A formula for neutron cross sections of heavy nuclei is derived on the basis of the Wigner-Eisenbud theory. The derived formula is the same as the single-level one introduced by Breit and Wigner except for the inclusion of additional interference parameters \((u, v)\) which represent the contribution of the interference effect between resonances. The present formula is therefore applicable to reactor calculations without much modifications of the existing resonance integral codes.

The present formula has been applied to the analyses of the 235\text{U} and 233\text{U} fission cross sections and the 238\text{U} total cross sections in the resolved resonance region. By the use of least squares fits of the experimental data, the interference parameters \((u, v)\) are obtained for resonance levels of these nuclei in their typical resonance regions. It is shown that the present formula well represents the experimental data.

In the unresolved resonance region, both the single-level resonance parameters and the present interference parameters are generated by using a random sampling method. The contributions of the interference between the resonances to the Doppler effect are also evaluated for the fission cross sections of 235\text{U} and 239\text{Pu} in the unresolved resonance energy region of 1 to 2 keV.

**KEYWORDS:** single-level formula, interference effects, resonance, interference parameters, least squares fits, Doppler effect, uranium 235, uranium 233, uranium 238, Breit-Wigner formula, multi-level analysis, total cross sections

**I. INTRODUCTION**

It has been often pointed out that the single-level formula derived by Breit & Wigner \(^{(2)}\) can not exactly represent the resonance cross section for fissile nuclei. This is due to an interference effect between resonances\(^{(2)}\). In order to take account of the interference effect, many researchers have attempted to represent the cross section by using a more general form than the Breit-Wigner formula. The methods developed by Reich-Moore\(^{(3)}\) and Vogt\(^{(4)}\) were based on the Wigner-Eisenbud resonance theory\(^{(5)}\). None of these methods, however, can easily represent the Doppler broadened cross section. Furthermore, the Vogt formula\(^{(4)}\) is too complicated to perform the least squares fit of cross sections for an energy range having many resonances. Adler & Adler\(^{(6)}\) introduced the multi-level formula which took these drawbacks away on representing the resonance cross sections. The Adler-Adler formula has therefore been used often for the cross section analysis of fissile nuclei. This formula is, however, very complex for the calculation of cross sections in the unresolved resonance region due to its S-matrix representation\(^{(7)}\).

In reactor physics, on the other hand, most resonance integral codes have usually adopted the Breit-Wigner single-level formula in the following considerations:

1. A large number of the single-level parameters have been already evaluated for many nuclei\(^{(8)}\).
2. The discrepancies between measured
and calculated cross sections are generally small, so that the differences can practically be corrected by considering appropriate background cross sections.

(3) The Doppler broadened cross sections can easily be calculated.

(4) The statistical distribution functions\(^{(9)}\)\(^{(10)}\) are known well for level widths and spacings of resonances.

(5) Doppler effect can be calculated for the unresolved resonance region\(^{(11)}\).

It will therefore be useful to improve the Breit-Wigner single-level formula so as to include the interference effect between the resonances without losing these useful characteristics. An improved formula is derived on the basis of the Wigner-Eisenbud theory\(^{(5)}\) in Chap. II. This formula contains a set of new parameters \((\eta, \nu)\). In Chap. III, examples of the least squares fits are shown for the cross sections of \(^{235}\text{U}\), \(^{233}\text{U}\) and \(^{238}\text{U}\) in the resolved resonance region. Furthermore, the interference effects are studied for both the energy variations in cross sections and the Doppler effects in the unresolved resonance region.

II. EXPRESSIONS OF REACTION CROSS SECTIONS

The reaction cross section is generally expressed by the use of the collision matrix \(U_{cc}\). In the \(R\)-matrix theory, the collision matrix is given as follows\(^{(11)}\):

\[
U_{cc} = \exp[-i\phi_c + \phi_c] 
\cdot \left[ \delta_{cc} + i \sum_{\lambda \lambda'} \sqrt{\Gamma_{\lambda c} \Gamma_{\lambda' c}} A_{\lambda \lambda'} \right], \quad (1)
\]

where \(\phi_c\) is the hard sphere scattering phase shift, \(\delta_{cc}\) the Kronecker's delta, \(\lambda\) denotes the resonance level, \(\Gamma_{\lambda \lambda'}\) is the partial width for decay of the state \((\lambda)\) through channel \(c\), and \(A\) the level matrix. The inverse of the level matrix \(A\) is given by\(^{(12)}\):

\[
A^{-1}_{\lambda \lambda'} = (E_\lambda - E) \delta_{\lambda \lambda'} - \frac{i}{2} \sum_{\alpha \beta} \left( \Gamma_{\lambda \alpha} \Gamma_{\lambda' \beta} \right), \quad (2)
\]

where \(E_\lambda\) is the resonance energy. Practically, the calculation of the cross sections is very difficult when many interacting levels are present. The perturbation approach\(^{(6)}\) is therefore useful for the inversion of the level matrix. Adler-Adler\(^{(6)}\) used this approach to obtain the relation between the \(S\)-matrix and the \(R\)-matrix representations. We can derive an approximate level matrix \(A'\) by using the method as follows:

