Resonance Reaction Theory Revisited: Thermal Neutron Capture Cross Sections

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Plan of Talk

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- 2) Thermal Neutrons
- 3) Fluctuations in cross section
- vs. A.
- 4)2p-1h Doorways and their role
- in the capture process.
- 4) Test of chaoticity of σ vs. A
- 5) Correlation width $\Gamma_{\rm A}$ and
- possible connection to
- nucleosynthesis.

Introduction

- It is a common knowledge that the capture cross section of nuclei such as ¹⁵⁷Gd is very large, 225,000.00 barns
- Other nuclei have much smaller cross sections.
- The reaction,
- •
- $n + {}^{10}B \rightarrow {}^{11}B \rightarrow {}^{7}Li + \alpha$

- has a cross section of 4,000.00 barns (very large and used in BNCT).
- The cross section on radioactive nuclei such as ¹³⁵Xe = 2.0 x 10⁶ barns!
- Doorway resonance could be cause of such large values.

Resonance cross section

 $\sigma_c = 4 \times 10^6 [\text{barns}] \Gamma_n \Gamma_v [(E - E_R)^2 + (\Gamma/2)^2]^{-1}$ For ¹⁵⁷Gd target, the thermal neutron width is of the order of $\Gamma_{\rm n} = 10^{-4} D[E(eV)]^{1/2} = 0.1 meV$ (taking D to be 42.6 eV for 158 Gd at E* = 6-8 MeV) and that of Γ_v =0.15 eV, and taking the compound resonance energy to be at about the neutron energy of 0.025 eV, the capture cross section acquires the value,

 $\sigma_c = 1.78 \times 10^4$ [barns]

- On the other hand if the CN resonance is at, say, 22 eV, which corresponds to D/2 then,
- σ_c = 2.0[barns] !
- A great order of magnitude difference!!

Fluctuations





2p-1h Doorways and their role

- We basically get the "background" cross sections in the barns – 100's barns range of values.
- The very large capture cross sections seem to require something else. Possible 2p-1h doorway resonances.
- Such doorways were used in the past in parity violation studies with epithermal neutrons.

The issue here is to find a physical situation where the neutron width is enhanced by order of magnitudes.

 2p-1h doorway resonance to which the neutron is exclusively coupled as it is captured by the target. Thus $\sigma_{c} = 4 \times 10^{6} [barns] \Gamma_{n,D} \Gamma_{\gamma,D} [(E - E_{D})^{2} + (\Gamma_{D}/2)^{2}]^{-1}$

• $\Gamma_{\rm D} = \Gamma_{\rm D}^{\uparrow} + \Gamma_{\rm D}^{\downarrow}$, where $\Gamma_{\rm D}^{\uparrow}$ is the doorway neutron escape width which comes out to be about 0.18keV and $\Gamma_{\rm D}^{\downarrow}$ is the doorway damping width which can be calculated using the 2p-1h density of states. The gives $\Gamma_{\rm D}^{\downarrow} =$ 1.0 keV. (We used $\Gamma_{\rm D}^{\uparrow} / D_{\rm D} = \Gamma_{\rm q} / D_{\rm q}$)

The gamma decay is predominantly through the compound nucleus. Accordingly we have for the cross section,

- $\sigma_c = (1/\pi)^2 \times 10^6 [\text{barns}] \Gamma_{D, n} \Gamma_{D, \gamma} [(E E_D)^2 + (\Gamma_D)^2/4]^{-1}$
- with
- $\Gamma_{D,\gamma} = \Gamma_{D}^{\downarrow} \Gamma_{q,\gamma} [(E_{D} E_{q})^{2} + (\Gamma_{q})^{2}/4]^{-1}$



Density of 2p-1h states

- The capture cross section becomes, after taking $E_q = E_D$ (the doorway resonance with a damping width of $\Gamma_D = 1.0$ keV contains a $\Gamma_D/$ $D_a = 1.0$ keV/42.6eV = 22 CN resonances)
- $\sigma_c \approx (2/\pi)^2 \times 10^6 [\text{barns}] \Gamma_{D,n} (\Gamma_D^{\downarrow})^2 [(E_D)^2 \Gamma_{q,\gamma}]^{-1}$
- or with $E_D = 50 \text{ keV}$,

