HANDLING OF EXTERNAL LEVELS IN NEUTRON RESONANCE FITTING; APPLICATION TO ^{52}Cr

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ABSTRACT

Nuclear resonance cross section data must be parametrized for most applications by fitting resonance-theoretic (R-matrix) curves to the data points. The curves depend on the "internal" levels inside the fitted energy range but also on all the "external" levels outside. Without due account of the external levels one gets troublesome edge effects and problems with potential scattering between resonances. As the external levels are mostly unknown, various ad hoc devices for their simulation are being used, for example energy-dependent nuclear radii or representation by "picket fence" resonances, although more convenient and theoretically sound techniques are available that describe external levels statistically in terms of familiar parameters (strength function, effective radius etc.). A novel, especially convenient approximation accounts for the external levels by just one fictitious pair of very broad resonances. Similarly, fine-tuning to accurately known thermal cross sections is often done by laborious adjustment of a number of bound levels, although again a simple analytical recipe involving just one bound level has been available for decades. For illustration, these analytical techniques are applied to the resolved resonance region of the nonfissile nuclide ^{52}Cr. The distinction between channel radii and effective radii, crucial in the present context, is emphasized.

1. THE PROBLEM OF UNKNOWN EXTERNAL LEVELS

The resonance formalism almost exclusively used in neutron physics is R-matrix theory introduced by Wigner and Eisenbud (1947),[1] in the standard form established by Lane and Thomas (1958).[2]

It describes the cross section resonances that are due to quasi-stationary states of the compound nucleus in terms of real and energy-independent resonance parameters (resonance energies, spins, parities, decay amplitudes for elastic scattering, radiative capture, fission etc.). For technical applications the resonance cross sections must be Doppler-broadened and parametrized, with resonance parameters determined by adjustment of theoretical curves to well resolved resonance data. At present the resolved resonance region extends typically from zero to several keV for actinides (Th, U, Pu,...), and to about 1 MeV for structural materials (Fe, Ni, Cr,...). Clearly its upper boundary is not sharp and has increased over the years as instrumental resolution has improved.
R-matrix theory shows that the cross sections for scattering, capture, fission etc. in a limited energy range depend not only on the "internal" levels in that range but also on the "external" levels below and above. Problems arise in practical resonance fitting and parametrization work because below the neutron threshold ($E < 0$) the compound levels are unobservable and therefore principally unknown. Above the analyzed range, resonances may still be observable but less and less well resolved as energy increases, because instrumental resolution worsens while level density grows and average widths increase - all of which makes the distinction between single resonance peaks and unresolved multiplets increasingly difficult and eventually impossible.

Various approaches have been developed to cope with the problem of unknown external levels, in particular

- **A.** simulation of the unknown external levels by equidistant "picket fence"[3] or Monte Carlo sampled resonance ladders,
- **B.** replication of the internal level sequence both below and above the internal region,[4–6]
- **C.** simulation of external levels by a smooth "background" cross section added to the internal resonance contribution. This procedure was used for several nuclides in the Joint Evaluated File JEF2.2, e. g. for ^{237}U and ^{242}Cm.[7]

Method C is restricted, unlike methods A and B, to the rather coarse "many-level Breit-Wigner approximation" where resonance cross sections are represented as sums of single-level Breit-Wigner terms. In the more rigorous multilevel approximations employed in practically all modern resonance analyses it is not the cross section but the R matrix that must be supplemented by an external-level contribution.
These recipes are still being used although conceptually simpler, more convenient and well functioning analytical techniques can be derived easily from level statistics and have, in fact, been available since decades. These techniques and an even simpler one that has been developed more recently are reviewed in the following sections. The last section is alloted to an illustration of their efficiency: A recent reevaluation of the resolved resonance range of ^{52}Cr offered an opportunity to compare the analytical techniques with the replication of the internal sequence.

2. R-MATRIX PARAMETRIZATION OF RESONANCE CROSS SECTIONS

In order to see where and how the external levels appear in the theory we review the relevant equations, using essentially the notation of Lane and Thomas.[2] The partial cross section for a

transition from an entrance channel c to an exit channel c' depends mainly on the collision matrix (or S matrix) $\mathbf{U}$,

$$\sigma_{cc'} = \pi\lambda\!\!\!^{-2}_c g_c |\delta_{cc'} - U_{cc'}|^2, \tag{1}$$

where g_c is the spin factor and $2\pi\lambda\!\!\!^{-}_c$ the de Broglie wave length of relative motion of incident particle and target nucleus in the center-of-mass system. Each channel c is specified by a partition α of the compound system in two collision partners (e. g. incident neutron plus target nucleus or outgoing photon plus residual nucleus), and by their spin and parity quantum numbers (total angular momentum J, orbital angular momentum ℓ, channel spin s), so that $c \equiv \{\alpha J \ell s\}$. From the unitarity of the collision matrix – which expresses conservation of overall probability – it follows that the total cross section for entrance channel c,

$$\sigma_c \equiv \sum_{c'} \sigma_{cc'} = 2\pi\lambda\!\!\!^{-2}_c g_c (1 - \mathrm{Re}\ U_{cc}), \tag{2}$$

depends linearly on the collision matrix, whereas the dependence of the partial cross sections is quadratic, see Eq. (1). These equations are quite general. Resonances are introduced if the collision matrix is expressed in terms of the R matrix (see Lane and Thomas,[2] Lynn,[8] Fröhner[9])

$$U_{cc'} = e^{-i(\varphi_c+\varphi_{c'})} P_c^{1/2} [(\mathbf{1} - \mathbf{RL^0})^{-1}(\mathbf{1} - \mathbf{RL^{0*}})]_{cc'} P_{c'}^{-1/2}\,, \tag{3}$$

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E}\,, \tag{4}$$

$$L^0_{cc'} = (S_c + iP_c - B_c)\delta_{cc'}\,. \tag{5}$$

Three groups of physical quantities appear in these equations.

First, there are the resonance parameters, viz. formal level energies E_λ and transition amplitudes $\gamma_{\lambda c}$ for decay (or formation) of compound states λ via exit (or entrance) channels c. Eq. (4) shows that the formalism has all resonance parameters neatly wrapped up in the R matrix to which each level contributes one sum term (a hyperbola in terms of E). The $\gamma_{\lambda c}$ can be positive or negative, with practically random signs. The E_λ are eigenvalues and the $\gamma_{\lambda c}$ are eigenvector coordinates of the quantum-mechanical scattering problem considered in R-matrix theory, where the configuration space of a given number of nucleons is taken as composed of an interior region corresponding to compound states and an exterior or channel region corresponding to states with two separated collision partners. Internal and external wave functions must be matched, of course, at the boundary between both regions.

The second group, hard-sphere phase shifts φ_c, level shifts S_c, and centrifugal-barrier penetrabilities P_c, are known functions of $k_c a_c = a_c/\lambda\!\!\!^{-}_c$, where a_c denotes the channel radius at which exterior wave functions (spherical Hankel functions for neutrons, Coulomb wave functions for protons) must smoothly join the interior wave functions describing nonpartitioned compound states. (The interior wave functions are unknown but for R-matrix theory it is enough that they can formally be written as eigenfunction expansions).

The quantities B_c and a_c form the third group. They define the eigenvalue problem. Their choice is largely a matter of convenience. The B_c are prescribed logarithmic derivatives of the radial eigenfunctions at the channel or matching radii a_c. These radii must be chosen so large that the short-range nuclear interaction can be safely neglected if the distance r_c between the collision partners is larger, otherwise they are arbitrary. It is best to take them just slightly larger than the radius of the compound nucleus (see Lynn[8]). A reasonable choice for neutron channels is $a_c = (1.23A^{1/3} + 0.80)$ fm (independent of c), where A is the number of nucleons in the target nucleus, but resonance fits are not very sensitive to the exact choice: A variation of a_c and thus of the "potential" part of the collision matrix can be compensated to quite some extent by a variation of the resonance parameters, especially those of the external levels. The best choice for the boundary parameters B_c in the resolved resonance region is $B_c = -\ell$. This eliminates the shift factors S_c rigorously for the s-waves and at least at low energies also for the higher-order partial waves, which means the cross section peaks occur at the formal resonance energies E_λ, as they should, instead of being shifted. For photon and fission channels the S_c and P_c are usually taken as constants that can be absorbed in the resonance energies and corresponding partial widths, respectively.
At this point it must be mentioned that all important resonance parameter tabulations, e. g. those due to Mughabghab et al.[10] and Sukhoruchkin et al.[11] or the evaluated nuclear data files, contain not decay amplitudes but partial widths $\Gamma_{\lambda c}$ and total widths Γ_λ. These are defined by

$$\Gamma_{\lambda c}^{1/2} \equiv \gamma_{\lambda c}\sqrt{2P_c}\,, \tag{6}$$

$$\Gamma_\lambda \equiv \sum_c \Gamma_{\lambda c}\,, \tag{7}$$

with the conventions that (a) the P_c are to be calculated at the energies $|E_\lambda|$ (the absolute value being needed for bound levels, $E_\lambda < 0$), (b) that the tabulated partial widths $\Gamma_{\lambda c}$ carry the relative signs of the decay amplitudes $\gamma_{\lambda c}$ where relevant. These somewhat awkward conventions ensure that the decay amplitudes can be calculated from the tabulated information if necessary. The reason is historical: Initially resonances were analyzed in single-level Breit-Wigner approximation for which one needs only partial widths, i. e. squared decay amplitudes. The use of widths was retained even after it had become clear later on that one needs the decay amplitudes themselves to describe level-level interferences properly. From a principal viewpoint it would be clearly more appropriate to tabulate the decay amplitudes instead of the partial widths because

- strictly speaking a neutron width has no meaning below the reaction threshold E_c since the penetrabilities P_c vanish there ($E_c = 0$ for elastic, $E_c > 0$ for inelastic neutron channels),
- for the multichannel case the signs of the width amplitudes are important which get lost when the widths are calculated,
- and also because inconsistencies may occur when several independent sets of neutron resonance parameters are combined which have been calculated with different values of the channel radius. This difficulty was encountered in the ^{52}Cr re-evaluation work[6] when old available neutron widths covering the first resonances (1.6 – 50 keV) were combined with the parameters of the newly evaluated energy range (50 – 1400 keV).

