Neutron width statistics in a realistic resonance-reaction model

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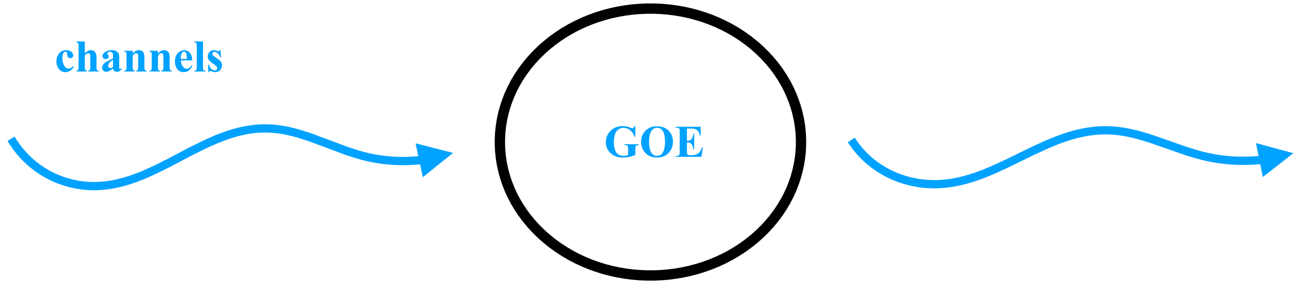
PF, G. F. Bertsch, and Y. Alhassid, arXiv:1710.00792 (2017)

- Statistical model of compound nucleus reactions.
- Recent experiment reporting violation of expected Porter-Thomas distribution (PTD) for neutron resonance widths in Pt isotopes.
- Overview of proposed theoretical explanations for PTD violation.
- Novel computational model for the simultaneous study of resonances and cross sections within the statistical model.
- Results for cross sections and neutron width fluctuations in the reaction n + ^{194}Pt.
- Conclusions: We find no violation of the PTD for neutron widths. Observation of apparent PTD violation could occur due to a common assumption in experimental analysis.
- Outlook for future work.

Statistical model of compound nucleus reactions



- Compound nucleus (CN): equilibrated system of incident particle and target nucleus. The rapid increase of the nuclear level density with energy makes a realistic description of CN states challenging.

- **Statistical model of CN reactions:** The CN states are described by the Gaussian orthogonal ensemble (GOE) of random-matrix theory [Mitchell, Weidenmüller, Richter RMP (2010)].

- Generic theory for chaotic quantum systems with time-reversal and rotational symmetries. Applications in atomic and mesoscopic physics.

- Widely used in reaction calculations. Significantly modifies Hauser-Feshbach theory of CN reactions.

- Used in experimental analysis, e.g. DICEBOX code to simulate gamma-ray cascades from CN resonances [Bečvár, NIM A (1998)].

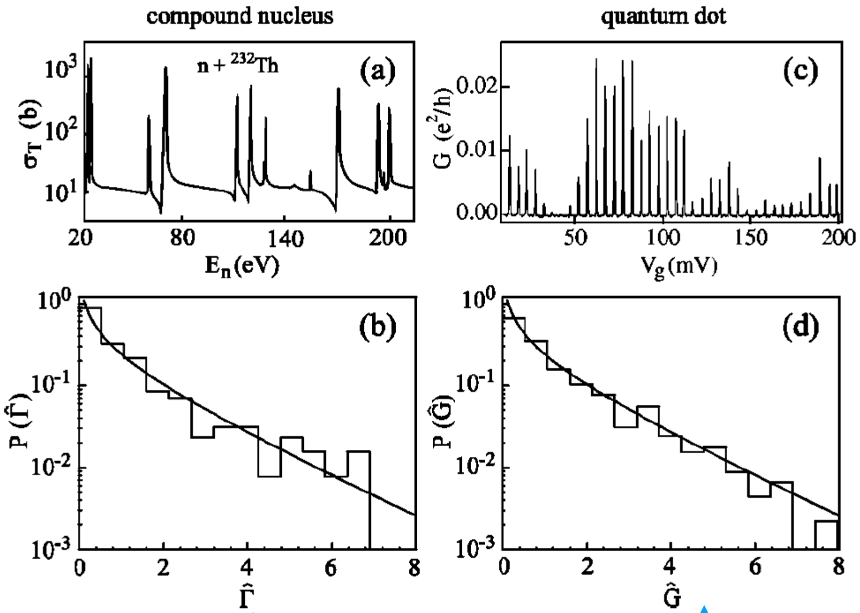
Experiment contradicts the statistical model

- Statistical model predicts the Porter-Thomas distribution for reduced width of any channel.

reduced neutron width

PTD

$$\gamma_{n,r} = \frac{\Gamma_{n,r}(E)}{\bar{\Gamma}_n(E)} \qquad \mathcal{P}_{\mathrm{PT}}\left(\frac{\gamma}{\langle\gamma\rangle}\right) = \frac{1}{\sqrt{2\pi\gamma/\langle\gamma\rangle}} e^{-\gamma/2\langle\gamma\rangle}$$



CN

quantum dot

- PTD observed in scattering through other chaotic quantum systems, e.g. quantum dots [Alhassid RMP (2000)].

- Experiment by Koehler *et al.* at Oak Ridge National Laboratory in 2010 measured many *s*-wave neutron resonances of Pt isotopes.

- Statistical analysis of reduced neutron widths excluded the PTD to a significance of 99.997%!