- $\sigma_c \approx (1/\pi)^2 \times 10^4 [barns/(eV)] \Gamma_{D, n}$
- which gives with $\Gamma_{\rm D, n} = \Gamma_{\rm D}^{\uparrow} = 0.18$ keV the value,
- $\sigma_c = 1.0 \times 10^5$ [barns]
- for the ¹⁵⁷Gd nucleus, to be compared to the empirical value of 2. 25 x 10⁵ [barns].
- It seems that a 2p-1h doorway could supply the mechanism of vary enhanced thermal cross section!

- How frequent this enhancement occurs? The ratio of the cross sections to that without the doorway is $\Gamma_{D,n}/\Gamma_{q,n}$. We calculated the probability of such an enhancement to be present in the sense that the width ratio attains a certain value η_0 and found it to be, $P(\eta_0) = (1/2\pi)[1 + \eta_0]^{-1}$,
- a very small number!!!

How Statistical is the cross section?

 The fluctuation seen in the capture cross section vs. A could be indicative of a random behavior which can be traced to the formation of the nuclei.

The correlation function:

- Energy: $C(\varepsilon) = 1/[1 + (\varepsilon/\Gamma_{\varepsilon})^2]$
- Or if an external parameter is varied,
- X : C(X) = $1/[1 + (X/\Gamma_X)^2]^2$

Density of Maxima

- The average density of maxima is given by
- $<n> = (1/2\pi)[C'''(z)|_{z=0}/(-C''(z)|_{z=0})]^{1/2}$

Brink and Stephen Phys. Lett. *5, 77 (1963)*

Density of Maxima

• Get, $< n_{s} > = 3^{1/2} / \pi \Gamma_{s}$ $x [(9p^2 - 18p + 10)/(5p^2 - 10p + 6)]^{1/2}$ And, $< n_x > = 3^{1/2}/2^{1/2}\pi\Gamma_x$ $[(7p^2 - 10p + 6)/(2p^2 - 3p + 2)]^{1/2}$ p is the tunneling probability, related to Γ/D . For our purpose of cross section fluctuation with A we take the second choice, namely, $< n_{\Delta} > = 3^{1/2}/2^{1/2}\pi\Gamma_{\Delta}$ $[(7p^2 - 10p + 6)/(2p^2 - 3p + 2)]^{1/2}$ and consider the case of p << 1 (isolated CN resonances (in energy). Get, $< n_{\Delta} > = 3/2^{1/2}\pi\Gamma_{\Delta}$ Thus $\Gamma_{\Delta} = 3/(2^{1/2}\pi < n_{\Delta} >)$







Numerical Simulations for open quantum dots

Random Matrix Theory (RMT)

 $S(\varepsilon) = 1 - 2\pi i W^{\dagger} (\varepsilon - H + i\pi W W^{\dagger})^{-1} W$



- We get 18 maxima in a range of A of 50. This gives us,
- $\Gamma_A = 1.8$ in units of A
- This value represents the range over which the chaotic system still maintains coherence

 Δ A = 1 or 2 is the number of neutrons captured in the nucleosynthesis process to form a certain element. We therefore attach a new and potentially important characteristic to the capture cross section vs. A, besides the historical connection to the strength function!

Conclusions

- Compound nucleus resonances can not explain the very large values of the capture cross section for a few nuclei.
- 2p-1h simple doorway resonances could supply the mechanism of enhancement of the cross section.
- The whole capture process vs. A is random.
- Can supply information about nucleosynthesis

Thank you !

