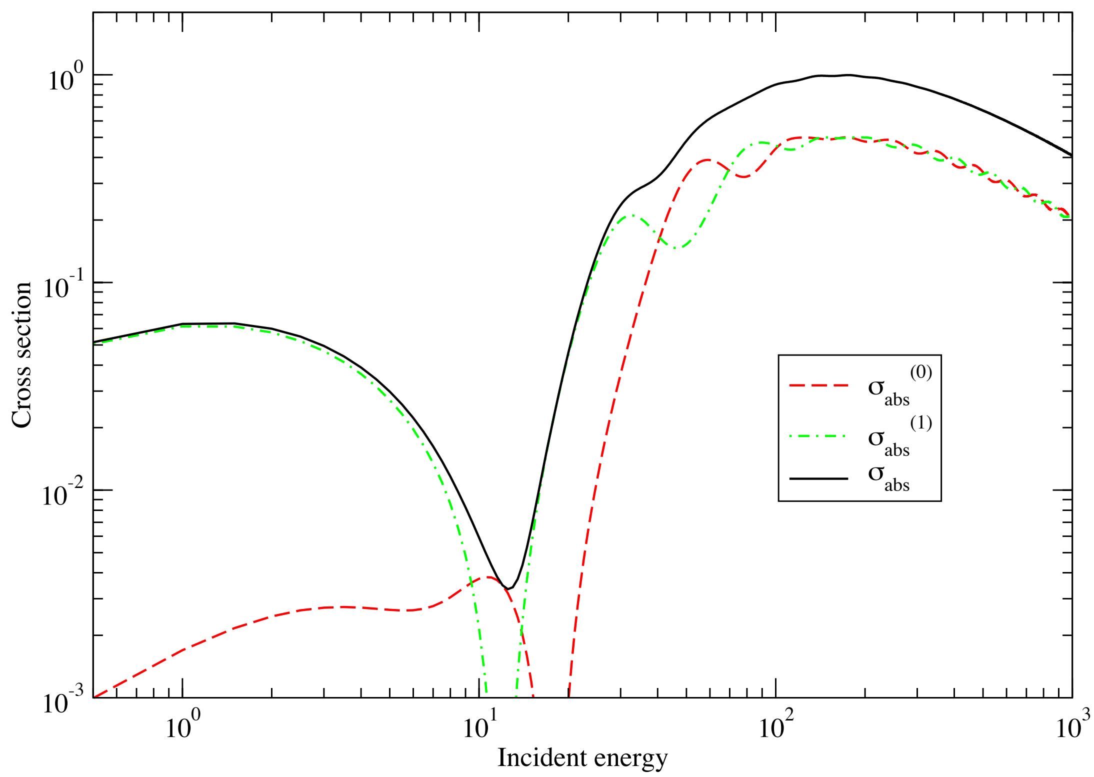
Cross sections

$$\frac{2m}{\hbar^2} = 0.05$$
$$V = 40$$
$$V_c = 20$$
$$a = 5$$



Let's take a closer look at the absorption cross section next

The absorption cross section, and its partial wave components



Can we understand the structure of the components?
What are those wiggles?

Analyzing σ_{abs}: plan of attack

- Wiggles ⇒ energies where σ_{abs} is enhanced ⇒ resonances
- We want to write $\sigma_{abs}(E)$ around those energies
  - Calculate logarithmic derivative of wave function at boundary

$$D \equiv \frac{a}{\Psi(r)} \frac{\partial}{\partial r} \Psi(r) \bigg|_{r=a}$$

    – Contains all info about $\Psi(x)$ and $V(x)$ needed to solve the TISE
  - Write $\sigma_{abs}(E)$ in terms of $D(E)$
  - Identify energies where $\sigma_{abs}(E)$ is enhanced
  - Taylor expand $\sigma_{abs}(E)$ around those energies

$$\sim \frac{\Gamma_\alpha \Gamma_\beta}{(E - E_r)^2 + \left(\frac{\Gamma_\alpha + \Gamma_\beta}{2}\right)^2}$$