\[
A = (D + N)^{-1} = D^{-1}(1 + ND^{-1})^{-1} \approx D^{-1} - D^{-1} ND^{-1}, \quad (3)
\]

where \(D\) and \(N\) are the diagonal and off-diagonal parts for the matrix \(A\) respectively, and the right-hand side of Eq. (3) is defined here as an approximate level matrix \(A'\):

\[
A'_{\lambda \lambda'} = \delta_{\lambda \lambda'} + \frac{i}{2} (1 - \delta_{\lambda \lambda'}) \frac{\Gamma_{\lambda \lambda'}}{Z_{\lambda} Z_{\lambda'}}, \quad (4)
\]

\[
Z_{\lambda} = (E_{\lambda} - E) - \frac{i}{2} \Gamma_{\lambda}, \quad (5)
\]

\[
\Gamma_{\lambda} = \sum_c \Gamma_{\lambda c} = \Gamma_{\lambda n} + \Gamma_{\lambda t} + \Gamma_{\lambda f}, \quad (6)
\]

\[
G_{\lambda \lambda'} = \sum_{\nu} \left( \frac{\Gamma_{\lambda \nu}}{Z_{\lambda}} \frac{\Gamma_{\lambda' \nu}}{Z_{\lambda'}} \right), \quad (7)
\]

and \(\Gamma_{\lambda n}, \Gamma_{\lambda t}\) and \(\Gamma_{\lambda f}\) represent respectively the neutron, capture and fission width.

The real and imaginary parts of \(A'_{\lambda \lambda'}\) are written as follows:

\[
R_\phi(A'_{\lambda \lambda'}) = \frac{1}{2} \frac{E_{\lambda} - E}{Z_{\lambda}^2} \delta_{\lambda \lambda'} + \frac{i}{2} (1 - \delta_{\lambda \lambda'}) G_{\lambda \lambda'} H_{\lambda \lambda'}, \quad (8)
\]

\[
I_\phi(A'_{\lambda \lambda'}) = \frac{1}{2} \frac{E_{\lambda} - E}{Z_{\lambda}^2} \delta_{\lambda \lambda'} + \frac{i}{2} (1 - \delta_{\lambda \lambda'}) G_{\lambda \lambda'} H_{\lambda \lambda'}, \quad (9)
\]

where

\[
H_{\lambda} = \frac{1}{2|Z_{\lambda} - Z_{\lambda'}|^2} \left[ \Gamma_{\lambda} (E_{\lambda} - E_{\lambda'}) + (E_{\lambda} - E_{\lambda'}) (\Gamma_{\lambda} - \Gamma_{\lambda'}) \right] |Z_{\lambda}|^2,
\]

\[
H_{\lambda'} = \frac{1}{2|Z_{\lambda} - Z_{\lambda'}|^2} \left[ \Gamma_{\lambda} (E_{\lambda} - E_{\lambda'}) - 2 (E_{\lambda} - E_{\lambda'}) (E_{\lambda} - E_{\lambda'}) \right] |Z_{\lambda'}|^2,
\]

\[
H_{\lambda \lambda'} = \frac{1}{2|Z_{\lambda} - Z_{\lambda'}|^2} \left[ \Gamma_{\lambda} (E_{\lambda} - E_{\lambda'}) - 2 (E_{\lambda} - E_{\lambda'}) (E_{\lambda} - E_{\lambda'}) \right] |Z_{\lambda}|^2
\]

\[
\left( \frac{\Gamma_{\lambda}^2 (\Gamma_{\lambda} - \Gamma_{\lambda'})}{|Z_{\lambda}|^2} - 2 (E_{\lambda} - E_{\lambda'}) (E_{\lambda} - E_{\lambda'}) \right) |Z_{\lambda}|^2 - \frac{\Gamma_{\lambda}^2 (\Gamma_{\lambda} - \Gamma_{\lambda'})}{|Z_{\lambda'}|^2}.
\]

Using the representation of the approximate level matrix \(A'\), the total cross section is given by the following formula:

---

\(628\)
\[ \sigma_f(E) = \frac{2\pi}{k^2} g_J R_a (1-U_{nn}) \]
\[ = \frac{2\pi}{k^2} g_J \left[ 2 \sin^2 \phi_n + \sum \frac{(E_x-E) \Gamma_{xn} \sin 2\phi_n + \frac{1}{2} \Gamma_{xn} \cos 2\phi_n}{(E_x-E)^2 + \frac{1}{4} \Gamma_i^2} \right] \]
\[ + \frac{1}{2} \sum \sum \sqrt{\Gamma_{xn} \Gamma_{x'n}} G_{x'k} (H_{x'k} \sin 2\phi_n + H_{x'k} \cos 2\phi_n) \right] \]
\[ = \frac{\pi E}{k^2} g_J \sum \sqrt{E} \left( \frac{1}{2} u_j \Gamma_x + v_j (E_x-E) \right) \]
\[ \approx 2 \sum \sqrt{\Gamma_x \Gamma_{x'e}} I_m(A_{xkk}) \]
\[ = \sum 2 \sqrt{\Gamma_x \Gamma_{x'e}} I_m(A_{x,k'e}) \]