Practical resonance fitting is always done by means of the least-squares method, either conventionally by merely maximizing the likelihood function or, more efficiently and rigorously, by Bayesian inference involving maximization of the entire posterior, i.e. the product of likelihood function and (Gaussian) prior, as is possible with the SAMMY code developed by N.M. Larson and F.G. Perey.[12] Since the dependence of observables such as transmission data or capture or fission yields on the resonance parameters is highly nonlinear one must iterate. In this context it ought to be understood that only the parameters of the first group, the E_λ and $\gamma_{\lambda c}$, must be adjusted. It is not advisable to adjust the channel radii, too. This would mean changing the entire eigenvalue problem and thus all eigenvalues and eigenvectors from one iterative step to the next. As a consequence, all penetration factors and hard-sphere phases of the second group would keep changing so that it would be hard to keep selected resonances invariant, for instance those that are already well fitted or the bound levels. In short, a sitting target would become a moving one, more difficult to hit. If, nevertheless, it is decided to adjust the channel radii, too, this ought to be done consistently: In any given iterative step the hard-sphere phases φ_c and the penetrabilities P_c and level shifts S_c should be calculated with the same channel radius. Notwithstanding popular practice (and misleading ENDF-6 conventions[13]) there is no decent theoretical justification to calculate φ_c with an "effective" or "scattering" radius R'_c differing from the channel radius a_c with which the P_c and S_c are calculated. This will become clearer in the next section.

3. RESONANCE-STATISTICAL REPRESENTATION OF EXTERNAL LEVELS

As only the resonance parameters proper are to be adjusted but not the channel radii, it might be asked how good fits can be achieved in regions where not resonances but potential scattering dominates the scattering and total cross section, notably in the valleys between resonances and in the thermal region below the first resonance. To answer this question we must take a look at the role played by the external level in the formalism. The only place where they appear is the R matrix. Certainly they do not appear in the hard-sphere phases.

Consider the practically most important variant of R-matrix theory introduced by Thomas (1955)[14] and independently by Reich and Moore (1958)[15]. It exploits the fact that the usually very many photon channels with relatively small partial widths can be "lumped together" which allows to replace the full R-matrix in the space of all reaction channels, Eq. (4), to a much smaller "reduced" R-matrix with elements

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} \qquad (c, c' \notin \gamma) \tag{8}$$

defined merely in the subspace of nonphotonic channels. The only trace left by the eliminated photon channels are the total radiation widths $\Gamma_{\lambda\gamma}$ in the denominators. The number of retained channels is quite small in practice. In neutron resonance fitting the elastic channel (c=c') and one or two inelastic or fission channels are all that is usually needed. For nonfissile nuclei there is only the elastic channel up to the first inelastic threshold so that for most applications the R matrix is actually an R function in Reich-Moore approximation. The capture cross section can be obtained as the difference between the total and the other partial cross sections.

Let us now split the reduced R matrix into a sum $\mathbf{R}^0$ over the external levels and a sum over the internal, explicitly considered levels ($\lambda = 1, 2, \ldots \Lambda$),

$$R_{cc'} = R^0_{cc'} + \sum_{\lambda=1}^{\Lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} \; . \tag{9}$$

The contribution of the external levels can be written as the difference between the sum over all levels and the sum over the internal levels, and these sums can be approximated by integrals,

$$\begin{aligned} R^0_{cc'} &= \Big(\sum_{\lambda} - \sum_{\lambda=1}^{\Lambda}\Big) \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} \\ &\simeq \Big(\int_{-\infty}^{\infty} - \int_{\bar{E}-I/2}^{\bar{E}+I/2}\Big) \frac{dE'}{D_c} \langle\gamma_c\gamma_{c'}\rangle \frac{E' - E + i\bar{\Gamma}_\gamma/2}{(E'-E)^2 + \bar{\Gamma}^2_\gamma/4} \, , \end{aligned} \tag{10}$$

where $\bar{E}$ and I are midpoint and length of the energy interval containing the internal levels. The reciprocal mean level spacing $1/D_c$ is the level density needed if the sum over levels is to be approximated by an integral, and $\bar{\Gamma}_\gamma$ is the average radiation width. Especially for heavy nuclei the radiation width, as a sum over very many partial radiation widths, does not fluctuate much from level to level, so that $\Gamma_{\lambda\gamma} \simeq \bar{\Gamma}_\gamma$. Since $(E' - E)^2 \gg \bar{\Gamma}^2_\gamma/4$ for the distant levels, we can neglect $\bar{\Gamma}^2_\gamma/4$ in the last expression. Furthermore, for pure compound reactions without direct interaction we may neglect the off-diagonal elements of the average matrix $\langle\gamma_c\gamma_{c'}\rangle$ because of the practically random signs of the $\gamma_{\lambda c}$. In addition, we introduce the pole strength s_c and its Hilbert transform, the so called distant-level parameter $R^\infty_c(E)$,

$$s_c \equiv \frac{\langle\gamma^2_c\rangle}{D_c}, \tag{11}$$

$$R^\infty_c(E) \equiv \mathop{\mathcal{C}\!\!\!\!\!\!\int}_{-\infty}^{\infty} dE' \frac{s_c(E')}{E' - E} \qquad , \tag{12}$$

where $\mathcal{C}\!\!\!\!\!\!\int$ denotes a principal-value (Cauchy) integral. With our approximations the real part of the first integral in Eq. (10) is then found to be $R^\infty_c(E)$. If we finally neglect the weak variation of s_c over the finite range of the remaining integrals we find [9,16]

$$R^0_{cc'}(E) = \Big[R^\infty_c(E) + 2s_c(\bar{E})\Big\{ \mathrm{ar\,tanh}\ \frac{E-\bar{E}}{I/2} + i\frac{\bar{\Gamma}_\gamma}{I}\Big[1 - \Big(\frac{E-\bar{E}}{I/2}\Big)^2\Big]^{-1}\Big\}\Big]\delta_{cc'}, \tag{13}$$

where the so-called area function $\mathrm{ar\,tanh}\ x \equiv (1/2)\ln[(1+x)/(1-x)]$, with $-1 < x < +1$, is the inverse hyperbolic tangent (often written arc tanh x although no arcus is involved or, in somewhat misleading fashion $\tanh^{-1} x$). The constant first term on the right-hand side is just the distant-level parameter, the second and third terms describe edge effects near the boundaries of the internal

range. Both edge terms become infinite at the boundaries of the range $(\bar{E} - I/2 \ldots \bar{E} + I/2)$, therefore these boundaries should be chosen outside the actual range of resonance analysis, for instance one mean spacing below and one mean spacing above the highest energy included in the analysis. The third term is often negligible. Employment of this analytical expression for $R^0_{cc'}(E)$ will be denoted **method D** in the next sections.

What about the rigorous non-reduced R matrix, without Reich-Moore approximation? The question is easily answered. We need only set $\Gamma_{\lambda\gamma} = \bar{\Gamma}_\gamma = 0$ everywhere in the derivation above to obtain

$$R^0_{cc'}(E) = \Big[R^\infty_c(E) + 2s_c(\bar{E})\,\mathrm{ar\,tanh}\;\frac{E-\bar{E}}{I/2}\Big]\delta_{cc'}. \tag{14}$$

This approximation for $R^0_{cc'}$ is available in the shape analysis codes FANAC[17] and SAMMY[12]. FANAC neglects the (weak) energy dependence of R^∞_c, SAMMY allows linear and quadratic components for $R^0_{cc'}(E)$ and also a linear behavior of the pole strength in the internal region (see ref. 12, section III.A.1.a). Practice has shown, however, that there is hardly any need for the refinements.

The replacement of sums by integrals and the associated introduction of the level density $1/D_c$ and of the pole strength via $\langle\gamma_c\gamma_{c'}\rangle/D_c = s_c\delta_{cc'}$ has resulted in a concise level-statistical description of the external levels which is much more convenient for resonance fitting than the use of fictitious external levels or of polynomial expansions of the type $R^0_{cc} = A(E-\bar{E}) + B(E-\bar{E})^2 + \ldots$ without any clear rationale for the choice of starting values. Our external-level matrix $\mathbf{R}^0$ is diagonal and contains only the three clearly relevant level-statistical quantities, R^∞_c, s_c and $\bar{\Gamma}_\gamma$. All three vary rather smoothly from nuclide to nuclide which makes it easy to find good starting values for a least-squares fit:

- The meaning of $\bar{\Gamma}_\gamma$ is obvious, and starting values need not differ from those for the radiation widths of the internal levels. Rough estimates can be obtained from the plots of measured average radiation widths given in the widely used "barn book" (Mughabghab et al.)[10] or from the systematics for transactinides given by Moore.[18]

- The pole strength $s_c = \langle\gamma_c^2\rangle/D_c$ is proportional to the neutron strength function $S_\ell = \langle\Gamma_n^\ell\rangle/D_c$ conventionally used in applied work,

  $$S_\ell = 2k_c a_c s_c\sqrt{1\ \mathrm{eV}/E}\,. \tag{15}$$

  This follows from the (historical) definition of the reduced neutron width as essentially the neutron width without the energy-dependence due to the centrifugal-barrier penetrability, hence proportional to the squared decay amplitude. The proportionality constant is chosen so that for s-wave channels the reduced width is simply the neutron width taken at the conventional reference energy $E_r = 1$ eV, i. e. $\Gamma_n^0 = 2P_0(E_r)\gamma_c^2$. With the same proportionality constant for other neutron channels, $c = \{nJ\ell s\}$, one gets the general form of the reduced neutron width

  $$\Gamma_n^c \equiv 2P_0(E_r)\gamma_c^2 = 2k_c a_c \gamma_c^2\sqrt{E_r/E}. \tag{16}$$

This entails Eq. (15) if we take $s_c = s_\ell$ and $S_c = S_\ell$ (i. e. depending only on ℓ) as is suggested by the optical model and agrees well with experiment. Estimates are readily obtained from the literature, for instance from the plots of s- and p-wave strength functions presented in the "barn book" (Mughabghab et al.).[10] For higher-order partial waves a rule of thumb says that the strength functions for $\ell = 0, 2, 4, \ldots$ are similar, and those for $\ell = 1, 3, 5, \ldots$ likewise.