Sample	E_{max} (keV)	a_0 ($eV^{-(1/2)}$)	n_0	$\hat{\nu}_{expt}$
^{192}Pt	4.98	7.00×10^{-8}	153	$0.57^{+0.16}_{-0.15}$
^{194}Pt	15.93	2.25×10^{-7}	161	$0.47^{+0.19}_{-0.18}$
^{196}Pt	15.99	3.19×10^{-7}	68	$0.60^{+0.28}_{-0.26}$

Koehler, Bečvár, Krtička, Harvey, and Guber, PRL (2010)

from maximum likelihood fits. ν = 1 for PTD

Statistical model explanations for PTD violation

- Assuming the validity of the statistical model, how could PTD violation occur?

- Explanation I [Weidenmüller PRL (2010)]

  - usual experimental assumption is that the average neutron width is proportional to $E^{1/2}$.

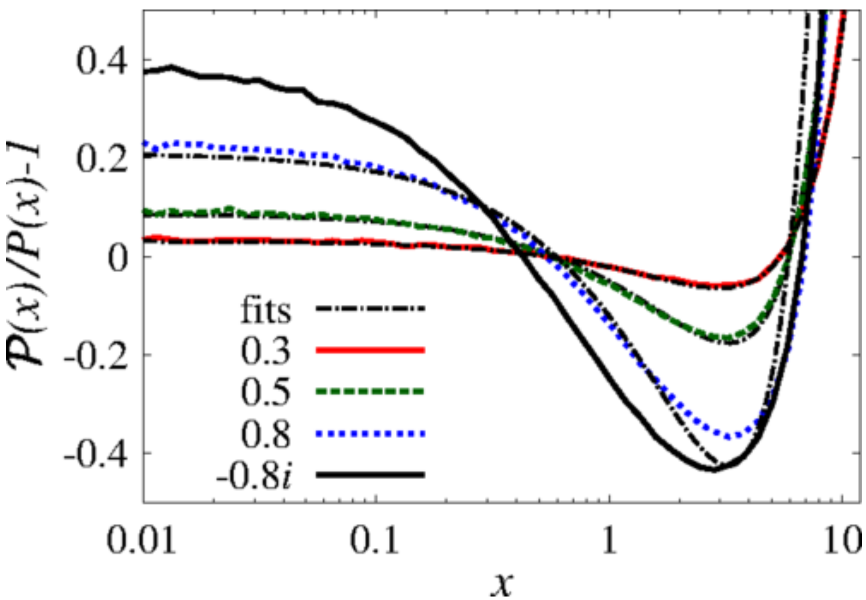
  - a near-threshold bound or virtual state of the neutron channel potential in Pt isotopes changes this energy dependence.

- Explanation II [Celardo, Auerbach, Izrailev, Zelevinsky PRL (2011); Volya, Weidenmüller, Zelevinsky PRL (2015)]

  - nonstatistical interactions of CN resonances through the channels can change reduced width distribution from PTD.

- No study of resonance width fluctuations of Pt isotopes in a realistic reaction model.