where \( k \) is the neutron wave number, \( g_J \) the spin statistical factor and \( J \) the spin quantum number of the compound nucleus. On the right-hand side of Eq. (12), the three terms in the brackets represent the contributions from the hard sphere scattering, the resonance reaction and the interference between resonances, respectively. The interference term can be rewritten by using two parameters \( u_j \) and \( v_j \) as follows:

\[ \sigma_f(E) \]
\[ = \frac{\pi E}{k^2} g_J \sum \sqrt{E} \left( \frac{1}{2} u_j \Gamma_x + v_j (E_x-E) \right) \]

where the two parameters are given by

\[ u_j = \sum \sqrt{\Gamma_x \Gamma_{x'n}} G_{x'k} (H_{x'k} \sin 2\phi_n + H_{x'k} \cos 2\phi_n) \]
\[ v_j = \sum \sqrt{\Gamma_x \Gamma_{x'n}} (\Gamma_{x'k} \sin 2\phi_n + 2(E_x-E) \cos 2\phi_n) \]

Using the unitarity of the collision matrix

\[ \sum \sum |U_{ce}|^2 = 1 \]

the following relation is obtained:

\[ \sum \sum |U_{ce}|^2 = 1 \]
In Eq. (21), the second term in the brackets shows the interference effect between resonance levels and is written as follows:

\[
\sigma_{v',y}(E) = \pi \frac{E}{k^2} g_y \sum I \left[ \frac{1}{E} \frac{1}{2} \frac{u_j^4 \Gamma_j^\prime + v_j^4 (E_j - E)^3}{(E_j - E)^3 + \frac{1}{4} \Gamma_j^\prime} \right] \tag{23}
\]

where

\[
u_j^4 = \sum_{\lambda} \frac{\sqrt{\Gamma_{j\lambda}^\prime \Gamma_{\lambda c}^\prime}}{\Gamma_{j\lambda}^\prime (E_j - E_c)^3 + \frac{1}{4} \Gamma_{\lambda c}^\prime} \tag{24}
\]

\[
u_j^4 = \sum_{\lambda} \frac{-2 \sqrt{\Gamma_{j\lambda}^\prime \Gamma_{\lambda c}^\prime}}{\Gamma_{j\lambda}^\prime (E_j - E_c)^3 + \frac{1}{4} \Gamma_{\lambda c}^\prime} \tag{25}
\]

The off-diagonal element for the capture channel is neglected because of the sign fluctuation for \((G_{lr})^{1/2}\), that is, \(\sum c' \sqrt{\Gamma_{j\lambda}^\prime \Gamma_{\lambda c}^\prime} \approx 0\). Hence, neglecting the second term of Eq. (21), the capture cross section is written as follows:

\[
\sigma_{v'}(E) = \pi \frac{E}{k^2} g_y \sum I \frac{\Gamma_{j\lambda}}{\Gamma_j^\prime} \tag{26}
\]

In Eqs. (12) and (21), each reaction cross section is represented by the summation of a symmetric and an asymmetric function. This expression for the reaction cross section is the same as the Breit-Wigner single-level formula except for the inclusion of the parameters \((u_j, v_j)\). From Eqs. (14), (15), (24) and (25), it is seen that the \((u_j, v_j)\) parameters decrease with an increase of the distances between the levels \(\lambda\) and \(\lambda'\). Hence the parameters \((u_j, v_j)\) can be considered as a kind of parameters that represent the measure of the interference between resonances. These will therefore be called as the interference parameters. However, these parameters can not generally be calculated from only the single-level parameters, because the signs of \((\Gamma_{j\lambda c}^\prime)^{1/2}\) are undetermined, with respect to each channel \(c'\), in the expression of Eq. (7) for \(G_{j\lambda}^\prime\). The Doppler broadened cross sections corresponding to Eqs. (12) and (21) can easily be derived and these are shown in APPENDIX. The calculation of the interference parameters will be performed for both the resolved and unresolved resonance region in the next chapter. Also, the contribution of the interference effect to the Doppler coefficient is evaluated from these parameters.

### III. INTERFERENCE PARAMETERS AND INTERFERENCE EFFECTS

#### 1. Resolved Resonance Energy Region

In the resolved resonance region, the many single-level parameters have been analyzed and evaluated\(^{(8)}\) on the basis of the Breit-Wigner single-level formula. The Breit-Wigner formula has been extensively used for the calculation of the reactor characteristics, because of the reasons described in Introduction. However, it is well known\(^{(2)}\) that the reaction cross section of fissile nuclei cannot adequately be represented by this single-level formula, because of the interference effect between the resonances levels. The interference effect may be accepted as the difference between the experimental cross section and the single-level cross section calculated by the Breit-Wigner single-level formula using the available single-level parameters. The interference effect will be represented by the formula derived in Chap. II. Therefore, the parameters \(u_4\) and \(v_4\) can be calculated\(^{(14)}\) to minimize the quantity:

\[
Q = \sum w_i \left| \sigma_{v, \exp}(E_i) - (\sigma_{v, B}(E_i) + \sigma_{v, M}(E_i)) \right|^2 \tag{27}
\]

where \(\sigma_{v, \exp}(E_i)\) is the measured cross section, \(\sigma_{v, B}(E_i)\) the Breit-Wigner single-level cross section, \(\sigma_{v, M}(E_i)\) the trial function for the term of the interference effect represented in Eqs. (A1), (A2) and (A3), and \(w_i\) the statistical weights.