- The distant-level parameter $R_c^\infty(E)$ is essentially the difference between the contributions to the R matrix from the resonances below and above E. It is negative if the levels below (usually the bound ones) have more strength than those above, positive if the levels above preponderate. The more distant levels contribute most (hence the name) whereas the contributions from levels around E cancel because there the integrand is practically an odd function of $E' - E$. Thus $R_c^\infty(E)$ is small and it is usually good enough to start a fit with $R_c^\infty(E) = 0$. In much of low-energy resonance work the concept of an effective nuclear radius

$$R_c' \equiv a_c(1 - R_c^\infty) \qquad \text{for s} - \text{wave channels} \tag{17}$$

is used instead of the distant-level parameters R_c^∞. Estimates of effective radii for given mass numbers are again readily available from plots in the "barn book".[10]

The concept of an effective nuclear radius originated as follows. In the general R-matrix formalism one can absorb the effect of the external levels approximately in the hard-sphere phases and the resonance parameters by means of the replacements

$$\varphi_c \to \varphi_c + \arg(1 - R_{cc}^0 L_c^0), \tag{18}$$

$$\gamma_{\lambda c} \to \frac{\gamma_{\lambda c}}{|1 - R_{cc}^0 L_c^0|} \equiv \alpha_{\lambda c}, \tag{19}$$

$$\gamma_{\lambda c} L_c^0 \gamma_{\mu c} \to \alpha_{\lambda c}(L_c^0 - R_{cc}^0 |L_c^0|^2)\alpha_{\mu c} \tag{20}$$

(cf. Preston[19], p.492). For the s-wave one has, with $B_c = 0$ (see, section 2), $L_c^0 = i\varphi_c = ik_c a_c$, so that at low energies, $k_c \to 0$, and with $R_{cc}^0 = R_c^\infty$ (Eq. (14) at $E = \bar{E}$), the replacement (18) is equivalent to replacement of the channel radius a_c by an effective radius for the calculation of the hard-sphere phase. For the potential scattering cross section one gets

$$\sigma_c^{\text{pot}} = 4\pi\lambda\!\!\!^{-2}_c g_c \sin^2\varphi_c \to 4\pi g_c R_c'^2 \qquad \text{for} \quad k_c a_c \to 0 \tag{21}$$

as if the channel radius were replaced by R_c', Eq. (17). It has been concluded that all hard-sphere phases ought to be calculated as $\varphi_c(k_c R_c')$ instead of $\varphi_c(k_c a_c)$, i. e. from effective radii, while the penetrabilities $P_c(k_c a_c)$ and the level shifts $S_c(k_c a_c)$ demand the unmodified channel radii a_c. This conclusion is wrong, notwithstanding fairly common practice and misleading ENDF-6 formats.

The effective radius is well defined and useful only for the s-wave, and even there only in the limit of vanishing energy, $k_c a_c \to 0$. The fundamental, generally valid concept is that of the distant-level parameter, not the effective radius, and all channel quantities, φ_c, P_c and S_c, ought to be calculated with the channel radius.

4. REPRESENTATION OF THE EDGE TERMS BY TWO BROAD RESONANCES (METHOD D')

The resonance-statistical representation of external levels is quite convenient for cross section parametrization but an even simpler one is obtained if one approximates the energy-dependent "edge" terms in Eq. (13) by the tails of two very broad resonances of equal strength, located symmetrically with respect to the mid-energy $\bar{E}$,

$$2s_c(\bar{E})\Big\{ \mathrm{ar\,tanh}\ \frac{E-\bar{E}}{I/2} + i\frac{\bar{\Gamma}_\gamma}{I}\Big[1-\Big(\frac{E-\bar{E}}{I/2}\Big)^2\Big]^{-1}\Big\}$$

$$\simeq \frac{\gamma^2}{E_- - E - i\Gamma_\gamma/2} + \frac{\gamma^2}{E_+ - E - i\Gamma_\gamma/2}. \tag{22}$$

We want to fix the three quantities $E_+ - \bar{E} = \bar{E} - E_-$, γ^2, and Γ_γ in such a way that the right-hand side becomes similar to the left-hand side. A suitable degree of similarity is attained if we demand, for example, that both sides have equal values, slopes (first derivatives) and curvatures (second derivatives) at the mid-energy $\bar{E}$. The resulting three equations can be solved exactly. The result can be further simplified with $\bar{\Gamma}_\gamma \ll I$ which yields the simple approximations

$$E_\pm \simeq \bar{E} \pm \frac{\sqrt{3}}{2} I, \tag{23}$$

$$\Gamma_{n\pm} = 2P_\ell(|E_\pm|)\gamma^2 \simeq \frac{3}{2} I S_\ell \sqrt{\frac{|E_\pm|}{1\ \mathrm{eV}}}, \tag{24}$$

$$\Gamma_\gamma \simeq \bar{\Gamma}_\gamma. \tag{25}$$

Insertion on the right-hand side of Eq. (23) (and utilization of Eqs. (6) and (15)) shows that they are tantamount to the approximations $\mathrm{ar\,tanh}\ x \simeq 3x/(3-x^2)$ and $1/(1-x^2) \simeq 3(3+x^2)/(3-x^2)^2$, where $x \equiv (E-\bar{E})/(I/2)$. Figure 1 shows the similarity between the level-statistical edge terms and the resonance pair approximation. The differences are small over most of the range. At the edges they become large but since the approximation stays finite there in contrast to the original expression this is not bad at all for parametrization purposes.

In the current ENDF-6 format it is trivial to store the parameters of two more resonances. There is, however, no place for the distant-level parameter (see section 6.2.1). In ENDF-6-oriented data

fitting it is therefore best to set it equal to zero – which implies $R'_c = a_c$, see Eq. (17) – and to adjust the two broad levels independently of each other, together with the internal resonances. Then one of them can become stronger than the other one which produces the imbalance originally described by the distant-level parameter. How well this worked in the ^{52}Cr resonance fitting work will be seen below.

5. NARROW BOUND LEVEL TO ENSURE CORRECT THERMAL CROSS SECTIONS

The simulation of external levels by the constant distant-level parameter and either the level-statistical edge terms in Eqs. (13) or (14) or a fictitious pair of broad levels with parameters given by Eqs. (23-25) is usually not accurate enough to guarantee, together with given internal levels, the thermal cross sections that for many nuclei are known very accurately. An exact reproduction of given thermal cross sections can be achieved, however, with just one more fictitious bound level[9,16].

We illustrate the approach with the case of a nonfissile nucleus ($\sigma_c = \sigma_{cc} + \sigma_{c\gamma}$, $\Gamma = \Gamma_n + \Gamma_\gamma$) for which the parameters of all internal levels ($\lambda = 1, 2, \ldots \Lambda$) and also a level-statistical approximation $\mathbf{R}^0$ for the external part of the R matrix are given. We want to determine the parameters E_0, Γ_n, Γ_γ of one additional bound ("negative") level so that prescribed thermal cross sections are reproduced exactly. At thermal energies the centrifugal-barrier penetrabilities P_ℓ for $\ell \geq 1$ are so small that only s-wave interaction need be considered. With the usual choice $B_0 = 0$ one has $L_c^0 = i\varphi_c = ik_c a_c$ and the Reich-Moore collision function for each s-wave channel is

$$U_{cc} = e^{-2ik_c a_c} \; \frac{1 + i\sum_\lambda \dfrac{\Gamma_{\lambda n}/2}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2}}{1 - i\sum_\lambda \dfrac{\Gamma_{\lambda n}/2}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2}} \qquad (c \in n). \tag{26}$$

The summation extends over all s-wave levels, internal as well as external ones, that have the spin and the parity implied by c. We now split the sum into three contributions, one from the internal levels ($\lambda = 1, 2, \ldots \Lambda$), another one from the special bound level that is to guarantee the correct thermal cross sections ($\lambda = 0$), and the third one from all the other external levels represented by R^0_{cc} as in Eq. (9). Solving for the second contribution ($\lambda = 0$) one gets

$$\frac{i\Gamma_n/2}{E_0 - E - i\Gamma_\gamma/2} = -\sum_{\lambda=1}^{\Lambda} \frac{i\Gamma_{\lambda n}/2}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} - ik_c a_c R^0_{cc} + \frac{U_{cc} - e^{-2ik_c a_c}}{U_{cc} + e^{-2ik_c a_c}} \equiv \Delta_{cc}. \tag{27}$$

The right-hand side, which we denote by Δ_{cc}, can be calculated from the given resonance parameters and from the prescribed cross sections if we use

$$U_{cc} = \left(1 - \frac{\sigma_c}{2\pi\lambda_c^2 g_c}\right) \pm i \sqrt{\frac{\sigma_{cc}}{\pi\lambda_c^2 g_c} - \left(\frac{\sigma_c}{2\pi\lambda_c^2 g_c}\right)^2} \qquad (c \in n) \tag{28}$$

which follows from the basic Eqs. (1) and (2). Separating real and imaginary part of Eq. (27) one finds

$$\text{Re } \Delta_{cc} = \frac{-\Gamma_n\Gamma_\gamma/4}{(E-E_0)^2 + \Gamma_\gamma^2/4} < 0, \tag{29}$$

$$\text{Im } \Delta_{cc} = \frac{-(E-E_0)\Gamma_n/2}{(E-E_0)^2 + \Gamma_\gamma^2/4} < 0 \quad \text{for} \quad E_0 < 0, \tag{30}$$

whence

$$E_0 = E - \frac{\text{Im } \Delta_{cc}}{\text{Re } \Delta_{cc}} \frac{\Gamma_\gamma}{2}, \tag{31}$$

$$\frac{\Gamma_n}{2} = -\frac{|\Delta_{cc}|^2}{\text{Re } \Delta_{cc}} \frac{\Gamma_\gamma}{2}. \tag{32}$$

With only two equations for the three unknowns E_0, Γ_n, Γ_γ we can choose one of them arbitrarily and then calculate the others. The weak variation of the radiation widths from level to level suggests to set Γ_γ equal to the average radiation width of the internal levels,

$$\Gamma_\gamma = \bar{\Gamma}_\gamma, \tag{33}$$

but other choices are possible. Obviously the three unknowns are determined only up to a common scale factor by the other cross section parameters and the prescribed thermal cross sections.
The sign ambiguity in Eq. (28) is due to the fact that the cross sections depend on $\text{Re } U_{cc}$ and $|U_{cc}|^2$ only. Usually the plus sign can be discarded immediately because it yields $E_0 > 0$ contrary to the assumption of a bound level. It should be noted that all the (s-wave) neutron widths in our equations are to be calculated at the thermal energy E from the nominal (tabulated) neutron widths as

$$\Gamma_{\lambda n}(E) = \Gamma_{\lambda n}(|E_\lambda|)\sqrt{\frac{E}{|E_\lambda|}}, \tag{34}$$

as the nominal neutron widths for all levels, bound or unbound, are defined by $\Gamma_{\lambda n} \equiv \Gamma_{\lambda n}(|E_\lambda|) = 2P_0(|E_\lambda|)\gamma_{\lambda n}^2$ in applied neutron resonance theory. This convention, already mentioned after Eq. (7), and used for the neutron width (Eq. (24)) of the broad bound level, allows to define and list neutron widths for bound as well as unbound levels on the same footing. Generalization to thermally fissile nuclei and to unknown level spins is possible at least in MLBW approximation. The resulting equations are given in reference 20.