Volya, Weidenmüller, Zelevinsky

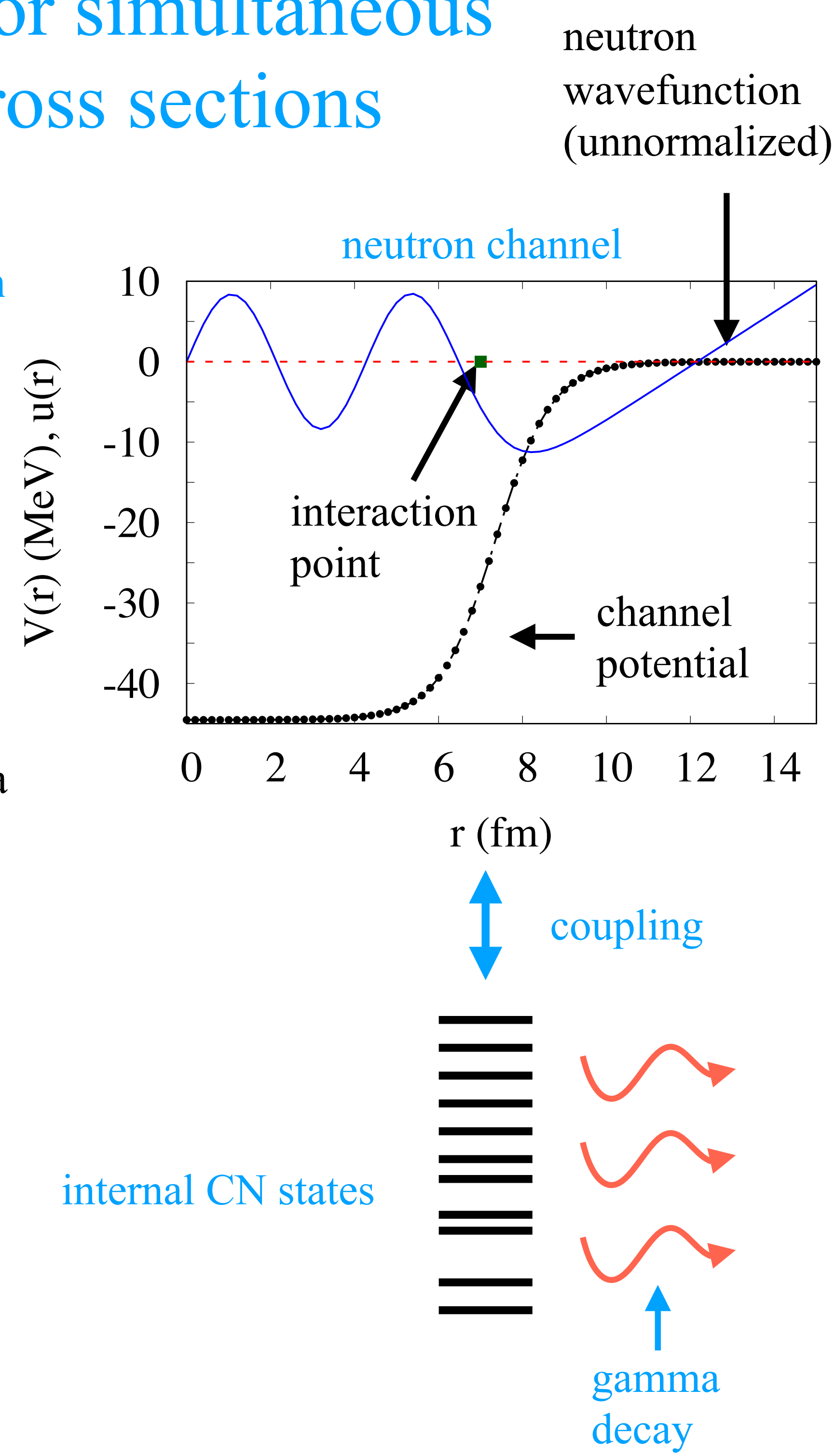


Novel computational model for simultaneous study of resonances and cross sections

- **Our model combines a realistic description of the entrance neutron channel with the usual GOE description of the internal CN states.**
- Based on the Mazama code of G. F. Bertsch [to be published].

$$\mathbf{H} = \begin{pmatrix} \mathbf{H_n} & \mathbf{V} \\ \mathbf{V}^T & \mathbf{H_c} \end{pmatrix}$$ ← model Hamiltonian

- Neutron channel described by discretized radial equation on a spatial mesh with Woods-Saxon channel potential.
- CN states have a GOE spectrum with average spacing D. Constant width Γ_γ added to each state to account for gamma decay.
- Coupling between neutron channel and each internal state μ at one spatial site r_e.
- Coupling strength: $v_\mu = (v_0 / \Delta r^{1/2})\, s_\mu$. v_0 is a coupling parameter. s_μ is a Gaussian random variable with zero mean, unit variance that accounts for GOE eigenvector fluctuations.



Resonance determination

- To find the complex resonance wavenumbers k_r, solve Schrödinger equation with appropriate boundary conditions

$$u(0) = 0$$

  - neutron wavefunction is regular at origin.

$$u(r) \to B(k)e^{ikr}$$ for large r

  - neutron wavefunction is purely outgoing.

$$\Rightarrow u(N_n + 1) = u(N_n)e^{ik\Delta r}$$

- With discretized approach, obtain a nonlinear eigenvalue problem (NEVP).

$$\mathbf{M}(k)\vec{u} = [\mathbf{H} - E - te^{ik\Delta r}\mathbf{C}]\vec{u}$$

$$t = \hbar^2/2m\Delta r^2 \ , \ \mathbf{C}_{ij} = \delta_{i,N_n}\delta_{ij}$$

- Solve NEVP with an iterative method to find resonance wavenumbers k_r.

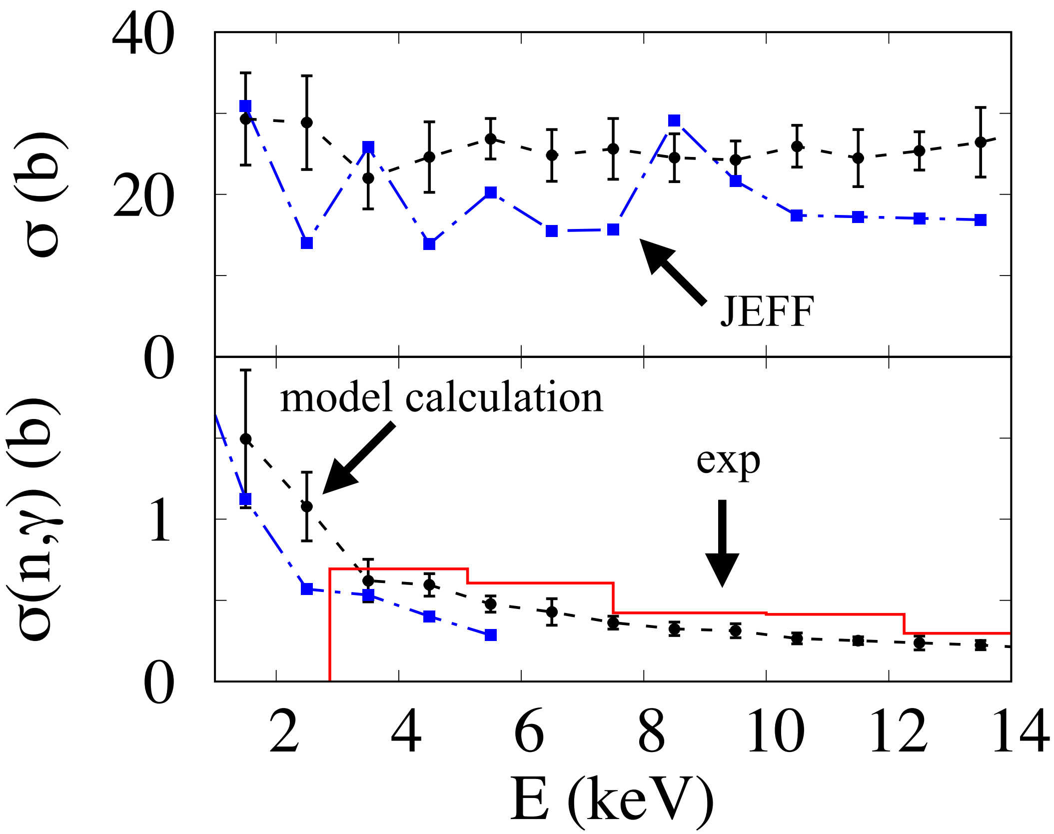
- Find resonance energies, total widths, and neutron widths from wavenumbers.