The least squares fits were performed for the \(^{232}\)U and \(^{233}\)U fission cross sections and for the \(^{238}\)U total cross section. The obtained results are as follows:

\(^{232}\)U: The fission cross sections for the energy range below 12.54 eV were studied by using the experimental data of Michauden\(^{(15)}\) (12.54~0.3788 eV) and of Shore & Sailor\(^{(2)}\) (0.37~0.1 eV). The single-level parameters \((E_2, \Gamma_{jln}, \Gamma_{jM}, \Gamma_{jL})\) used for the calculation of the cross section \(\sigma_{v, B}\) are shown in Table 1\(^{(13)(14)}\). These single-level parameters were analyzed...
Table 1 Single-level parameters of $^{235}$U used for present calculation and obtained interference parameters

<table>
<thead>
<tr>
<th>$E_i$ (eV)</th>
<th>$g_J$</th>
<th>$\Gamma_J^R$ ($\times 10^{-1}$ (meV))</th>
<th>$\Gamma_J^R$ (meV)</th>
<th>$\Gamma_J^I$ (meV)</th>
<th>$\nu_J^L$ ((eV)$^{1/2}\times 10^{-6}$)</th>
<th>$\nu_J^I$ ((eV)$^{1/2}\times 10^{-6}$)</th>
</tr>
</thead>
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<td>27.6</td>
<td>169.4</td>
<td>-656.4</td>
<td>76.30</td>
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</tr>
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<td>4.453</td>
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<tr>
<td>5.732</td>
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<td>0.04887</td>
<td>49.0</td>
<td>443.0</td>
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<tr>
<td>6.19</td>
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<td>36.0</td>
<td>3.5</td>
<td>3.470</td>
<td>-0.4448</td>
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Single-level parameters $E_i$, $\Gamma_J^R$, $\Gamma_J^I$ and $\Gamma_J^L$ were analyzed by Michauden, and Shore & Sailor.

Fig. 1 Comparison of $^{235}$U fission cross sections from 12.5 to 0.1 eV

The circles are experimental data of Michauden (12.54~0.3788 eV) and of Shore & Sailor (0.37~0.1 eV). The dotted line is the cross sections calculated by using the single-level parameters in Table 1. The solid line is the present least squares fit.
from the resonance experiments by Michauden and by Shore & Sailor. The least squares fits were performed for 576 data points with the 19 levels below 11.66 eV to determine the parameters $u_f$ and $v_f$. The obtained parameters $u_f$ and $v_f$ are shown in columns 6 and 7 in Table 1, respectively. Figure 1 shows the comparison between the measured values.

### Table 2

<table>
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<tr>
<th>$E_i$ (eV)</th>
<th>$g_J$</th>
<th>$\Gamma_{66}^\theta$ (meV)</th>
<th>$\Gamma_{66}^\delta$ (meV)</th>
<th>$u_f$ $(\text{eV})^{1/2} \times 10^{-4}$</th>
<th>$v_f$ $(\text{eV})^{1/2} \times 10^{-6}$</th>
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<td>0.086</td>
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<td>-2.261</td>
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</table>

Single-level parameters $E_i$, $\Gamma_{66}^\theta$, $\Gamma_{66}^\delta$ and $\Gamma_{ij}$ were analyzed by Bergen(17).
(\sigma_{y,\text{exp}}), the single-level cross sections (\sigma_{y,B}) and the modified cross sections (\sigma_{y,B+\sigma_{y,M}}). This figure shows that Eq. (A2) can nicely reproduce the measured fission cross section in the lower energy region.

The integral quantities were also compared with the experimental values. The averaged cross sections \langle \sigma_{y,\text{exp}} \rangle, \langle \sigma_{y,B} \rangle and \langle \sigma_{y,B+\sigma_{y,M}} \rangle and the resonance integrals \text{RI}_{y,\text{exp}}, \text{RI}_{y,B} and \text{RI}_{y,B+\text{RI}_{y,M}} were calculated. The deviations of \langle \sigma_{y,B} \rangle and \langle \sigma_{y,B+\sigma_{y,M}} \rangle from \langle \sigma_{y,\text{exp}} \rangle were -11.5 and -1.78\%, respectively, and those of \text{RI}_{y,B} and \text{RI}_{y,B+\text{RI}_{y,M}} from \text{RI}_{y,\text{exp}} were -14.7 and -0.246\%, respectively. The single-level cross section considerably underpredicts the integral quantities but the present least squares fit extremely improves the situation though somewhat in underprediction.