Resonance cross section

- Recall $\ell = 0$ component of 1D wave function:

$$\Psi_{\text{ext}}(x) = \cos kr + \frac{i}{k} f_k^{(0)} e^{ikr}, \quad f_k^{(0)} = \frac{k}{2i}\left(\eta_0 e^{2i\delta_0} - 1\right)$$

- Calculate the logarithmic derivative at the boundary

$$D_0 = ika \frac{-e^{-ika} + \eta_0 e^{2i\delta_0} e^{ika}}{e^{-ika} + \eta_0 e^{2i\delta_0} e^{ika}}$$

- Solve for η_0 and calculate cross section assuming η_0 is real ($\Rightarrow \eta_0^2 = |\eta_0|^2$)

$$\sigma_{\text{abs}}^{(0)} = \frac{1}{2}\left(1 - \eta_0^2\right) = \frac{-2kay_0}{x_0^2 + (y_0 - ka)^2}, \quad D_0 \equiv x_0 + iy_0$$

Resonance cross section

- So far we have:

$$\sigma_{\rm abs}^{(0)} = \frac{-2kay_0}{x_0^2 + (y_0 - ka)^2}$$

- Note that $\sigma_{abs}^{(0)} > 0 \Rightarrow y_0 < 0$ and also $(y_0 - ka)^2 \neq 0$
  - So $\sigma_{abs}^{(0)}$ reaches local max when $x_0(E = E_r) = 0$
- Expand $x_0(E)$ about E_r:

$$x_0(E) \approx \left.\frac{dx_0(E)}{dE}\right|_{E=E_r} (E - E_r)$$

From R-matrix theory:

$$\left.\frac{dx_0(E)}{dE}\right|_{E=E_r} < 0$$

- Plug back into equation for $\sigma_{abs}^{(0)}$ above

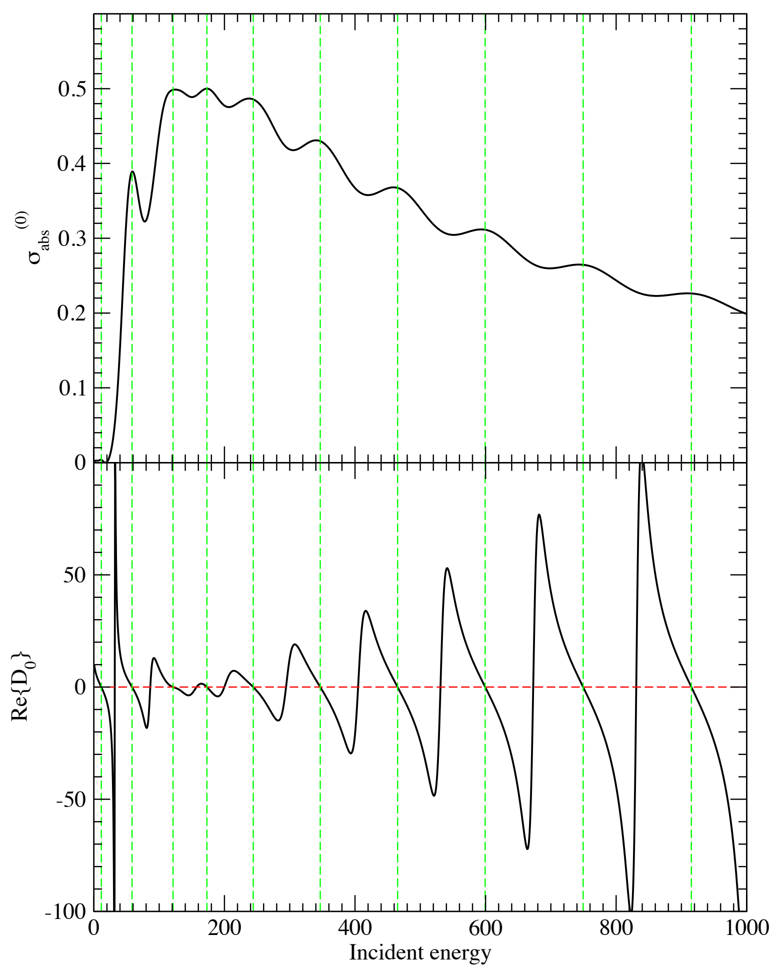
$$\sigma_{\rm abs}^{(0)} \approx \frac{1}{2}\frac{\Gamma_\alpha\Gamma_\beta}{(E-E_r)^2 + \left(\frac{\Gamma_\alpha+\Gamma_\beta}{2}\right)^2}$$