$$E_r - \frac{i}{2}\Gamma_r = \frac{\hbar^2 k_r^2}{2m}$$

$$\Gamma_{n,r} = \Gamma_r - \Gamma_\gamma$$

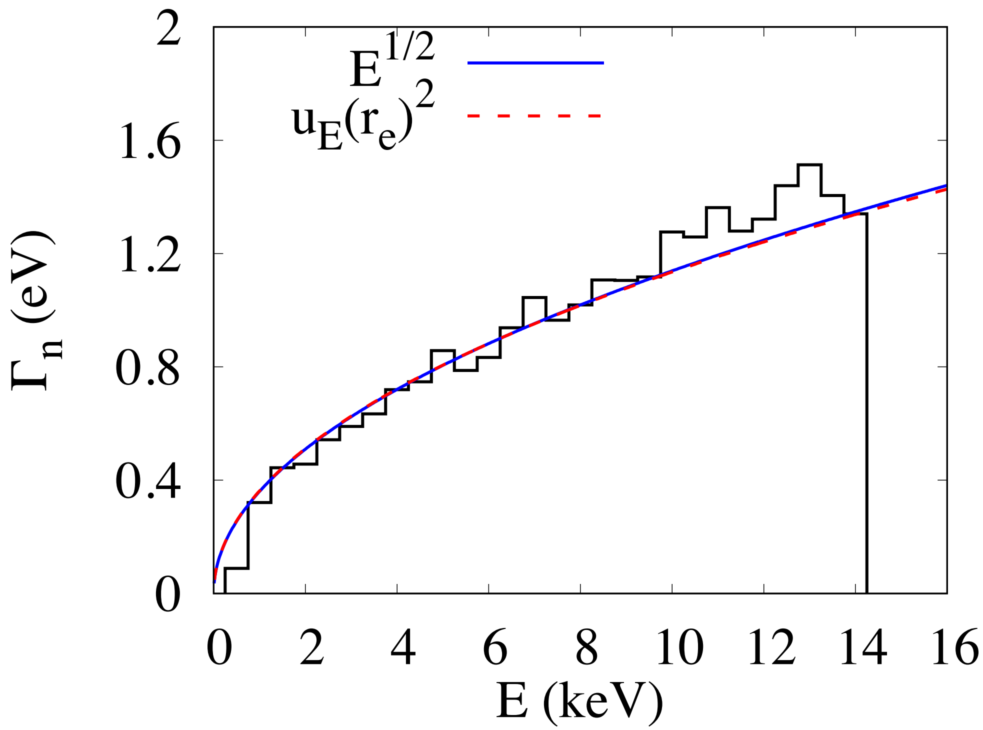
- Can calculate elastic and capture cross sections [details in additional slides].

Application to n + ^{194}Pt: Baseline Parameter Set



- (V_0, r_0, a_0) = (-44.54 MeV, 1.27 fm, 0.7 fm) from Bohr and Mottelson Vol I. D = 82 eV and Γ_γ = 72 meV from RIPL-3.
- Tune v_0 = 11 keV-fm$^{1/2}$ to reproduce roughly RIPL-3 neutron strength function parameter at 8 keV neutron energy.
- Compared our calculations with the JEFF-3.2 library (calculation based on the reaction code TALYS) and experimental capture cross sections [Koehler and Guber PRC (2012)].
- We know of no published elastic scattering cross sections for this reaction.