\textit{233U:} The experimental data of the fission cross sections were obtained for the energy range of 45~20 eV from the data table given in Ref. (16). The data of 495 points with 44 resonance levels were analyzed by using the least squares fit with the trial function of Eq. (A2). The single-level parameters used for the present calculation are given in Table 2 (17), together with the obtained parameters u'_{f} and v'_{f}. The results calculated by using these parameters u'_{f} and v'_{f} and the single-level parameters are compared with the experimental values in Fig. 2. As seen from Fig. 2, both the Breit-Wigner single-level formula and the expression derived in this article well reproduce the measured cross sections. In the comparison of the integral quantities, however, the deviations of \langle \sigma_{y,B} \rangle and \langle \sigma_{y,B+\sigma_{y,M}} \rangle from \langle \sigma_{y,\text{exp}} \rangle were -2.95 and 0.094\%, respectively, and those of \text{RI}_{y,B} and \text{RI}_{y,B+\text{RI}_{y,M}} from \text{RI}_{y,\text{exp}} were -3.15 and 0.127\%, respectively. This result also shows that the present formula gives an improvement to the Breit-Wigner single-level formula.

---

**Fig. 2** Comparison of \textit{233U} fission cross sections from 45.5 to 20.0 eV

The circles are the experimental data from Petrel bomb explosion\textsuperscript{(16)}. The dotted line is the cross sections calculated by using the single-level parameters in Table 2. The solid line is the present least squares fit.
It is well-known that the Breit-Wigner single-level formula gives a very good representation for the cross section of the non-fissile nuclide with a large level spacing such as $^{238}\text{U}$. However, we experience the case where the total or scattering cross sections given by the single-level formula become negative at the lower energy side of the resonance which interferes strongly with the potential scattering. It is seen easily that this negative cross section appears only for the case of $\lambda \geq 2$ in Eq. (A1) or (A3).

For example, the $^{238}\text{U}$ total cross section calculated by using the single-level parameters shown in Table 3 takes a large negative value ($-5$ barns) at energy of 1,961 eV. But the experimental data of Garg et al.\(^{(18)}\) show about 4 barns near 1,961 eV. Using Eq. (A1) the total cross sections were analyzed by the least squares fit for the energy range of 2,020–1,920 eV. The parameters $(u_2, v_2)$ thus obtained are shown for two resonances of 1,974.65 and 1,968.66 eV in Table 3. The total cross sections calculated by using the single-level parameters and the parameters $(u_2, v_2)$ are compared with the experimental data in Fig. 3. This figure shows that the present formula of Eq. (A1) can reproduce the reasonable curve of the total cross section of $^{238}\text{U}$ also in the case where the resonance interferes strongly with the potential scattering. In addition, it is seen from Table 3 that for the two resonances, the contribution from the $u_2$-interference term to the total cross section is very small as compared with the single-level symmetry terms. On the other hand, the $v_2$-interference terms give the influence of $-16$ and $-7\%$ on the single-level asymmetry terms, as shown at the last column in Table 3.

From the results described above, it can be said that the interference parameters $(u_2, v_2)$ introduced for an improvement of the single-level formula play a very significant role in the analyses of the measured cross sections. The calculation of the parameters can easily be performed from the least squares fitting to the measured data.

For fertile materials, it should be noticed that the parameters $(u_2, v_2)$ can be calculated

\begin{table}
\centering
\begin{tabular}{cccccccc}
\hline
$E_1$ & $g_\nu$ & $\Gamma_\nu^{\text{ep}}$ & $\Gamma_\nu^{\text{pp}}$ & $\nu_1^\prime$ & $\nu_2^\prime$ & $\nu_1^\prime/2\Gamma_\nu^{\text{ep}}$ & $\sigma_0\nu_1^\prime/2\sigma_0\nu_2^\prime$ \\
(eV) & & (meV) & (meV) & (eV)$^{1/2} \times 10^{-4}$ & (eV)$^{1/2} \times 10^{-4}$ & & \\
\hline
1,808.26 & 1.0 & 0.4000 & 13.6 & & & & \\
1,845.6 & 1.0 & 0.3101 & 11.8 & & & & \\
1,902.27 & 1.0 & 0.4801 & 12.1 & & & & \\
1,917.1 & 1.0 & 0.4999 & 24.64 & & & & \\
1,968.66 & 1.0 & 13.00 & 24.64 & 0.5085 & & -7.8861 & 0.0021 & -0.16 \\
1,974.65 & 1.0 & 10.50 & 24.64 & 1.3545 & & -2.9279 & 0.0065 & -0.07 \\
2,023.58 & 1.0 & 4.500 & 24.64 & & & & \\
2,031.26 & 1.0 & 1.11 & 24.64 & & & & \\
2,088.63 & 1.0 & 0.2998 & 24.64 & & & & \\
2,096.49 & 1.0 & 0.2201 & 24.64 & & & & \\
\hline
\end{tabular}
\caption{Single-level parameters of $^{238}\text{U}$ used for present calculation and obtained interference parameters}
\end{table}

The circles are the experimental data of Garg et al.\(^{(18)}\) The dotted line is the cross sections calculated by using the potential scattering cross section of 10.6 barns and the single-level parameters in Table 3. The solid line is the present least squares fit.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{Comparison of $^{238}\text{U}$ total cross sections from 2,020 to 1,920 eV}
\end{figure}
from single-level parameters by considering only the entrance channel for neutron channel, that is, \( G_{i\kappa} = \sqrt{\Gamma_{i\kappa} \Gamma_{\kappa\kappa}} \). And then we could reproduce a similar total cross section curve to the fitted cross sections in Fig. 3. Furthermore, we have already proved also for the unresolved resonance regions that the present multi-level formula could correct such a failure of the single-level formula as \(^{238}\text{U}\) total cross sections became negative values in the case where resonance generated by random sampling method interferes strongly with the potential scattering.

