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Coherent neutron scattering amplitudes of fissionable nuclei, ²³³U, ²³⁵U, and ²³⁹Pu.* By MASAO ATOJI, Chemistry Division, Argonne National Laboratory, Argonne, Illinois, U.S.A.

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The fissionable nuclei 233 U, 235 U and 239 Pu possess a number of prominent neutron resonances in close proximity to the neutron-diffraction energy region. We may thus expect a certain wavelength dependency of their coherent scattering amplitudes having significant imaginary components. These aspects have been examined following Vogt's (1960) multilevel resonance formulation which includes the interferences among the fission levels. Accordingly, we derive the formula for the coherent scattering amplitude, *b*, as

$$b = R' - 227 \cdot 6 \sum_{j,k} g(\Gamma_{nj}^0 \Gamma_{nk}^0)^{\frac{1}{2}} A_{jk} +$$
(similar term for the other spin). (1)

where the amplitude and energy quantities are in units of 10^{-12} cm and eV, respectively; R' is the reaction nuclear radius, g the statistical factor and Γ_n^0 , the reduced neutron width. A_{jk} is the element of the symmetric complex matrix A and its reciprocal matrix A^{-1} has the form,

where E_j is the resonance energy, E the neutron energy, and Γ_{fj} the fission width at E_j ; the total resonance width, Γ_j , is the sum of $(E/1eV)^{+}\Gamma_n^0$, Γ_f and the radiation width Γ_y ; θ_{jk} is the interference parameter between the resonances at E_j and E_k . When $\cos \theta_{jk} = 0$, equation (1) is reduced to the Breit–Wigner single-level multiterm formula.

We write b = R' + b' + ib''. The summation in (1) for b' converges very slowly with respect to $|E_j - E|$, in contrast to the rapidly converging b''. Hence, for the former in particular, the unmeasured distant levels both in the virtual and bound states must be taken into account. The distant-level contribution for b' is approximated by

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$$b' \text{ (distant)} \simeq -227 \cdot 6 \langle g\Gamma_n^0 \rangle \sum_j \frac{1}{E_j}$$
$$\simeq -227 \cdot 6 \frac{\langle g\Gamma_n^0 \rangle}{\langle D \rangle} \left(\sum_{n=1}^{m_1} \frac{1}{a_1 + n} - \sum_{n=1}^{m_2} \frac{1}{a_2 + n} \right), \quad (2)$$

where $\langle g \Gamma_n^0 \rangle$ is the weighted-average reduced neutron width and $\langle D \rangle$ is the mean level spacing. In addition to the positive integers, n, m_1 and m_2 , the summation terms include $a_1 = E_j^{(1)} \langle D \rangle$ and $a_2 = |E_j^{(2)}| \langle D \rangle$, where $E_j^{(1)}$ and $E_j^{(2)}$ are the highest measured positive and negative resonance energies, respectively (cf. Atoji, 1964). The summation in (2) is a generalized Riemann zeta function, numerical tables of which have been given by Atoji & Clark (1965). The b'' (distant) can similarly be evaluated (Atoji & Clark, 1965), although it is usually negligibly small.

The resonance amplitudes, b' and b'' in Table 1, were computed with the use of the resonance and interference parameters which were deduced from the total (virtually y-ray capture plus fission) and fission cross-section analyses (Vogt, 1960[†]). The g-factors for ²³⁹Pu are those reported by Frazer & Schwartz (1962). The reliable g-factors for the high-spin targets, ²³³U and ²³⁵U, are not known, but all of the possible combinations of the g-factors gave insignificantly different values. The distant level contributions (m_1, \dots, m_n) $m_2 \sim 100$) with $E_i^{(1)}$ and $E_i^{(2)}$ used by Vogt have been included in the tabulated values. The calculations with higher $E_i^{(1)}$ values (see references in Lynn, 1964) led to insignificantly different results. The average resonance parameters employed were those compiled by Garrison (1963). The R' values computed from the total elastic scattering cross sections (Sher & Felberbaum, 1962) and our b' and b'' data are 1.01 ± 0.08 , 0.88 ± 0.09 and 0.83 ± 0.10 for ^{233}U , ²³⁵U and ²³⁹Pu respectively. The large uncertainties in R' are due to the scattering cross sections being minute fractions of the total cross sections. For ²³⁹Pu, Roof, Arnold & Gschneidner (1962) have reported $|b| = 0.75 \pm 0.03$ at

† In Table 1 of Vogt's paper (1960), the interference parameters, $\theta_2 = 277.5^\circ$ for 235 U and $\theta_3 = 126.9^\circ$ for 239 Pu should read 278.5° and 143.1°, respectively; the correct values for $\cos \theta_{45}$ and $\cos \theta_{48}$ in the 233 U column are -0.017 and 0.005, respectively.