Average neutron width for baseline parameter set



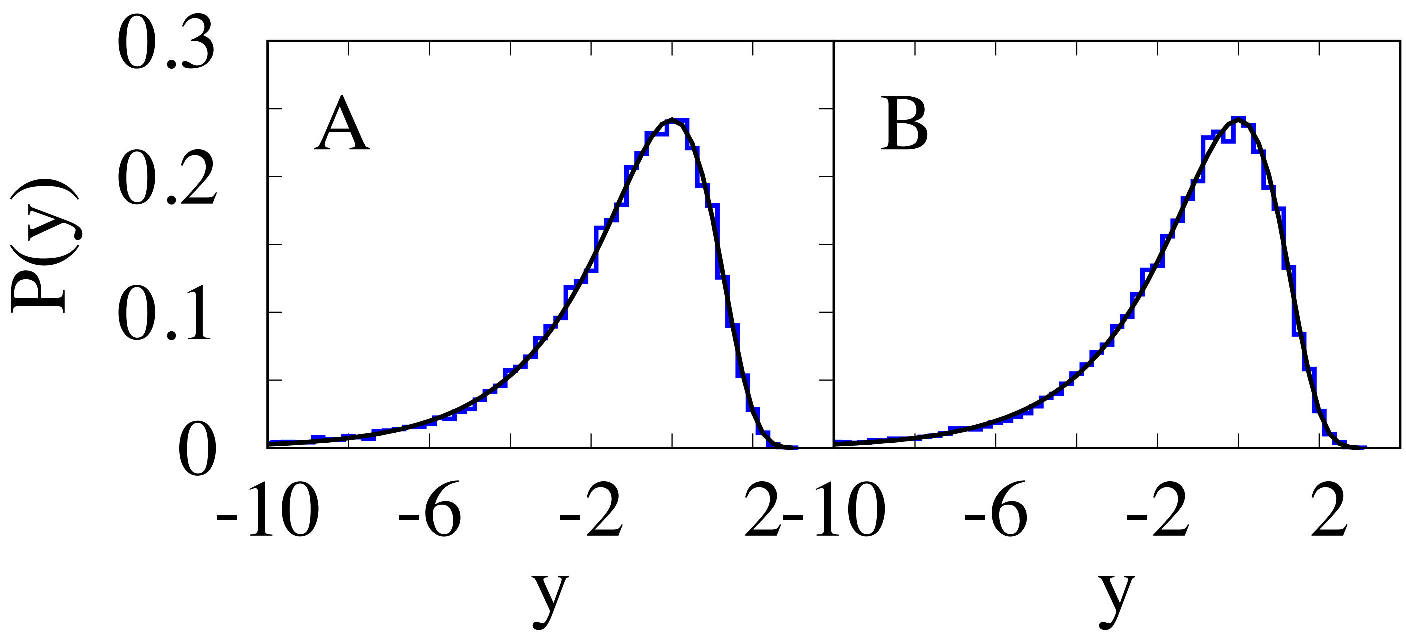
histogram is model calculations

- Reduced neuron width: $\gamma_{n,r} = \dfrac{\Gamma_{n,r}(E)}{\bar{\Gamma}_n(E)}$ ← neutron width; ← **average neutron width**

- We calculate the average neutron width by averaging all widths from 100 GOE realizations over bins of 0.5 keV width.

- Compare with $E^{1/2}$ and with neutron probability density (square of neutron wave function) at interaction point $u_E(r_e)^2$

Reduced neutron width distributions for baseline parameter set



Histograms are model calculations, solid lines are PTD

- Reduction A: extract reduced neutron widths with calculated average neutron widths.
- Reduction B: extract reduced neutron widths using assumption $\bar{\Gamma}_n(E) \propto \sqrt{E}$
- y = ln(x), where $x = \gamma/\langle\gamma\rangle$ is the normalized reduced neutron width.
- Model with baseline parameters follows statistical model predictions.

Physical parameter variation

- Do we see evidence for explanations for PTD violation within a reasonable parameter range?
- Two neutron channel potential depths
  - Baseline depth V_0 = -44.54 MeV from Bohr and Mottelson.
  - V_0 = -40.85 MeV with near-threshold bound state $E_0 \cong$ -0.54 keV.
- For each depth, we fit the coupling v_0 to the RIPL-3 strength function parameter $S_0 = 2 \times 10^{-4}$ $eV^{-1/2}$ at 8 keV.
- We varied v_0 by a factor of 2 smaller and larger than this fit value.

V_0 (MeV)	-44.54			-40.85		
v_0 (keV-fm$^{1/2}$)	11.0	5.5	22.0	1.97	0.98	3.94
$S_0 \times 10^4$ (eV$^{-1/2}$)	1.4	0.4	4.6	2.1	0.5	8.5
$\bar{\sigma}_{el}$ (b)	25.	19.0	28.	288.	300.	118.
$\bar{\sigma}_{\gamma}$ (b)	0.44	0.34	0.46	0.49	0.43	0.54