2. Unresolved Resonance Energy Region

Several techniques\(^{(20)-(22)}\) have been developed for the generation of resonance parameters by random sampling from the distribution functions of the resolved resonance parameters and level spacing. Starting with some initial energy, resonance parameters are generated over the complete energy range of interest. The merits of generating resonance parameters are that both the effects of the self-interference between resonances in one nuclide and of the mutual resonance-interactions between different nuclei can accurately be taken into account for the calculation of effective cross sections\(^{(23)}\). In the unresolved resonance region, the interference parameters \((u_j, v_j)\) can be calculated by using the generated resonance parameters and energies, where according to the Vogt’s definition\(^{(4)}\) the off-diagonal elements of the level matrix are defined as follows:

\[
G_{ij} = \sqrt{\Gamma_{jn} \Gamma_{n\kappa} + (\Gamma_{j\kappa})^{1/2}(\Gamma_{j\kappa})^{1/2}} \cos \theta_{ij}, \\
\kappa \neq \lambda',
\]

in which the capture channel is neglected\(^{(4)}\) because of the sign fluctuation for \((\Gamma_{j\kappa})^{1/2}\). For the neutron channels, only the entrance channel is taken into consideration. The off-diagonal terms for the fission channel is defined\(^{(4)}\) by the scalar product of two vectors whose components are equal to \((\Gamma_{j\kappa})^{1/2}\). For the fissile nuclei, especially, the value of the neutron width is always sufficiently small compared to that of the total width and hence the neutron channel can be neglected. The main contribution to the off-diagonal elements comes from the fission channels.

In the calculation of the interference parameters \((u_j, v_j)\), the assumption \(|N/D| \ll 1\) used in the expansion for the level matrix must be examined for the unresolved resonance region. This assumption is generally valid because \(|E_i - E|\) is larger than the total width except for the case of \(E_i \approx E\). For \(E \approx E_i\), however, the diagonal element is the main contributor to the cross section, and \(N \ll D\) is satisfied for the other elements \((\lambda = \lambda')\). The acceptance of this assumption will therefore be reasonable in the calculation of the resonance cross sections. This fact can be ascertained also from numerical experiments.

In order to assess the validity of the first order perturbation approach, the resonance parameters for \(^{235}\text{U}\) were generated for the energy range of 1~2 keV using the ARCFIT-3 code\(^{(24)}\). The average resonance parameters used were \(\langle \Gamma_f \rangle = 0.353\) eV, \(\langle \Gamma_\gamma \rangle = 0.152\) eV, \(\langle \Gamma_n \rangle = 0.000132\) (eV)\(^{-1}\) and \(\langle \Gamma_\gamma \rangle = 0.0479\) eV, and the average level spacing was 1.16 eV. The fission channel number was 3 and the \(\chi^2\) distribution with the degree of freedom one was assumed for each fission channel. The examination of the validity of the perturbation approach becomes cumbersome when a sizable number of levels and energy points are considered. The interference effects of a level \((\lambda)\) with the neighboring levels are main contributors to off-diagonal elements in the vicinity energy \(E_i\). Hence, many studies have been done for two-level interference effects\(^{(5),(25),(26)}\). In the case of two levels, the direct inversion for the level matrix \(A^{-1}\) is given by

\[
A = D^{-1}(1 + ND^{-1})^{-1}
\]

\[
= \begin{pmatrix}
D_{11} & 0 & -N_{12} \\
0 & D_{22} & -N_{21} \\
N_{12}D_{22} & N_{21}D_{11} & 1
\end{pmatrix}
\]

where \(|B| = 1 - N_{12}N_{21}/D_{11}D_{22}\). (30)

If the approximation, \(|B| \approx 1\), is satisfied, hence, \(A \approx D^{-1}(1 - ND^{-1})\), the perturbation approach is valid. Therefore, the validity of the perturbation approach can be examined by calculating the values of \(|N_{12}N_{21}/D_{11}D_{22}|, |\lambda = \lambda'|\) for neighboring levels \(\lambda\) and \(\lambda'\) in the vicinity

---
of the resonance energy $E_k$. The values were calculated for 180 levels over the range of 1,712~1,800 eV. Figure 4 shows the values of $|N_{i+1} N_{j+1} D_{i+1} D_{j+1}|_{l+1}$ for the three cases of $E=E_{k1}$, $E=E_{k1}+0.1$ eV and $E=E_{k1}+0.2$ eV. It is seen from this figure that the perturbation approach is generally valid. Though the values show the largest values in the case of $E=E_{k1}$, fortunately, asymmetric term of Eq. (23) becomes zero and, furthermore, $u_{k}$ is generally smaller than $2\Gamma_{2k} \Gamma_{2k} / \Gamma_{2k}$ because $(E_{k}-E_{k})^{2}$ in the denominator of Eq. (24) is normally larger than the total width. Therefore, the perturbation approach is valid also for $E=E_{k}$ in the calculation of the resonance cross sections.