With the bound-level parameters calculated analytically in this way measured cross sections are usually well reproduced not only at the thermal energy, $E = 25.3$ meV, but in the entire region below the first resonance.
Sometimes it happens, however, that the calculated fictitious bound level is closer to the neutron threshold than the first unbound resonance (i. e. $|E_0| < E_1$). Although the calculated cross section curve goes then through the prescribed thermal point, the typical $1/v$ behavior of σ_γ is obtained only below $|E_0|$. Above that energy the curve tends towards a $1/v^5$ behavior until the resonance at E_1 causes it to rise again. This behavior follows already from the single-level Breit-Wigner formula,

$$\sigma_\gamma = \pi\lambda^2 \frac{g\Gamma_n(E)\Gamma_\gamma}{(E-E_0)^2 + \Gamma(E)^2/4} \,, \tag{35}$$

with $\Gamma(E) = \Gamma_n(E) + \Gamma_\gamma + \Gamma_f$ and $\Gamma_n(E) = \Gamma_n(|E_0|)\sqrt{E/|E_0|}$, in the limit of very small or very large E. The asymptotic behavior due to a *bound level* at $E_0 < 0$ is the same as that due to an *unbound level* at the mirror energy $|E_0| > 0$ as shown in Fig. 2. If the experimental data show a similar deviation from $1/v$ this constitutes clear evidence for a bound level close to the neutron threshold. If on the other hand the experimental data below the first unbound resonance do not deviate much from $1/v$ (which entails a Westcott factor[21] close to unity) one must shift the computed onset of the deviation (near $|E_0|$) to energies above the first resonance where it becomes unimportant because other resonances dominate. This is easily accomplished, without further change of the computed cross sections at the thermal energy, by common upscaling of the resonance energy and the partial widths of the fictitious narrow levels (see Eqs. 32-33) until $|E_0| > E_1$.

6. ILLUSTRATIVE COMPARISON OF SEVERAL METHODS

6.1 REPLICATION METHOD (B)

We can illustrate how well the analytical methods D and D' work if we compare them with a recent re-evaluation of the resolved resonance region of the nonfissile medium-mass nucleus ^{52}Cr (Bouland [6]) that was performed with the replication method B: The unknown external s-wave levels had been simulated by shifting a sample of 19 true s-wave resonances taken from the internal energy range both into the energy region below the neutron threshold and into the region above the resolved resonance range (0 - 1400 keV). In this method, already used in previous re-evaluation work for heavy isotopes,[4,5] the replicated neutron widths must of course be corrected for their energy dependence, so that in effect the reduced neutron widths (or decay amplitudes) are replicated and the value of the s-wave strength function ($S_0 = \bar{\Gamma}_n^0/D_0$) obtained in the internal energy range is preserved. In contrast to heavy nuclides the resolved-resonance range of ^{52}Cr is so wide that the energy dependence of the level density cannot be neglected. The resonance spacings of the external levels were therefore modified so as to be consistent with the level density formula of Gilbert and

Cameron.[22] Furthermore, the parameters of the first two bound levels were adjusted to the experimental thermal capture and scattering cross sections ($\sigma_\gamma = 0.76 \pm 0.06$ b[23] and $\sigma_n = 2.96 \pm 0.02$ b[24] at $E = 25.3$ meV).
Figs. 3-6 show the excellent fit obtained with the fictitious levels thus determined to the low-energy capture cross sections of Pomerance[23] and of Kapchigashev and Popov[25], and simultaneously to the ORNL transmission data[26] between 45 keV and 1400 KeV. The quality of the latter fit is indicated by the value 1.71 of the goodness-of-fit parameter (chi-square divided by the number of data points, χ^2/n). Clearly method B simulates the influence of the external s-wave levels quite well, in particular the edge effects described by the $\mathrm{ar\,tanh}\ x$ term of Eqs. (13) and (14). As mentioned already the effect of external levels is sometimes approximated by calculating the hard-sphere scattering phase shifts from an effective nuclear radius R' instead of the channel radius as would be more correct. In the particular case of ^{52}Cr there was no need for an R' value differing from the s-wave channel radius. This indicates similar strength of the fictitious levels below and above the internal energy range as is, indeed, to be expected from the replica construction.
The disadvantage of method B is that it requires a large number of iterations to converge. Moreover, when it is applied to heavy isotopes with typically hundreds of internal levels, complete replication of the internal level sequence in an evaluated file is impractical and calls for reduction to a smaller number of fictitious resonances. In the recent ^{235}U re-evaluation,[5] for example, the 6330 fictitious levels (2×3165) were reduced to 20 external levels, 10 below and 10 above the resolved resonance range (0-2250 keV). With the analytical methods D and D' presented in this paper there is no such storage problem. Moreover, they converge much faster as will be shown in the next sections.

6.2 ANALYTICAL METHODS

6.2.1 LEVEL-STATISTICAL REPRESENTATION OF THE EXTERNAL PART OF THE R MATRIX (METHOD D)

As already mentioned, the program SAMMY[12] permits statistical representation of the external part, Eq. (14), of the general R matrix. Strictly speaking, for the Reich-Moore approximation employed in SAMMY Eq. (13) would be more appropriate but the difference is negligible as long as the radiation widths are much smaller than the length of the internal range, $\bar{\Gamma}_\gamma \ll I$, which is certainly true for ^{52}Cr: The radiation widths are of order 1 eV while the length of the analyzed interval is 1400 keV. (In order to keep the calculation finite the limits of the internal range were taken as $\bar{E} - I/2$=-30 keV and $\bar{E} + I/2$=1430 keV, about one mean level spacing outside the lower and upper boundaries of the analyzed interval.)
At first the external-level calculation was restricted to the s-wave contribution, with the following prior values of the level-statistical parameters,

$$R_0^\infty = -0.1, \qquad s_0 = 0.12208$$

(treated as constant over the internal range). This s-wave pole strength corresponds to the strength function $S_0 = 3.031(\pm 0.7)$ and the channel radius $a_0 = 5.76$ fm obtained in the recent re-evaluation.[6] The Bayesian SAMMY fit to the ORNL transmission data[26] in the energy range 0

– 1400 keV yielded a perfectly satisfactory adjustment ($\chi^2/n = 1.83$) with the posterior values

$$R_0^\infty = +0.0975, \qquad s_0 = 0.1253.$$

With this distant-level parameter and the chosen channel radius of 5.76 fm one gets $R' = 5.2$ fm for the effective radius, in complete agreement with the JEF2.2 evaluation[7] and the "barn book".[10] Inclusion of the external $p_{1/2}$ and $p_{3/2}$ levels, via a p-wave strength function of $S_1 = 0.51(\pm 0.08)$ and equal channel radii for both p-wave channels, $a_1 = 5.76$ fm, as given in ref. 6, improved the fit only slightly (to χ^2/n = 1.70) since the external parts of the R matrix elements due to p-wave channels are small. Note that the goodness-of-fit parameter was practically the same as that achieved with method B, but the effort required was considerably smaller. The thermal cross sections were, however, not exactly reproduced yet.

The current ENDF-6 format[13] of the evaluated files does not allow storage of the level-statistical parameters of Eq. (13) – strength function, distant-level parameter, average radiation width – together with the individual Reich-Moore parameters for a given level sequence. (Only in the general R-matrix and in the hybrid R-function options one can supply background R-matrix elements.) In principle, resonance cross sections calculated with processing codes like NJOY could be corrected for the deficiencies caused by the ENDF-6 format restrictions by adding pointwise correction ("background") cross sections. This *ad hoc* recipe is, however, cumbersome and problematic because usually the corrections show as much structure as the resonance cross sections themselves which leads to difficulties with storage and Doppler broadening. Addition of a smooth background cross section calculated from $\mathbf{R}^0$ alone is not correct either: As the cross sections do not depend linearly on the R matrix, addition of the external and internal parts of the R matrix is not the same as addition of the cross section components calculated separately from those parts.

6.2.2 REPRESENTATION OF THE EXTERNAL TERM $R^0_{cc'}(E)$ BY TWO BROAD RESONANCES (METHOD D')

Method D' is even simpler than Method D since the parameters of the two broad levels, given in good approximation already by the simple set of Eqs. (23-25), require but little adjustment. The storage of their parameters in ENDF-6 format poses absolutely no problem. There is, however, no place for the distant-level parameter (see section 6.2.1, above). It is therefore best to put it equal to zero (which implies $R'_c = a_c$, see Eq. (17)) and to adjust the two broad levels independently of each other together with all the internal resonances. One of the two will then become stronger than the other which produces the strength imbalance originally described by the distant-level parameter.