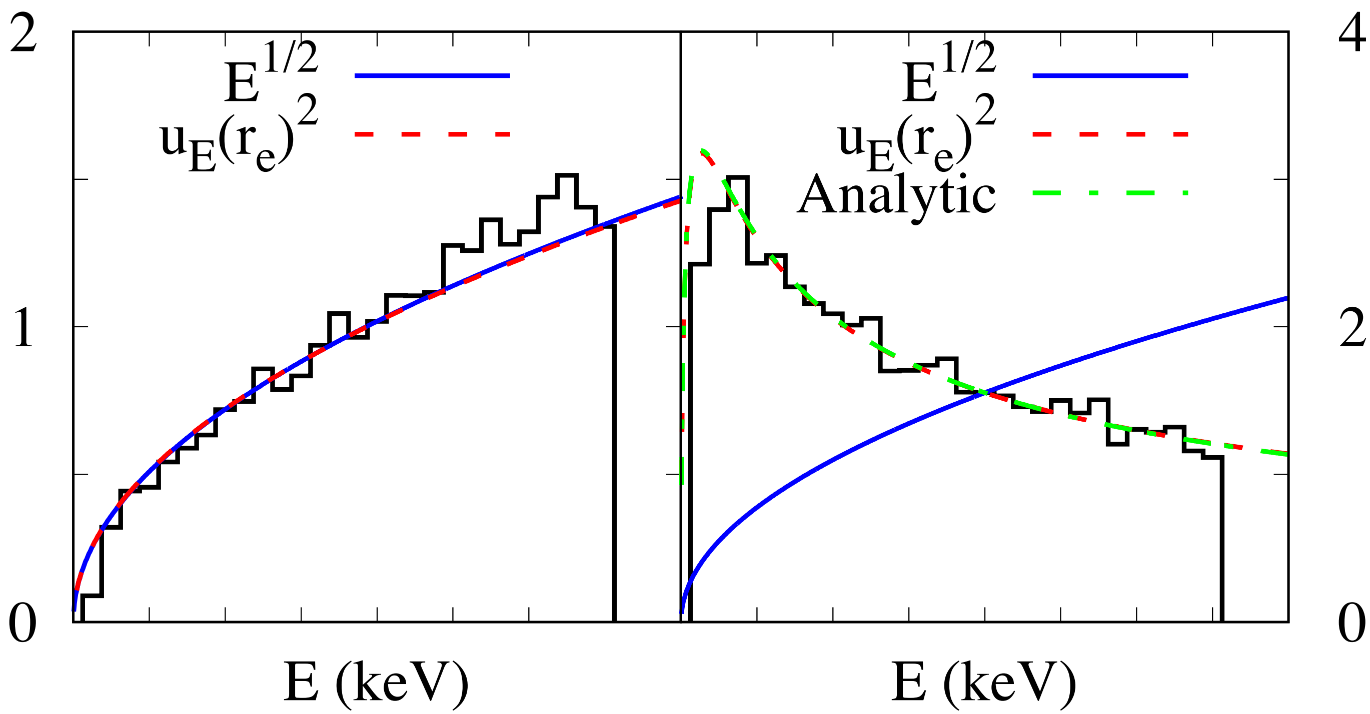
← $\bar{\sigma}_{el}$: at 8 keV

← $\bar{\sigma}_{\gamma}$: over bin 5-7.5 keV.
exp value: 0.6 b

Effect on average neutron widths

V_0 = -44.54 MeV
baseline depth

V_0 = -40.85 MeV
has bound state $E_0 \cong$ -0.54 keV



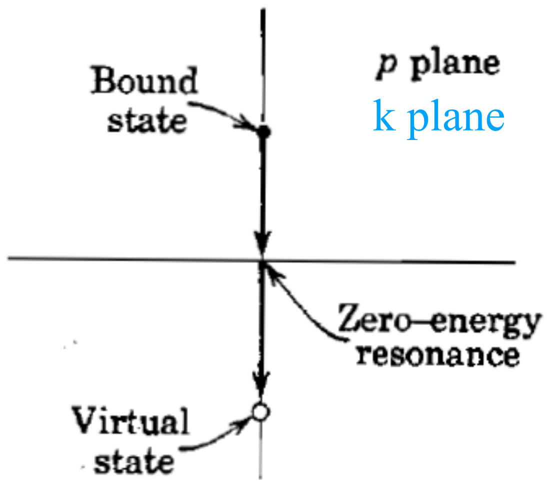
couplings fitted to RIPL-3 neutron strength function at 8 keV

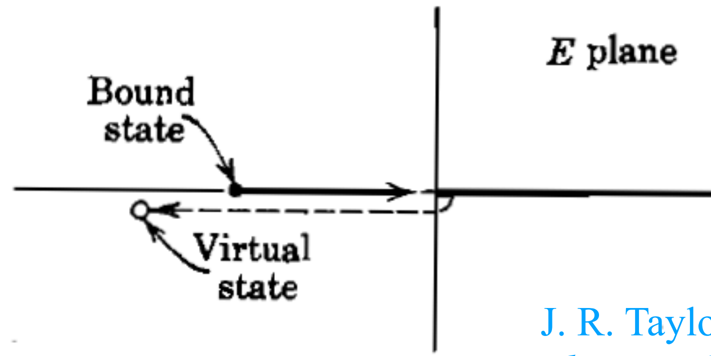
- In the presence of a near-threshold bound state of neutron channel potential, average neutron widths deviate noticeably from $E^{1/2}$.
- Analytic form for energy dependence of average neutron width derived by Weidenmüller [PRL 2010] fits model calculations if bound state energy E_0 = -0.54 keV is used.

$$u_E^2(r_e) \propto \frac{\sqrt{E}}{E + |E_0|}$$

- No dependence of the average width curve on the coupling strength.

Bound and virtual states





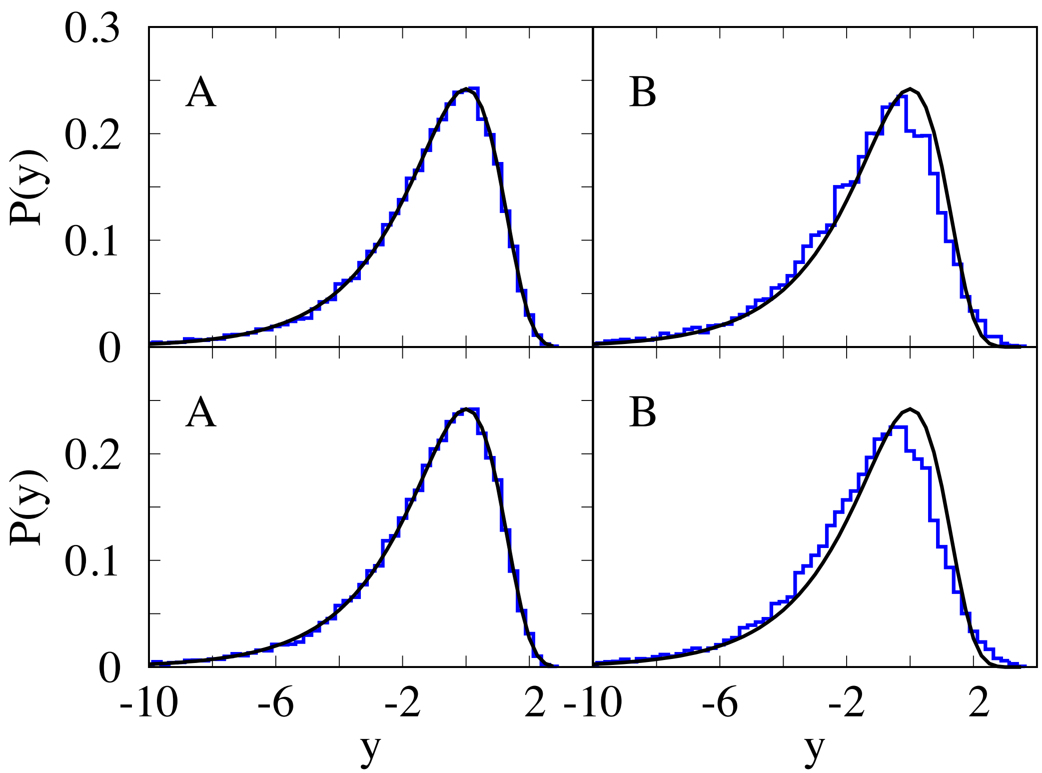
J. R. Taylor, *Scattering Theory: The Quantum Theory of Nonrelativistic Collisions* (Wiley, New York, 1972)