Table 1. The resonance scattering amplitudes (in 10^{-12} cm) and the distant-level contributions for ^{233}U , ^{235}U and ^{239}Pu

		233U		235U		²³⁹ Pu	
E(eV)Å)	λ($-b^{\prime\prime}$		$-b^{\prime\prime}$		$-b^{\prime\prime}$
0.0253	1.798	0.019	0.014	0.199	0.018	0.042	0.029
0.04	1.430	0.019	0.012	0.196	0.018	0.036	0.031
0.05	1.279	0.019	0.015	0.195	0.018	0.032	0.032
0.06	1.168	0.019	0.015	0.193	0.017	0.027	0.033
0.07	1.081	0.019	0.012	0.191	0.012	0.023	0.035
0.08	1.011	0.019	0.012	0.189	0.017	0.017	0.036
0.09	0.953	0.019	0.016	0.188	0.016	0.012	0.038
0.10	0.905	0.018	0.014	0.186	0.016	0.006	0.041
0.14	0.764	0.018	0.016	0.179	0.012	-0.022	0.055
0.20	0.640	0.018	0.017	0.169	0.016	-0.086	0.110
Distant-level contribution		0.069	0.000	0.034	0.000	0.046	0.000

Fig. 1. The resonance scattering amplitudes and the total cross section of ²³⁹Pu as a function of neutron energy.

1.391 Å, from which we obtain a more accurate value, $R' = 0.73 \pm 0.03$.

In spite of the proximate resonance levels, b' and b'' of ²³³U and ²³⁵U are very small and practically constant. The amplitude variation and the imaginary amplitude of ²³⁹Pu are also small but by no means negligible in the high-precision structure analysis. In Fig. 1, the resonance amplitudes of ²³⁹Pu are plotted in the wider range of the neutron energy. The total cross-section curve is also shown in Fig. 1 so as to *demonstrate* the effect of the 0·296 eV resonance on the scattering amplitudes. The functional correlation here represents a typical, common feature of the resonance scattering. A resemblance between the b'' and total cross-section curves implies that the neutron structure analysis analogous to the X-ray dispersion technique has to overcome a rapidly increasing absorption effect for the larger b'' value.

The multilevel analysis has suffered from many adjustable parameters and the refined experiment and interpretation have recently revealed a number of smaller probable levels in these nuclei (for example, Lynn, 1964). Moreover, the bound levels will not be determined unambiguously without the direct method that has yet to be established. Regardless of this apparently provisional status, the following conclusions can be drawn. (1) It is very unlikely that further resonance analysis would alter our b'' values significantly since b'' is strongly related to the capture and fission cross-sections. (2) The (R'+b') values are reliable, although the uranium cases possess large statistical errors. (3) The individual real components, R' and b' are sensitive to the refinement in the resonance analysis, although our conclusion regarding the wavelength dependence of b' will not be affected. (4) The coherent amplitude of naturally occurring uranium, 0.845 ± 0.015 , a statistical average of the reported values (Atoji, 1961; Roof et al. 1962), can also be assigned to depleted uranium. Finally, the determination of these small b' and b'' by means of the coherent-intensity analysis using non-centrosymmetric single crystals would require exceedingly high-accuracy measurement.

Note added in proof: – For 235 U, it was gratifying to find a reasonable agreement between our result, $|b| = 1.07 \pm 0.09$, and an experimental value, $|b| = 0.98 \pm 0.06$, reported by Willis (1963).

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References

- ATOJI, M. (1961). J. Chem. Phys. 35, 1950.
- Атол, М. (1964). Acta Cryst. 17, 1087.
- ATOJI, M. & CLARK, F. L. (1965). Argonne National Laboratory Report, ANL-6970.
- FRAZER, J. S. & SCHWARTZ, R. B. (1962). Nucl. Physics, 30, 269.
- GARRISON, J. D. (1963). Symposium Report on Statistical Properties of Atomic and Nuclear Spectra, State University of New York at Stony Brook, New York.
- LYNN, J. E. (1964). Phys. Rev. Letters, 13, 412.
- ROOF, R.B. JR., ARNOLD, G. P. & GSCHNEIDNER, K.A., JR. (1962). Acta Cryst. 15, 351.
- SHER, R. & FELBERBAUM, J. (1962). Brookhaven National Laboratory Report, BNL-722.
- VOGT, E. (1960). Phys. Rev. 118, 724.
- WILLIS, B.T. M. (1963). Proc. Roy. Soc. A, 274, 122.

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The crystal structure of the copper complex of L-alanine. By A. DIJKSTRA*, Central Laboratory, Dutch State Mines, Geleen, The Netherlands

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Knowledge of the crystal structure of the copper complex of L-alanine was required in order to elucidate the optical properties (in the visible region) of single crystals of this copper complex (Dijkgraaf, 1964*a*, *b*). The structure was determined by two-dimensional Fourier methods.

Rotation and Weissenberg photographs gave the following unit-cell dimensions:

$$a=9.24\pm0.04, b=5.05\pm0.02, c=9.59\pm0.04 \text{ Å};$$

 $\beta=95.2^{\circ}\pm0.3^{\circ}.$

The density as calculated with two formula units $Cu(C_3H_6O_2N)_2$ per unit cell is 1.785 g.cm⁻³, whereas the observed density is approximately 1.81 g.cm⁻³. Reflexions 0k0 with k odd are systematically absent. Since the copper complex of L-alanine has no centre of symmetry, the monoclinic space group must be $P2_1$.



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