In the case of ^{52}Cr a very satisfactory fit was obtained by adjustment of the two broad levels only. The distant-level parameter was kept equal to zero and the channel radius was set to 5.76 fm again. Starting from prior parameters calculated from Eqs. (23-25), and with the radiation width fixed at $\Gamma_{\gamma\pm} = \bar{\Gamma}_\gamma = 1.32$ eV, the following posterior estimates were obtained:

$$E_- = -553 \text{ keV}, \qquad E_+ = 1787 \text{ keV},$$
$$\Gamma_{n-} = 385.34 \text{ keV}, \qquad \Gamma_{n+} = 918.89 \text{ keV}.$$

How well the replacement of all the external resonances by just two broad levels works can be seen from Figures 7-9. They show the fit to the ORNL transmission data in the energy range 45 - 1400

keV. The overall fit ($\chi^2/n = 1.73$) is again as good as that obtained with method B, but as with method D the calculated thermal cross sections (2.57 b for scattering, 0.13 b for capture) were not yet equal to the best current experimental estimates (2.96 b for scattering, 0.76 b for capture). To make up for the deficiency another fictitious level was introduced as described in section 5. The parameters of this narrow bound level were calculated from Eqs. (27-28) and (31-32), with the radiation width at first set equal to the average observed in the internal range. The result was

$$E_0 = -1.274 \text{ keV}, \quad \Gamma_n = 7.069\text{eV} \quad \text{for} \quad \Gamma_\gamma = 1.32\text{eV}.$$

This gave the prescribed point cross sections but the overall shape of the capture cross section deviated significantly from the $1/v$ shape indicated by the data, tending towards a $1/v^5$ behavior above a few hundred electron volts (see Figure 10). As explained in the text preceding Eq. (35) this indicates that the fictitious narrow bound level is located too close to the neutron threshold, closer than the first unbound level ($|E_0|$=1.274 keV $< E_1$=31 keV). This was remedied easily. As the radiation width is an undetermined scale factor in Eqs. (31) and (32) one needs only increase all three resonance parameters by the same factor until the mirror energy $|E_0|$ of the bound level exceeds the resonance energy E_1 of the first unbound level sufficiently. This leaves the thermal cross sections invariant but changes the capture cross section shape towards a $1/v$ slope below the first unbound level. Figure 11 shows the $1/v$ capture cross section shape recovered with the resonance parameters upscaled by a factor of 50,

$$E_0 = -63.7 \text{ keV}, \quad \Gamma_n = 2.5\text{keV} \quad \text{for} \quad \Gamma_\gamma = 66\text{eV}.$$

It is interesting to note, and points to the general consistency of the methods employed, that the original ^{52}Cr re-evaluation[6] of the resolved resonance range, and of the thermal range in particular, by means of the replica method B, required a comparable upscaling of the radiation width for the nearest bound level (by a factor of 44). The rather high values of the radiation widths in both cases are a reminder that the combined effect of many true levels is described by (the tail of) just one fictitious level. Obviously this works, but the resonance parameters may be equally fictitious.

CONCLUSION

In this paper we discuss methods for taking into account the (mostly unknown) external levels in resonance cross section calculations, with special emphasis on sound physical foundations and convenience of application. A special effort is made to clarify the definitions of, and relationships between, the basic quantities of resonance theory (decay or width amplitudes, channel radii, pole strengths, distant-level parameters) on one hand, and the quantities used in applied work and evaluated files (partial and total widths, reduced widths, strength functions, effective nuclear radii) on the other – about which there has been occasional confusion. A clear understanding of these concepts is crucial if modern resonance fitting codes and file formats are to be used properly, or if one has to compare or combine resonance parameter sets for a given isotope that have been obtained with different channel radii or different representations of external levels. Approximations that work only at low energies, and only for s-wave interactions, for instance calculation of hard-sphere scattering phase shifts with effective nuclear radii, but centrifugal-barrier penetrabilities and level shifts with

channel radii, are definitely inadequate for the wide energy ranges and higher-order partial waves encountered in modern resonance analyses, in particular for medium-mass and light nuclides.
The most rigorous and straightforward treatment of unknown external levels (method D) is based on level statistics. It provides a simple analytical form for the external part of the (reduced) R matrix depending only on the three relevant statistical parameters of the external levels: The strength function and the average radiation width determine edge effects mostly due to nearby levels, the distant-level parameter represents the strength imbalance of the more distant levels. As predicted by the optical model and the giant dipole resonance model all three parameters depend so weakly on energy that they can usually be taken as constant in the resolved resonance region. Strictly speaking, the strength function and the distant-level parameter can be taken as constant for actinides but not for structural materials with their very wide (hundreds of keV to MeV) analysis ranges.
Although this approach has a solid theoretical underpinning, is practically convenient, well tested, and implemented in widely used fitting codes (FANAC, SAMMY) it has one handicap: ENDF-6 format conventions do not permit mixtures of individual parameters (for internal levels) and average parameters (for external levels) in resonance parameter files.
A more approximate but also well working approach (method D'), newly proposed here, avoids this handicap. It replaces the two statistical ensembles of external levels below and above the internal resonance range by just two very broad fictitious levels. Demanding that their tails closely approximate the level-statistical edge terms of method D one finds that the two broad levels depend, of course, on the strength function and the average radiation width again, but in a very simple way. Moreover, if they are adjusted along with all the internal levels, they can acquire different strengths and thus imitate the strength imbalance described by the distant-level parameter that is then not needed any more. The problem of the ENDF-6 format, which does not allow the storage of the distant-level parameter in the Reich-Moore option, is thus avoided: The same level-statistical information is utilized as with method D but now in the form of (fictitious) individual resonance parameters rather than average parameters, so that nothing but individual resonance parameters must be adjusted and stored, all on the same footing.
A merely statistical treatment of the external levels is rarely accurate enough to give the right thermal cross sections. Local discrepancies in the thermal region are often removed with much effort by trial-and-error adjustment of the parameters of a few nearby bound levels, although a simple analytical recipe has been available for a long time which requires only one (narrow) bound level whose parameters can be directly calculated, up to a scale factor, from the discrepancies between the calculated and the prescribed thermal cross sections. The prescribed cross section values are then guaranteed at the thermal energy for any value of the scale factor, while the cross section shapes in the entire thermal region depend on its specific choice, and thus on the exact location of the narrow bound level. If it is farther from the neutron threshold than the first unbound level one finds the usual behavior: constant for scattering and $1/v$ for capture (and fission). If it is closer, one has a transition from $1/v$ towards $1/v^5$ near the "mirror energy" of the bound level. Varying the scale factor one can usually get not only the desired cross sections at the thermal energy but also their correct shapes throughout the low-energy region up to the first unbound level.
These methods were practically tested and compared with a recent re-analysis of the resolved resonance region of ^{52}Cr that had been performed with the replica method B and provided a convenient reference for the SAMMY fits. The main result was that both method D (level-statistical representation of external levels with adjusted average resonance parameters) and method D' (two broad

fictitious levels with adjusted individual resonance parameters, starting values depending on the same level statistics as D) gave equally good overall fits as method B, but with much less effort. The recommended thermal cross sections were easily reproduced by adding one narrow fictitious bound level with parameters calculated analytically (up to a scale factor). The calculated capture cross section shape differed, however, from the observed $1/v$ shape, indicating that the narrow fictitious bound level was too close to the neutron threshold. This meant that the chosen scale factor (corresponding to a fictitious radiation width equal to the average radiation width from the internal region) was too small. Upscaling by a factor of 50 gave low-energy cross sections in good agreement with the experimental data.
A final remark concerns the difficulties caused by the different ways of accounting for external levels which are being used. In particular, comparison and combination of neutron widths from different sources is by no means straightforward if they have been obtained with different recipes for the external levels and with different channel and effective radius-parameters. Apart perhaps from special pathological cases a useful standardization for neutron resonance fits could be envisaged with the following recommendations:

- Use as default option the ENDF-6 recommendation for channel radii of neutron channels, $a = (1.23A^{1/3} + 0.80)$ fm, where A is the nucleon number of the target nucleus.
- Use the same channel radius for all partial waves, i.e. for all s-, p-, d- ... wave channels of a given compound system.
- Use, for each neutron channel, the approximation of two broad fictitious levels with adjustable parameters to represent the external levels below and above the internal range of the resonance analysis. Calculate starting values of the parameters from average resonance parameters, see Eqs. (23)-(25). Any strength imbalance can then be taken into account by adjustment, without need for distant-level parameters or effective nuclear radii.
- Use one additional narrow fictitious level per s-wave channel for fine-tuning in the thermal region as explained in section 5.

In any case it ought to be clear that no list of resonance parameters is complete without the associated channel radii and the parameters quantifying external-level effects.

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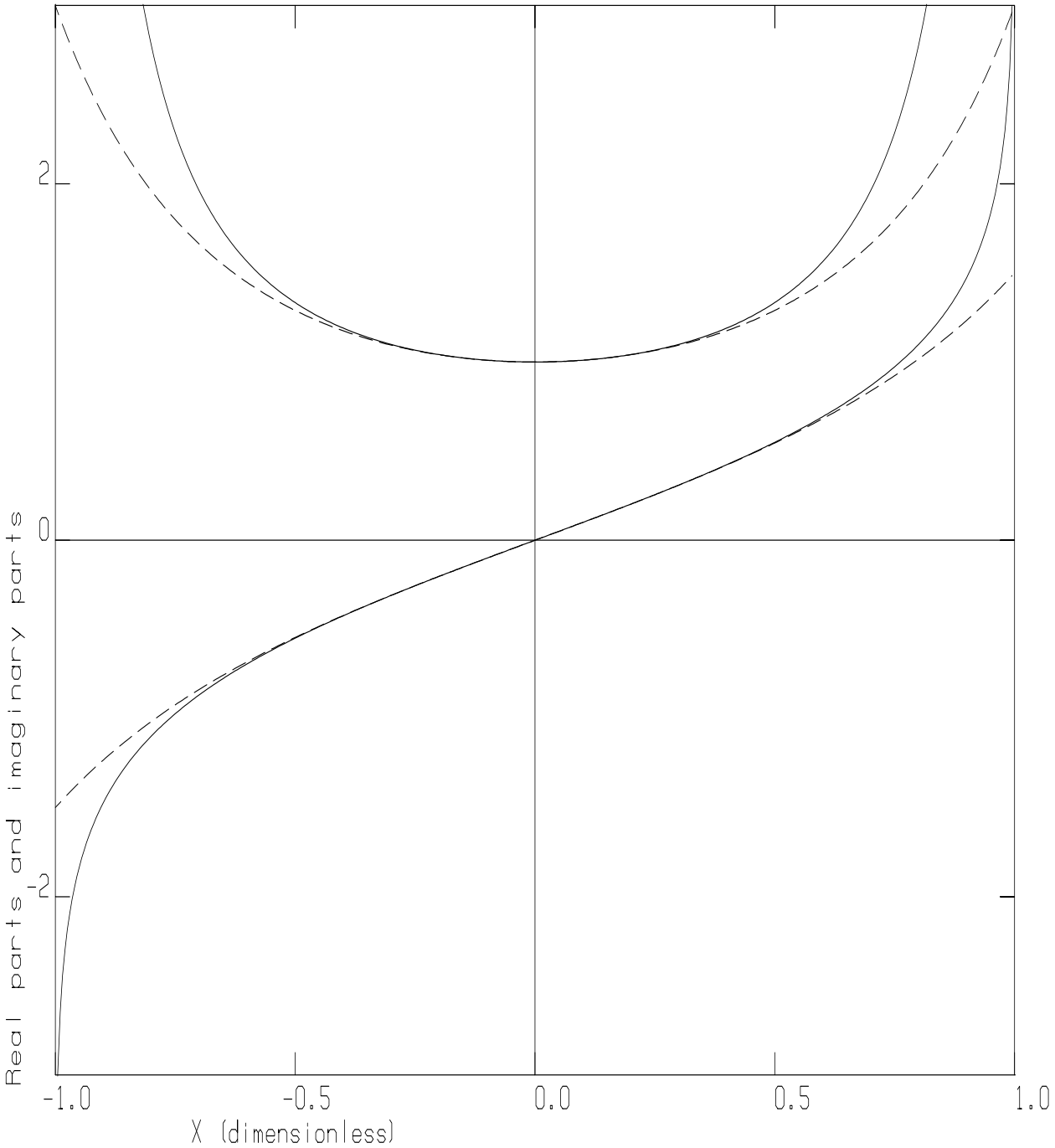