- Bound states of a potential are poles of the S matrix on the positive imaginary k axis.
- As an *s*-wave potential is made less attractive, a bound state crosses zero and becomes a virtual state on the negative imaginary k axis.
- The only parameter in the formula $u_E^2(r_e) \propto \dfrac{\sqrt{E}}{E + |E_0|}$ is the magnitude of the negative bound or virtual state energy $|E_0|$.
- If $|E_0|$ is relatively large compared to resonance energies, $E^{1/2}$ is a good approximation to average width energy dependence.
- Maximal deviation from $E^{1/2}$ is for zero-energy resonance $E_0 = 0$, where $u_E(r_e)^2 \propto E^{-1/2}$

Effect on reduced neutron widths

V_0 = -40.85 MeV, bound state with $E_0 \cong$ -0.54 keV

V_0 = -40.773 MeV, zero-energy resonance



histograms are model calculations
solid lines are PTD

couplings fitted to RIPL-3 neutron strength function at 8 keV

- Distributions extracted using reduction A match PTD well.
- Distributions extracted with reduction B, i.e. $\bar{\Gamma}_n(E) \propto \sqrt{E}$, are noticeably broader than the PTD.
- When the neutron channel has a zero-energy resonance, reduction B shows increased deviation from the PTD vs. the case of a near-threshold bound state.
- Maximum-likelihood fits of reduction B to a chi-squared distribution yield $\nu < 1$, in qualitative agreement with experimental value $\nu \cong 0.5$.
- No observable dependence of reduced width distribution on coupling strength.

Conclusions

- We find no violation of the PTD within the statistical model!
- Nonstatistical interactions of the resonances through the continuum do not significantly affect the reduced neutron width distribution.
- When the neutron channel potential has a near-threshold bound or virtual state, the energy dependence of the average neutron width deviates significantly from the usually assumed $E^{1/2}$ form.
- Distributions of reduced neutron widths extracted using the assumption $\bar{\Gamma}_n(E) \propto \sqrt{E}$ in this case deviate from the PTD and yield $\nu < 1$ when fitted to a chi-squared distribution.
- Omission of the modified energy dependence of the average neutron width in experimental analysis is the only viable explanation for the experimental findings within the statistical model.

Outlook

- Caveat: we can fully explain the experiment only if there is a weakly bound or virtual state with energy of only a few keV ($\lesssim$ 5 or so keV) for each of the three isotopes ^{192,194,196}Pt.

- A reanalysis of the experimental results using appropriate analytic form for the average neutron width with $|E_0|$ as a free parameter would be useful.

- Improvement of model predictions for neutron width fluctuations

  - Comparison with experimental elastic cross sections, which are sensitive to neutron channel potential.

  - Use of microscopic theory to limit possible values of v_0.

- How to expand the model to describe other reactions?

  - Realistic description of other channels. Multiple channels? Coupled channels?

  - Theory of average channel-CN coupling.

Thank you for your attention!

Cross section calculation in Mazama

- Developed by G. F. Bertsch [to be published]

$$u(r) \to A[e^{-ikr} - S_{nn} e^{ikr}]$$

S-matrix element for neutron channel

- Asymptotic scattering boundary condition for neutron wave function

- In the mesh representation, this BC holds for points N_n of the mesh edge and $N_n + 1$ just beyond the mesh edge. Thus:

$$\frac{u(N_n)}{u(N_{n+1})} = \frac{1 - \tilde{S}_{nn}}{e^{-ik\Delta r} - \tilde{S}_{nn} e^{ik\Delta r}}$$

$$\tilde{S}_{nn} = S_{nn} e^{ik(2N_n)\Delta r}$$

- Mazama Schrödinger equation becomes

$$[H - E]u(i) = tu(N_n + 1)]\delta_{i,N_n}$$

- Solving this equation yields:

$$\frac{u(N_n)}{u(N_n + 1)} = tG(E)_{N_n,N_n} \qquad G(E) = [H - E]^{-1}$$

$$\Rightarrow S_{nn} = e^{-i(2N_n)\Delta r} \left[\frac{1 - tG(E)_{N_n,N_n} e^{-ik\Delta r}}{1 - tG(E)_{N_n+1,N_n+1} e^{ik\Delta r}} \right]$$