Landauer Formula

The above S-Matrix can be written as

$$S = \left(\begin{array}{cc} r & t \\ t' & r' \end{array}\right)$$

where r is the reflection matrix and t is the transmission matrix. The conductance is calculated from the transmission matrix through the Landauer formula

$$G = \frac{2e^2}{h}T$$
 with $T = \operatorname{tr}(t^{\dagger}t)$

T is the dimensionless conductance which we analyse in the following.

The Correlation Functions

$C(\delta \epsilon)$ is expected to be a Lorentzian.



FIG. 2: Normalized transmission autocorrelation function $\widetilde{C}_{\varepsilon}(\delta \varepsilon) = C_{\varepsilon}(\delta \varepsilon)/\operatorname{var}(T)$ as a function of the energy $\delta \varepsilon$. Symbols correspond to ensemble averages for different number of channels N.

The agreement with a Lorentzian function is excellent.

The Average Density of Maxima for Energy Fluctuations



FIG. 3: Density of maxima $\langle \rho_{\varepsilon} \rangle \Gamma$ as a function of the number of open channels N. The symbols with statistical error bars correspond to our numerical simulations. The dashed line stands for the Gaussian process prediction.

Expect to approach to 0.55

Correlation Function for Fluctuation due to Variation of the Hamiltonian

 $C(\delta X)$ is expected to be a squared Lorentzian.



FIG. 4: Normalized transmission autocorrelation function $\tilde{C}_X(\delta X) = C_X(\delta X)/\operatorname{var}(T)$ as a function of the parameter δX . Dots correspond to numerical simulations for different N. Solid line is given by theory, Eq. (15). Insert: Fitted X_c versus $N^{1/2}$ showing a linear behavior, as indicated by the solid line.

The agreement with a squared Lorentzian function is excellent.

The Average Density of Maxima for External Parameter Variation



FIG. 5: Density of maxima $\langle \rho_X \rangle$ as a function of the number of open channels N in units of X_c . The symbols with statistical error bars correspond to our numerical simulations. The dahed line stands for the theoretical prediction

Expect to approach to 0.68

Correlations Functions in Open Quantum Dots with Finite Tunnel Barrier

* Introduce tunnel probability, Γ, for electrons to enter the QD.



FIG. 1. (Color online) Correlation function as a function of the parametric variation of energy. Transition from Lorentzian (dashed lines) to anticorrelation (solid line) as a function of symmetric Γ . The inset diagram $(\delta \varepsilon / \gamma) \times \Gamma$ show values of the correlation function in each color.

Correlations Functions in Open Quantum Dots with Finite Tunnel Barrier * For $\delta \epsilon = 0$, only magnetic field variation $\frac{C(\delta X)}{1/8\beta} = \frac{2\Gamma(1-\Gamma)}{1+(\delta X)^2} + \frac{2+\Gamma(3\Gamma-4)}{[1+(\delta X)^2]^2}$ * For $\delta B=0$, only electronic energy variation $\frac{C(\delta\epsilon)}{1/8\beta} = \frac{3\Gamma(2-\Gamma)-2}{1+(\delta\epsilon)^2} + \frac{4[1+\Gamma(\Gamma-2)]}{[1+(\delta\epsilon)^2]^2}$ Both cases show highly non-Lorentzian shape.

Number of Maxima in Case with Tunneling







FIG. 4. (Color online) The top (bottom) diagram shows the density of peaks $\langle \rho_{\varepsilon} \rangle$ ($\langle \rho_X \rangle$) for parametric variation of the electron energy (perpendicular magnetic field). The darker and lighter regions are explained in the strip on the right.

$$\langle \rho_{\varepsilon} \rangle = \frac{\sqrt{3}}{\pi} \sqrt{\frac{9\Gamma^2 - 18\Gamma + 10}{5\Gamma^2 - 10\Gamma + 6}}, \quad \langle \rho_x \rangle = \frac{\sqrt{3}}{\pi\sqrt{2}} \sqrt{\frac{7\Gamma^2 - 10\Gamma + 6}{2\Gamma^2 - 3\Gamma + 2}}$$

 \Rightarrow Get excellent agreement with numerical simulation "data".