Figure 1: Similarity between the level-statistical edge terms $\mathrm{ar}\tanh\, x$ and $1/(1-x^2)$ (solid lines) and the corresponding resonance pair approximations $3x/(3-x^2)$ and $3(3+x^2)/(3-x^2)^2$ (dashed lines).

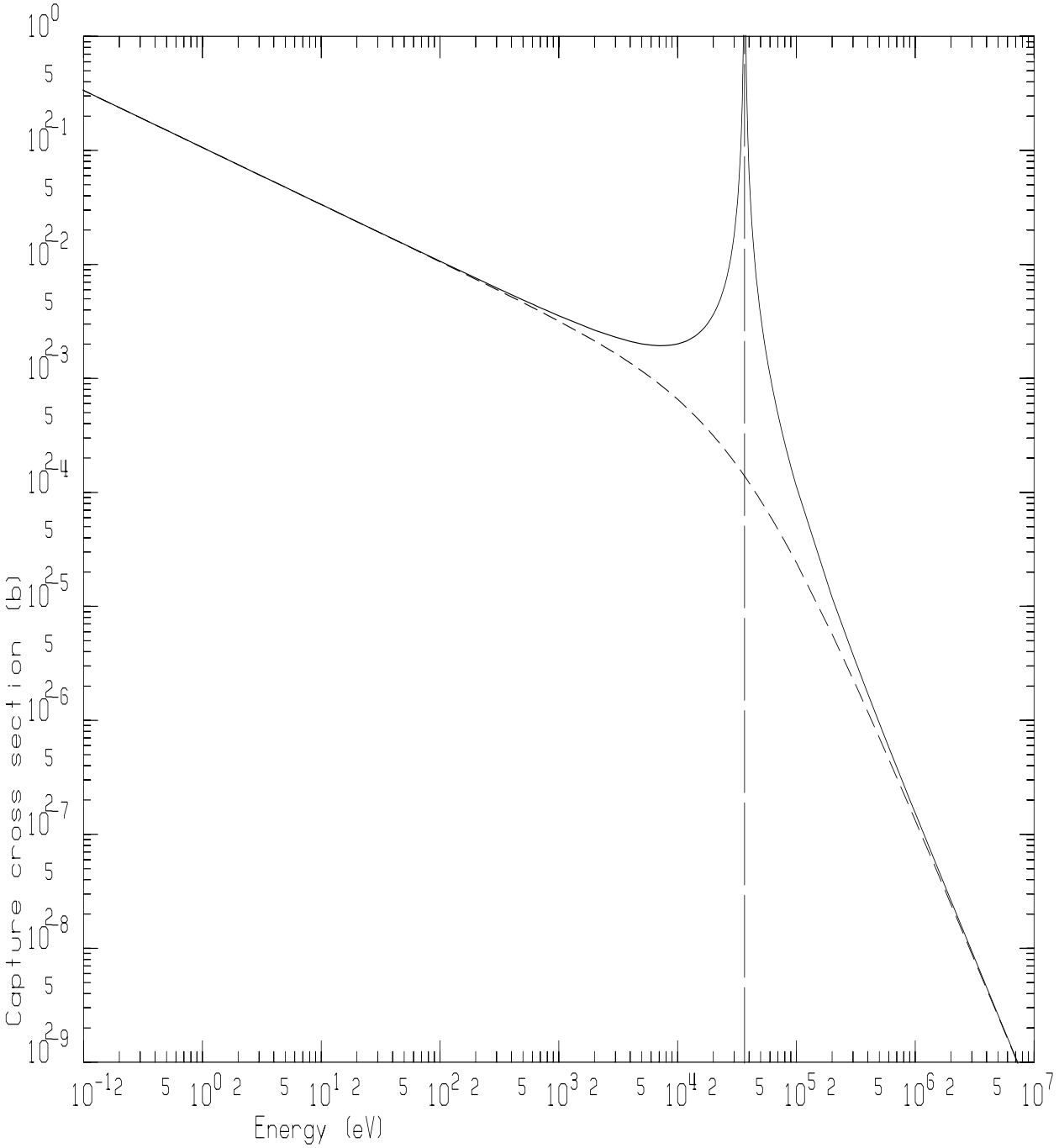

Figure 2: Single-level Breit-Wigner capture cross section of an unbound level at 37 keV (solid line) and of a bound level with the same partial widths at -37 keV (short dashes). The vertical dashed line indicates the (absolute value of) the resonance energy. Note the same asymptotic behavior in both cases: $1/v$ at low, $1/v^5$ at high energies.

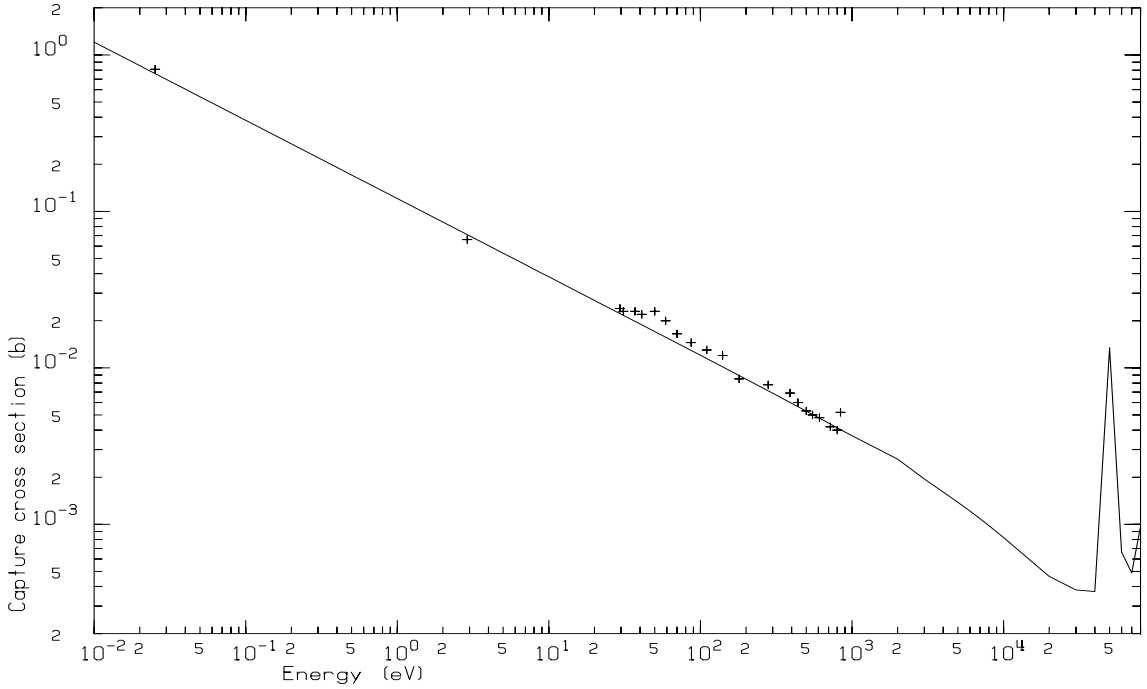

Figure 3: Fit to ^{52}Cr low energy capture cross section data (crosses) of Pomerance[23] and Kapchigashev and Popov[25]; the calculated curve (solid line) is based on replication of the internal level sequence.

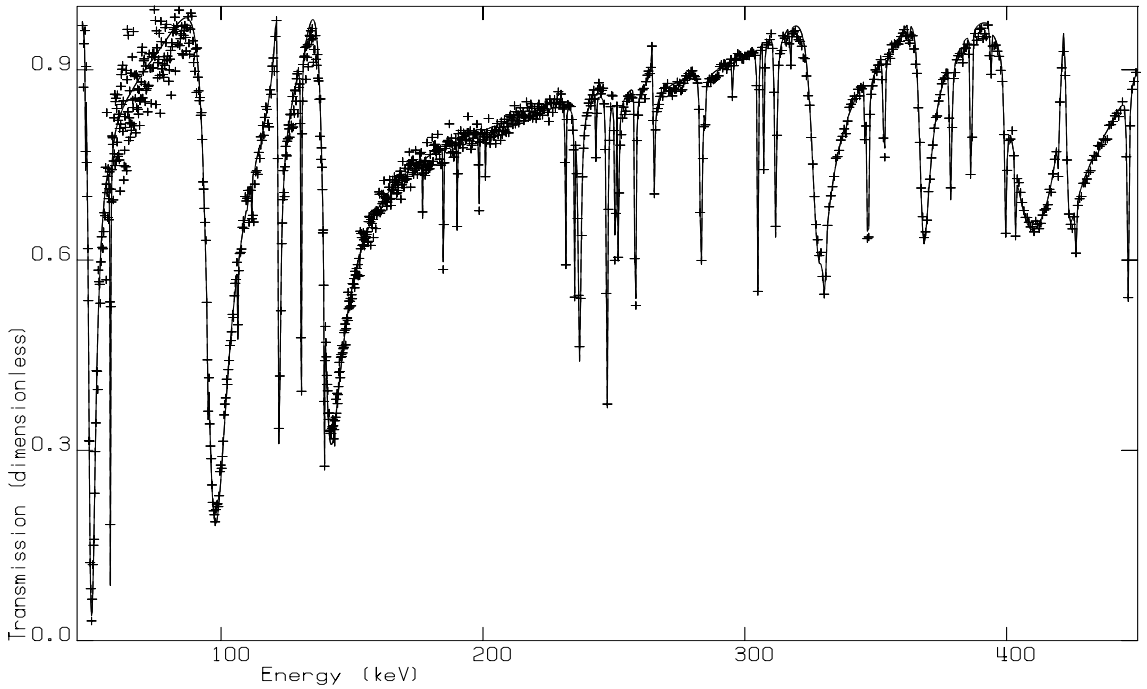

Figure 4: Transmission data fit in the energy range 45-500 keV; the crosses represent the ORNL experimental data[26] on ^{52}Cr (without uncertainties) and the solid line represents the calculated transmission based on replication of the internal level sequence.