$$\Gamma_\alpha \equiv \frac{-2ka}{(dx_0/dE)|_{E=E_r}} > 0$$

$$\Gamma_\beta \equiv \frac{y_0}{(dx_0/dE)|_{E=E_r}} > 0$$

This result does not depend on the explicit form of $V(x)$

Resonances in our numerical example



Note: wherever x_0 = Re{D$_0$} has a negative slope, $\sigma_{abs}^{(0)}$ has a maximum!

$$\left.\frac{dx_0(E)}{dE}\right|_{E=E_r} < 0$$

You can check for yourselves that the same type of resonant behavior occurs in the ℓ = 1 component, i.e. $\sigma_{abs}^{(1)}$

Alternate approach: the optical model

- Not to be confused with the optical theorem!
- Mimic absorption through complex potential:

$$V(x) = \begin{cases} -V - iW & |x| \leq a \\ 0 & |x| > 0 \end{cases}$$

- Solution outside is

$$\Psi(x) = Ae^{i\kappa x} + Be^{-i\kappa x}, \quad \kappa = \sqrt{\frac{2m}{\hbar^2}(E + V + iW)}$$

- Next: calculate *j*(*x*) (i.e., flux in 1D)
  - If *W* = 0 then *j*(*x*) doesn't depend on *x* ⇒ no absorption
  - If *W* ≠ 0 then *j*(*x*) depends on *x* ⇒ absorption!

In realistic 3D problems, the optical model potential looks more complicated and is tuned to data

Resonances: link between time and energy pictures

- **Consider state $\Psi(t)$ with decay lifetime τ:**

$$\text{Prob}\,(t) = |\Psi\,(t)|^2 = |\Psi\,(0)|^2\, e^{-t/\tau}$$
$$\Rightarrow \Psi\,(t) = \Psi\,(0)\, e^{-iE_r t/\hbar} e^{-t/(2\tau)}$$

- **To get energy dependence, take Fourier transform:**

$$\Phi\,(E) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dt\, e^{iEt/\hbar} \Psi\,(t) = \frac{\hbar i \Psi\,(0)}{\sqrt{2\pi}} \frac{1}{(E - E_r) + \left(\frac{\hbar i}{2\tau}\right)}$$

- **Probability of finding state at energy E:**

$$\text{Prob}\,(E) = |\Phi\,(E)|^2 = \underbrace{\frac{\hbar^2\,|\Psi\,(0)|^2}{2\pi}}_{N_0 = \text{norm}} \frac{1}{(E - E_r)^2 + \frac{1}{4}\left(\frac{\hbar}{\tau}\right)^2}, \qquad \frac{\hbar}{\tau} \equiv \Gamma = \text{width}$$

Relation between width and lifetime of resonance peak: $\Gamma = \hbar/\tau$

Multiple resonances

- Suppose there are many resonances in some interval ΔE
- Want compound cross section: a + A → C (or C → a + A)
  - Nucleus trapped behind barrier, making repeated attacks
  - Reaction rate: $$\frac{1}{\tau_\alpha} = \underbrace{T_\ell}_{\text{crossing prob.}} \times \underbrace{R_b}_{\text{attack rate}}$$
- Model: equidistant resonances: $E_n = \bar{E} + nd, \quad n = 0, \pm 1, \pm 2, \ldots$
- Solution of TDSE related to TISE solutions ψ_n via

$$\Psi(t) = \sum_n a_n \psi_n e^{-iE_n t/\hbar} \quad \Rightarrow \quad |\Psi(t)|^2 = \left| \sum_n a_n \psi_n e^{-indt/\hbar} \right|^2$$

- Prob repeats at t, t+h/d, t+2h/d, … Therefore: $R_b = d/h$

$$\Rightarrow \quad \boxed{T_\ell = \frac{h/d}{\tau_\alpha} = 2\pi \frac{\Gamma}{d}}$$