The values for some levels were smaller than $10^{-3}$, so that these were not presented in this figure.

The calculations of the cross sections of $^{235}$U and $^{239}$Pu were performed by considering many level interference effects for the energy range of 1~2 keV. Figures 5(a) and (b) show two examples of the calculated fission cross sections for $^{235}$U and $^{239}$Pu at the temperature 300°K. There are considerable discrepancies between the energy variations of the fission cross sections calculated by the Breit-Wigner single-level formula and the present formula. Such discrepancies due to the interference effect between resonances are especially important when their contributions to the Doppler reactivity effect is to be evaluated for a nuclear reactor.

In order to estimate the contribution, the resonance shielding factors of $^{235}$U and $^{239}$Pu were calculated for the temperatures 300 and 900°K using the MCROSS-2 code(27). The energy range considered in the calculation were 2~1.5 and 1.5~1.0 keV. Table 4 shows comparisons of the results calculated by the two different formulas. The differences in the Doppler effect between the two calculated results are 5~7% for $^{235}$U and smaller for $^{239}$Pu. These differences are exactly due to the interference effect between the resonances, because the infinitely dilute cross sections given by the two formulas are almost equal to each other. This can easily be examined by performing the $\omega$-integration of Eq. (A7) as follows:

\[\sum_{l} \int_{-\infty}^{\infty} \sigma_{\omega l} \chi_{l}(\theta, \omega) d\omega = 0,\]

\[\sum_{l} \int_{-\infty}^{\infty} \sigma_{\omega l} \phi_{l}^{2}(\theta, \omega) d\omega = -\frac{\pi}{2} \sum_{l} \sigma_{l} \Gamma_{l} u_{l} = 0.\]

Therefore, the infinitely dilute cross sections for a sufficiently wide energy range are the

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<th>Present results</th>
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<td>1.5~1.0</td>
<td>6.014 0.7090</td>
<td>0.0732</td>
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$\Delta f = f(900°K) - f(300°K)$
Fig. 5 Comparison of energy variations of fission cross sections of $^{235}$U and $^{239}$Pu calculated by Breit-Wigner single-level and present formulas
same for these two formulas. In other words, the present formula can represent the same experimental data as those evaluated by using the single-level formula for the unresolved resonance region. In addition this formula can take into account the interference effect between resonances by using the Breit-Wigner single-level parameters.

IV. CONCLUSIONS

Without losing the useful characteristics of the Breit-Wigner single-level formula, we have developed a simple way to take into account the interference effect between resonances. The improved formula contains the interference parameters \((u_i, v_i)\) which represent the interference effect, in addition to the usual single-level parameters.

In the resolved resonance region, the present formula can well represent the measured cross sections, which can not sufficiently be analyzed by the single-level formula. The interference parameters \((u_i, v_i)\) were calculated for typical resonance regions of \(^{235}\text{U}, ^{237}\text{U}\) and of \(^{239}\text{U}\) by using the least squares fit.

In the unresolved resonance region, the interference parameters \((u_i, v_i)\) can be reproduced with random sampling method using the single-level average resonance parameters and spacings. Infinitely dilute cross sections calculated by the Breit-Wigner single-level formula are substantially identical to those by the present formula. Therefore, the present expression reproduces the same experimental data as obtained from the single-level formula in the unresolved resonance region. The contribution of the interference effect to the Doppler effect has been examined from a comparison of the resonance shielding factors given by the two formulas. The differences in the Doppler effects caused by these two approaches are 5~7\% for \(^{235}\text{U}\) and smaller for \(^{239}\text{Pu}\).

Although the interference parameters \((u_i, v_i)\) can readily be generated for the unresolved resonance region, their statistics are not studied in the present paper. The study will be an interesting problem.

ACKNOWLEDGMENTS

The authors would like to express their gratitude to Mr. K. Kobayashi (JAERI) for his helpful support in the programming of the least squares fit.

REFERENCES

(3) Reich, C.W., Moore, M.S.: ibid., 111, 929 (1958); 118, 718 (1960).
[APPENDIX]

Doppler Broadened Cross Sections

The expressions given in Chap. II are derived on the basis of absorber nuclei at rest. In actual fact, however, the absorber nuclei are in thermal motion and hence the influence of the motion on the neutron absorption must be taken into consideration. In the present paper, Maxwellian distribution is assumed for the velocity of the absorber nuclei. Then, using the method developed by Buckler & Pull (13), the Doppler broadened cross sections corresponding to Eqs. (21) and (22) are easily given as follows:

\[ \sigma_{i}^{D}(E) = \sigma_{p}(E) + \frac{4\pi}{k^2} \sqrt{\frac{\alpha}{2m_\pi}} g_j \sum_{l} \left( \Gamma_{ln}^{\text{m}} + \frac{u_{l}^{j}}{2} \right) \Phi_{l}^{i} \]
\[ + \frac{8\pi R}{k} \sqrt{\frac{\alpha}{2m_\pi}} g_j \sum_{l} \left( \Gamma_{ln}^{\text{m}} + \frac{v_{l}^{j}}{4kR} \right) \Phi_{l}^{i}, \]
\[ \sigma_{s}^{D}(E) = \frac{4\pi}{k^2} \sqrt{\frac{\alpha}{2m_\pi}} g_j \sum_{l} \left( \Gamma_{ln}^{\text{m}} + \frac{u_{l}^{j}}{2} \right) \Phi_{l}^{i} \]
\[ + \frac{v_{l}^{j}}{2} \Phi_{l}^{i}, \]

where \( \Phi_{l}^{i} = R_{l}(F(w_{1}) - F(w_{2})) \)
\[ \Phi_{l}^{i} = I_{m}(F(w_{1}) - F(w_{2})) \]
\[ F(w) = \int_{0}^{\infty} \exp(-x^{2}) \frac{w}{x^2 + w^2} dx \]
\[ w_{1} = \sqrt{\alpha} \left( b + i(a - v_{0}) \right) \]
\[ w_{2} = \sqrt{\alpha} \left( b + i(a + v_{0}) \right) \]
\[ a - ib = (2E_{j} - i\Gamma_{j})^{1/2} \]
\[ \alpha = A_{m}/2kT, \]
and \( K, T, v_{0}, R \) and \( \sigma_{p} \) represent the Boltzmann constant, absolute temperature, neutron velocity, atomic radius and potential scattering cross section, respectively. The resonance scattering cross section is now given by

\[ \sigma_{s}^{D}(E) = \sigma_{p}(E) - \sigma_{s}(E) - \sum_{l} \sigma_{s}^{D}(E) \]
\[ = \frac{4\pi}{k^2} \sqrt{\frac{\alpha}{2m_\pi}} g_j \sum_{l} \left( \Gamma_{ln}^{\text{m}} + \frac{u_{l}^{j}}{2} \right) \Phi_{l}^{i} \]
\[ + \frac{8\pi R}{k} \sqrt{\frac{\alpha}{2m_\pi}} g_j \sum_{l} \left( \Gamma_{ln}^{\text{m}} + \frac{v_{l}^{j}}{4kR} \right) \Phi_{l}^{i}, \]
\[ (A3) \]

where \( u_{l}^{j} = u_{l}^{j} - \sum_{l} u_{l}^{j} \)
\[ (A4) \]
\[ v_{l}^{j} = v_{l}^{j} - \sum_{l} v_{l}^{j} \]
\[ (A5) \]

When \( \sqrt{E_{j}/E} \) is nearly equal to unity and \( \Gamma_{j}/E_{j} \ll 1 \), the functions \( \Phi_{l}^{i} \) and \( \Phi_{l}^{j} \) are reduced to the usual Doppler line shape functions \( \phi_{l}(\theta, x) \) and \( \lambda_{l}(\theta, x) \), respectively. The assumptions will approximately hold near resonance energy in the relatively high energy region, and Eqs. (A1), (A2) and (A3) can be written as follows:

\[ \sigma_{s}^{D}(E) = \sigma_{s}(E) + \sum_{l} \left[ \sigma_{a}(1 + u_{l}) \phi_{l}(\theta, x) \right. \]
\[ + \frac{\sigma_{a}^{\text{pl}}(1 + \frac{\sigma_{a}^{\text{pl}}}{\sigma_{a}^{\text{pl}}})}{\sigma_{a}^{\text{pl}}} \phi_{l}(\theta, x) \right], \]
\[ (A6) \]
\[ \sigma_{s}^{D}(E) = \sum_{l} \left( \Gamma_{ln}^{\text{m}} + u_{l} \right) \phi_{l}(\theta, x) \]
\[ + \phi_{l} \lambda_{l}(\theta, x), \]
\[ (A7) \]
\[ \sigma_{s}^{D}(E) = \sum_{l} \left( \Gamma_{ln}^{\text{m}} + u_{l} \right) \phi_{l}(\theta, x) \]
\[ + \phi_{l} \lambda_{l}(\theta, x), \]
\[ (A8) \]

where \( \sigma_{a} = \frac{4\pi}{k^2} g_j \Gamma_{ln}^{\text{m}}, \)
\[ \sigma_{a}^{\text{pl}} = 2 \sqrt{\sigma_{a}^{\text{pl}}} g_j \Gamma_{ln}^{\text{m}} / \Gamma_{ln}, \]
\[ \sigma_{p} = 4\pi R^2, \]
\[ u_{l} = u_{l}^{j} / 2 \Gamma_{ln}^{\text{m}}, \]
\[ v_{l} = v_{l}^{j} / 2 \Gamma_{ln}^{\text{m}}, \]
\[ u_{l} = u_{l}^{j} / 2 \Gamma_{ln}^{\text{m}}, \]
\[ v_{l} = v_{l}^{j} / 2 \Gamma_{ln}^{\text{m}}, \]
\[ (A9) \]
\[ (A10) \]
\[ (A11) \]
\[ (A12) \]
\[ (A13) \]