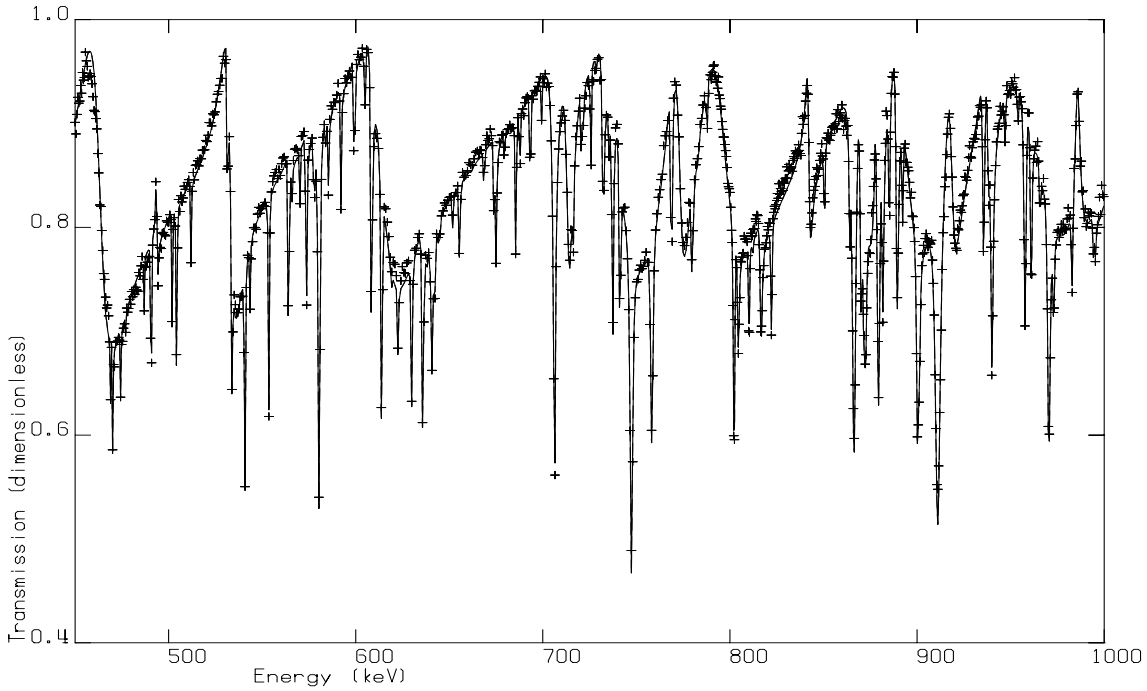

Figure 5: Transmission data fit in the energy range 500-1000 keV; the crosses represent the ORNL experimental data[26] on ^{52}Cr (without uncertainties) and the solid line represents the calculated transmission based on replication of the internal s-wave level sequence.

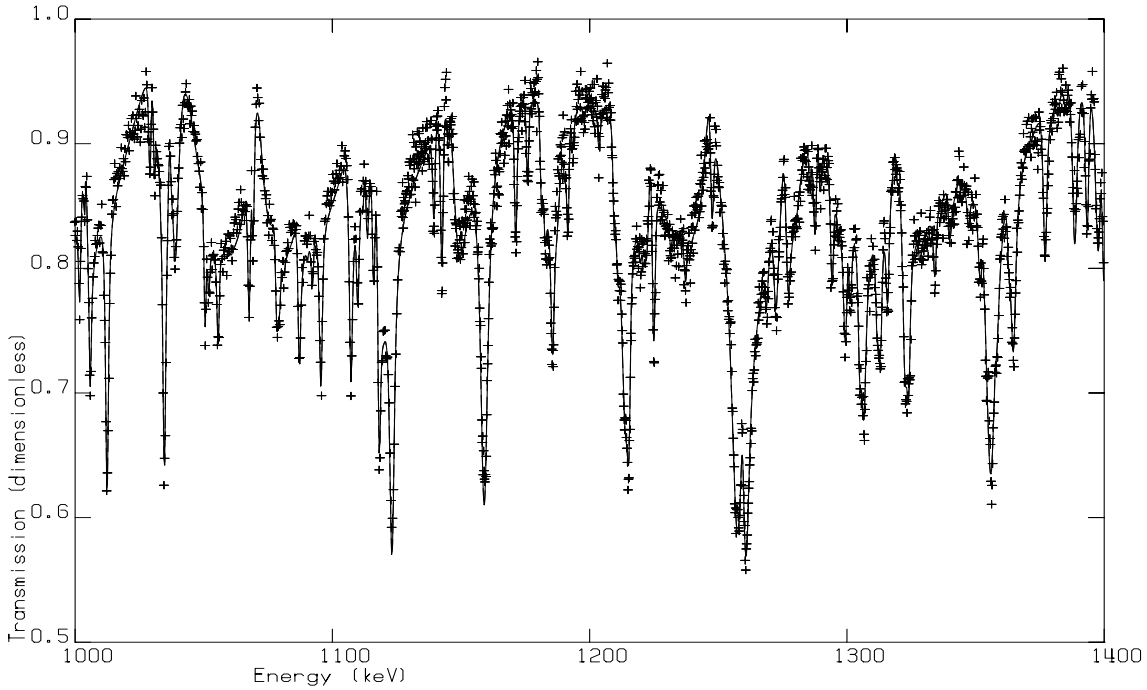

Figure 6: Transmission data fit in the energy range 1000-1400 keV; the crosses represent the ORNL experimental data[26] on ^{52}Cr (without uncertainties) and the solid line represents the calculated transmission based on replication of the internal s-wave level sequence.

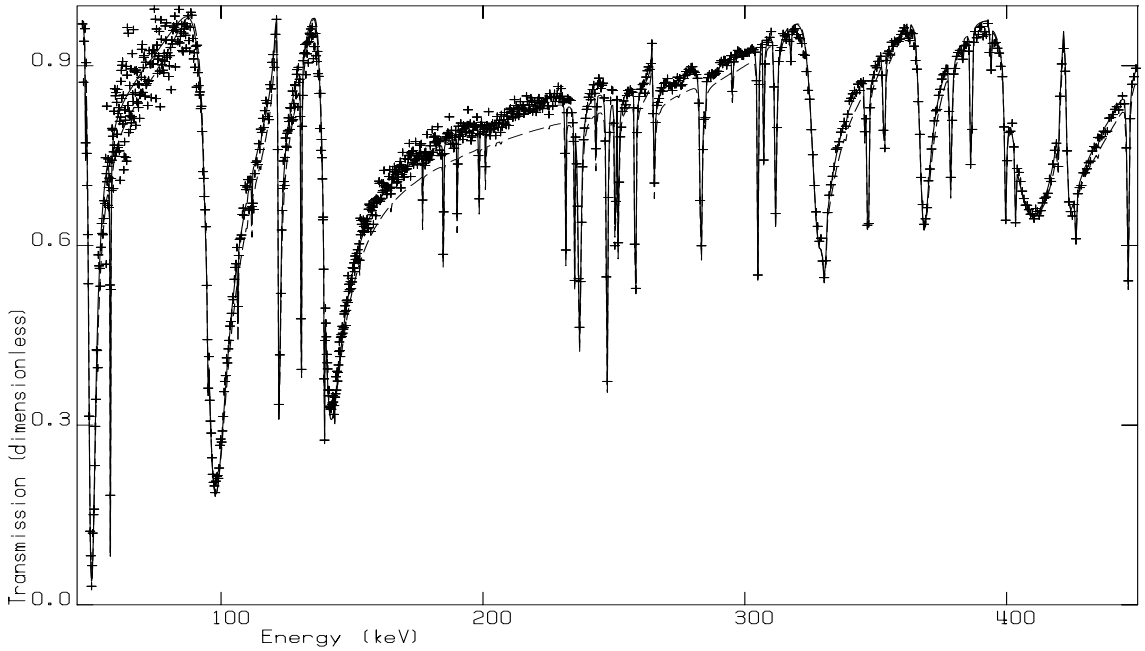

Figure 7: Transmission data fit in the energy range 45-500 keV; the crosses represent the ORNL experimental data[26] on ^{52}Cr (without uncertainties) and the solid and dashed lines represent respectively the calculated transmission based on two broad external s-wave levels (and $R_c^\infty = 0$) and the calculated transmission without these two external levels.