- Calculate cross sections: $\sigma_{\text{el}} = \frac{\pi}{k^2} |1 - S_{nn}|^2 \ , \ \sigma_{\text{cap}} = \frac{\pi}{k^2} (1 - |S_{nn}|^2)$

Iterative method for finding resonances

- Nonlinear eigenvalue problem: **H** = Mazama Hamiltonian, $\mathbf{C}_{ij} = \delta_{i,N_n+1}$

$$\mathbf{M}(k)\vec{u} = [\mathbf{H} - E\mathbf{1} - te^{ik\Delta r}\mathbf{C}]\vec{u} = 0 \qquad E = \frac{\hbar k^2}{2m} \quad t = \frac{\hbar^2}{2m\Delta r^2}$$

- Taylor expand **M** at resonance solution k_r about guess k_g.

$$\mathbf{M}(k_r)\vec{u} = \mathbf{M}(k_g)\vec{u} + \left.\frac{d\mathbf{M}}{dk}\right|_{k=k_g}(k_r - k_g)\vec{u} = 0$$

$$\Rightarrow \mathbf{M}(k_g)\vec{u} = (k_g - k_r)\left.\frac{d\mathbf{M}}{dk}\right|_{k=k_g}\vec{u}\,.$$

← **generalized eigenvalue problem (GEVP)**

- GEVP is easily solved by inversion because dM/dk is diagonal

$$\mathbf{M}'(k_g) = -i\Delta r t e^{ik\Delta r}\mathbf{C} - 2k\frac{\hbar^2}{2m}\mathbf{1}$$

- Find complex eigenvalue $\lambda_{\min}$ of $[\mathbf{M}'(k_g)]^{-1}\mathbf{M}(k_g)$ with minimal modulus

- Iterate: $k_{g+1} = k_g - \lambda_{\min}$ until convergence is reached.

Bykov and Doskolovich
J. Lightwave Techno.
2013

Iterative method contd.: initial guesses

- To find initial guesses k_g expand nonlinear EVP to second order in $k\Delta r$. Obtain a quadratic eigenvalue problem (QEVP)

$$\left[\mathbf{U} - k\mathbf{V} - k^2\mathbf{W}\right]\vec{u} = 0 \qquad \mathbf{U} = \mathbf{H} - t\mathbf{C} \qquad \mathbf{V} = it\Delta r\mathbf{C}$$

$$\mathbf{W} = (\hbar^2/2m)\mathbf{1} - (t\Delta r^2/2)\mathbf{C}$$

- Solve QEVP by linearization: introduce $\vec{v} = k\vec{u}$ and obtain

$$\mathbf{U}\vec{u} - \mathbf{V}\vec{v} - k\mathbf{W}\vec{v} = 0$$

- Combine two conditions into GEVP

Tisseur and Meerbergen, SIAM Rev. 2001)

$$\begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{U} & -\mathbf{V} \end{pmatrix} \begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix} - k \begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{W} \end{pmatrix} \begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix} = 0$$

- Easily solved because **W** is diagonal. Yields $2(N_n + N_c)$ guesses k_g. We place restrictions on real and imaginary parts of corresponding guess energies to select initial guesses for neutron resonances.

Goodness of PTD fit to distributions

Model	baseline	M2	M3	M4	M5	M6
V_0 (MeV)	-44.54			-40.85		
v_0 (keV-fm$^{1/2}$)	11.0	5.5	22.0	1.97	0.98	3.94
χ_r^2 PTD A	0.9	0.9	1.1	0.9	0.9	1.2
χ_r^2 PTD B	0.8	0.9	1.9	202	206	2017

reduction A: with average width from code → (χ_r^2 PTD A)

reduction B: with √E ansatz → (χ_r^2 PTD B)

- Reduced chi-squared value:

$$\chi_r^2 = \frac{1}{N_b - 1} \sum_{i=1}^{N_b} \frac{(O_i - E_i)^2}{E_i}$$

O_i: number of counts in bin i; E_i: expected number from PTD; N_b: number of bins

- Rough criterion for a good fit is $\chi_r^2 \approx 1$
- Reduction A always matches PTD well.
- Baseline depth V_0 = -44.54 MeV: reduction B matches PTD.
- Depth with shallow bound state V_0 = -40.85 MeV: poor fit to PTD.

Maximum-likelihood fits

V_0 (MeV)	-44.54			-40.85		
v_0 (keV-fm$^{1/2}$)	11.0	5.5	22.0	1.97	0.98	3.94
$\nu_{\rm fit}$ A	1.0	1.0	0.99	1.0	1.0	0.98
χ^2_r fit A	0.9	0.9	1.1	0.9	0.9	1.1
$\nu_{\rm fit}$ B	1.0	1.0	0.97	0.88	0.88	0.88
χ^2_r fit B	0.8	0.9	1.6	46	47	248

PTD: ν = 1

- We found the best fit value of ν for a chi-squared distribution by maximizing the likelihood function.
- Our results for reduction B in the case of a near-threshold bound state yield ν < 1, in qualitative agreement with experimental value $\nu_{\rm fit} \approx 0.5$.

$$\mathcal{P}(x|\nu) = \frac{\nu(\nu x)^{\nu/2-1}}{2^{\nu/2}\Gamma(\frac{\nu}{2})} e^{-\nu x/2}$$

$$L(\nu) = \prod_{i=1}^{N_{\rm data}} \mathcal{P}(x_i|\nu)$$

likelihood function

normalized reduced width data points