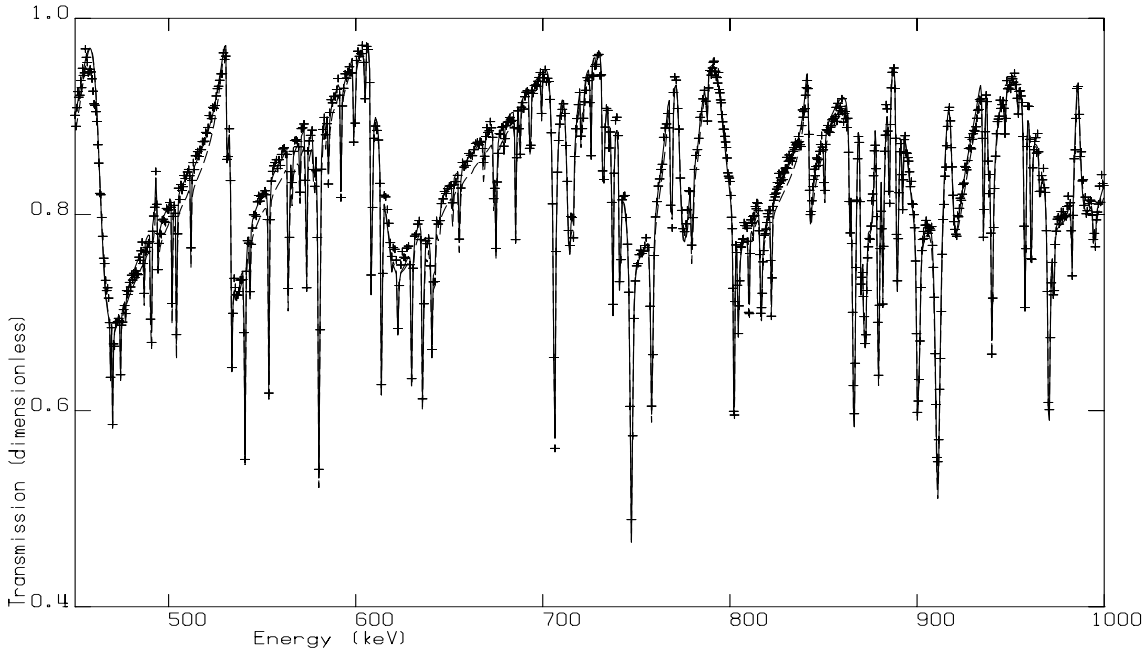

Figure 8: Transmission data fit in the energy range 500-1000 keV; the crosses represent the ORNL experimental data[26] on ^{52}Cr (without uncertainties) and the solid and dashed lines represent respectively the calculated transmission based on two broad external s-wave levels (and $R_c^\infty = 0$) and the calculated transmission without these two external levels.

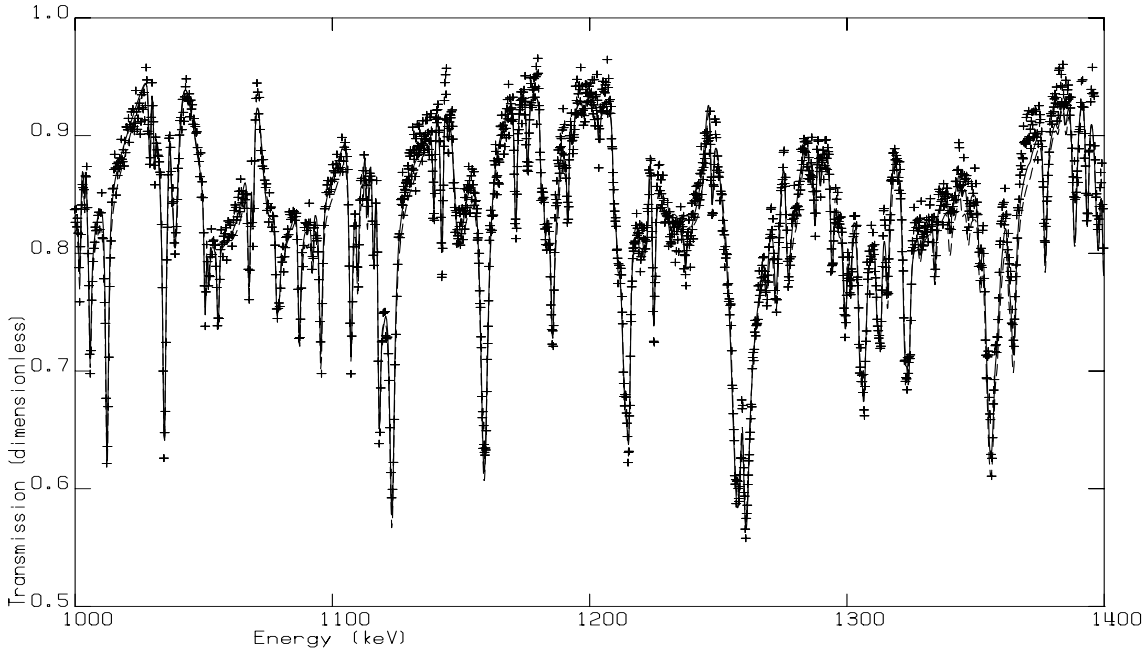

Figure 9: Transmission data fit in the energy range 1000-1400 keV; the crosses represent the ORNL experimental data[26] on ^{52}Cr (without uncertainties) and the solid and dashed lines represent respectively the calculated transmission based on two broad external s-wave levels (and $R_c^\infty = 0$) and the calculated transmission without these two external levels.

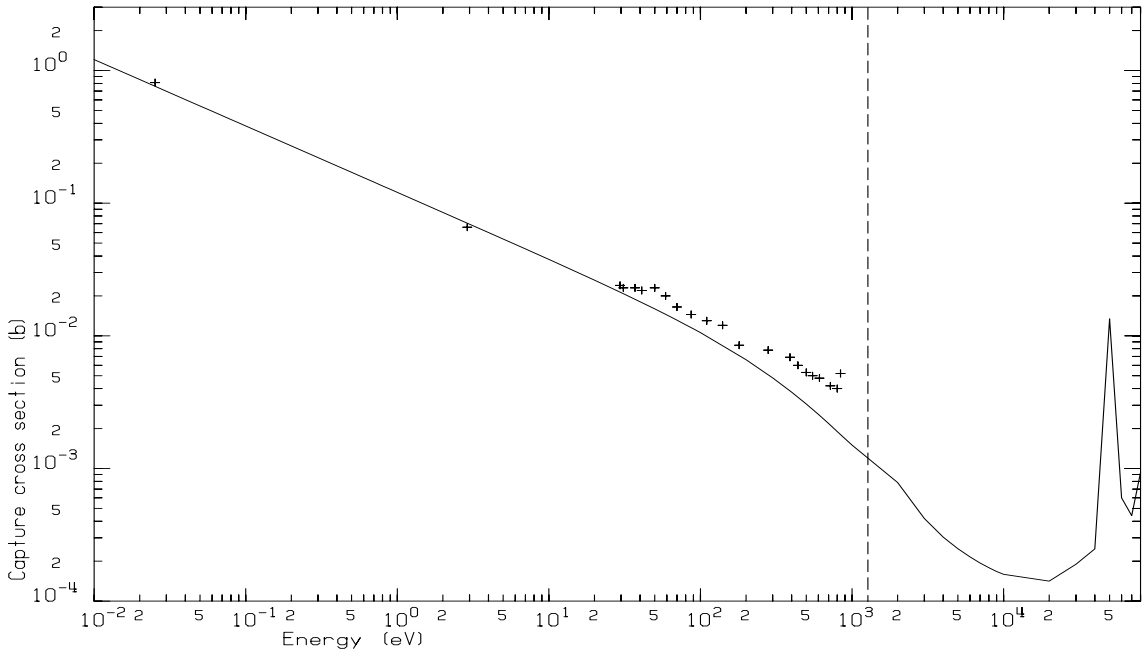

Figure 10: Calculated ^{52}Cr capture cross section (solid line) compared to the low energy data (crosses) of Pomerance[23] and Kapchigashev and Popov[25]; the calculated curve is based on two fitted broad external resonances and a narrow bound resonance (with $R_c^\infty = 0$); the vertical line represents the mirror energy ($|E_0|$=1.274 keV) of the narrow bound level.

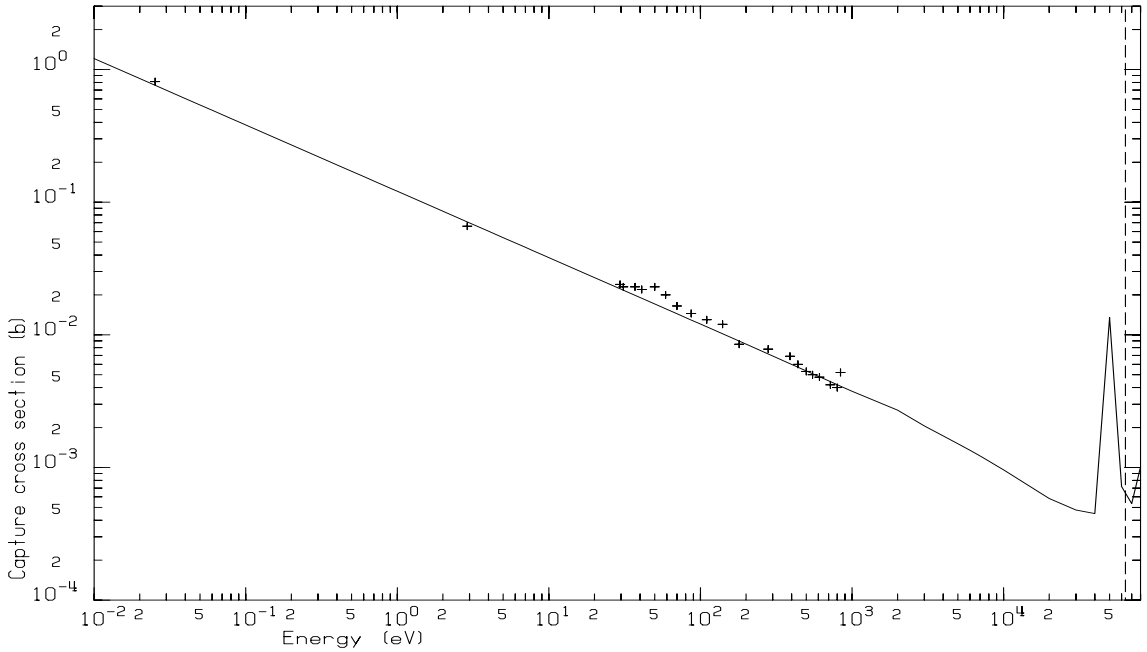

Figure 11: Calculated ^{52}Cr capture cross section (solid line) compared to the low energy data (crosses) of Pomerance[23] and Kapchigashev and Popov[25]; the calculated curve is based on the two fitted broad external resonances and the narrow bound resonance (with $R_c^{\infty} = 0$) but the capture width of the negative broad level was shifted to preserve the $1/v$ slope; the vertical line represents the upscaled mirror energy ($|E_0|$=63.71 keV) of the narrow bound level.