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CALCULATION OF PROMPT FISSION NEUTRON SPECTRA

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We present a new calculation of the prompt fission neutron spectrum N(E) as a function of both the fissioning nucleus and its excitation energy. The calculation, based upon standard nuclear-evaporation theory, accounts for the physical effects of (1) the distribution of fission-fragment residual nuclear temperature, and (2) the energy dependence of the cross section for the inverse process of compound-nucleus formation. Using a residual nuclear temperature distribution based upon the Fermi-gas model, we have performed calculations for two different assumptions concerning the cross section for compound-nucleus formation. Use of a constant cross section leads to a closed expression for the neutron energy spectrum while use of an energy-dependent cross section, calculated with the optical model, yields a numerical integration. Results obtained for the two assumptions agree well with experimental data although there is a preference for the energy-dependent cross section calculation.

[RADIOACTIVITY, FISSION Calculation of prompt fission neutron spectrum as function of fissioning nucleus and excitation energy. Nuclear-evaporation model, Fermi-gas model. Comparisons to $^{235}U(n,f)$ and $^{252}Cf(sf)$ experimental prompt neutron spectra.]

Introduction

Nuclear reactor design and other applications require knowledge of the prompt fission neutron spectrum N(E) as a function of both the fissioning nucleus and its excitation energy. The dependence upon fissioning nucleus and incident neutron energy is particularly important in cases where fission neutron spectrum measurements do not exist or are not possible. We study these dependencies by use of standard nuclear-evaporation theory to calculate the neutron energy spectrum in the fission-fragment center-of-mass system, and then transform these results to the laboratory system.

The center-of-mass neutron energy spectrum is obtained by integrating the nuclear-evaporation spectrum[1] for fixed residual nuclear temperature over the distribution function of this temperature. The nuclear temperature is that of the residual nucleus following neutron emission from the evaporating fission fragment. The physical origins of the residual nuclear temperature distribution are the initial distribution of fission-fragment excitation energy and the subsequent fragment cooling as neutrons are emitted. Following the integration, the resulting center-of-mass neutron energy spectrum is transformed to the laboratory system under the assumption that the neutrons are emitted isotropically from the moving fragments.

Our calculations have been performed using a triangular approximation to the residual nuclear temperature distribution determined by Terrell on the basis of experiment and the Fermi-gas model.[2] Two different assumptions have been tested for the inverse process of compound-nucleus formation. Use of a constant compound-nucleus formation cross section yields a closed expression for N(E) involving the exponential integral and the incomplete gamma function. Use of an energy-dependent formation cross section, calculated with the optical model, yields a numerical double-integral expression. Comparisons to experimental data demonstrate the importance of including both the distribution of residual nuclear temperature and the energy-dependent compound-nucleus formation cross section. The calculations and results obtained using the constant compound-nucleus cross section are discussed in the next section and those obtained with the energy-dependent cross section in the section following that. We then compare the results of both calculations with experimental data. Our conclusions are presented in the final section.

Constant Compound-Nucleus Cross Section

The nuclear-evaporation spectrum corresponding to a fixed residual nuclear temperature T is given approximately by[1]

$$\phi(\varepsilon) = c(T)\ \sigma_c(\varepsilon)\ \varepsilon\ \exp(-\varepsilon/T)\ , \qquad (1)$$

where ε is the center-of-mass energy, $\sigma_c(\varepsilon)$ is the cross section for the inverse process of compound-nucleus formation, and c(T) is the normalization integral defined such that $\phi(\varepsilon)$ is normalized to unity when integrated from zero to infinity. All distributions in this paper are normalized in this way. In the case of a constant compound-nucleus cross section σ_c, the normalization integral c(T) has the value $1/\sigma_c T^2$.

The initial distribution of total fission-fragment excitation energy is approximately Gaussian in shape, with a total average value given by

$$\langle E^* \rangle = \langle E_r \rangle + B_n + E_n - \langle E_f^{tot} \rangle\ . \qquad (2)$$

Here $\langle E_r \rangle$ is the average energy release, B_n and E_n are the separation energy and kinetic energy of the neutron inducing fission, and $\langle E_f^{tot} \rangle$ is the total average fission-fragment kinetic energy. For spontaneous fission both B_n and E_n in Eq. (2) are zero. In calculating $\langle E_r \rangle$ and B_n we use the experimental and systematic masses compiled by Wapstra and Bos[3] where available and otherwise the droplet-model mass formula of Myers.[4] Measured values of $\langle E_f^{tot} \rangle$ are also used where available and otherwise the formula

$$\langle E_f^{tot} \rangle = c_1(Z^2/A^{1/3}) + c_2\ ,$$

where Z and A are the atomic number and mass number of the fissioning nucleus and c_1 and c_2 are determined by least-squares adjustment to experimental data. For low-excitation fission we use (c_1, c_2) values of (0.13323 Mev, -11.64 MeV) determined by Unik *et al.*,[5] and for high-excitation fission the values (0.1071 MeV, 22.2 MeV) obtained by Viola.[6]

In a study of experimental distributions of fission-fragment kinetic energy and neutron number Terrell obtained the distribution of kinetic energy that governs neutron emission.[2] This distribution was transformed into the distribution P(T) of fission-fragment residual nuclear temperature by use of the Fermi-gas model where the excitation energy E^*, the nuclear temperature T, and the nuclear level-density parameter a are related by $E^* = aT^2$. Terrell observed that if the resulting temperature distribution is approximated by the sharp cutoff triangular distribution

$$P(T) = \begin{cases} 2T/T_m^2 , & T \le T_m \\ 0 , & T > T_m \end{cases} \qquad (3)$$

then the maximum temperature T_m is related to the initial total average fission-fragment excitation energy $\langle E^* \rangle$ by

$$T_m = (\langle E^* \rangle / a)^{1/2} . \qquad (4)$$

For the present studies we use the approximation summarized by Eqs. (3) and (4) to calculate the residual nuclear temperature distribution. We use the simple relationship

$$a = A/(11\ \text{MeV}) \qquad (5)$$

for the nuclear level-density parameter, where A is the mass number of the fissioning nucleus. It must be noted that a slight adjustment in T_m from the value predicted by Eqs. (4) and (5) could in principle be required.

The neutron energy spectrum in the fission-fragment center-of-mass system, $\Phi(\varepsilon)$, is obtained by integrating Eq. (1) over the temperature distribution given by Eq. (3). This yields

$$\Phi(\varepsilon) = \int_0^\infty \phi(\varepsilon)\ P(T)\ dT \qquad (6a)$$

$$= (2\varepsilon/T_m^2)\ E_1(\varepsilon/T_m) , \qquad (6b)$$

where $E_1(x) = \int_x^\infty [\exp(-u)/u]du$ is the exponential integral. This result has been obtained previously by Kapoor et al.[7] The average center-of-mass neutron energy $\langle \varepsilon \rangle$ is the first moment of Eq. (6b) and has the value $(4/3)T_m$.

The transformation of the fission-fragment center-of-mass neutron energy spectrum $\Phi(\varepsilon)$ to the laboratory system, under the assumption that the neutrons are emitted isotropically from a fission fragment moving with average kinetic energy per nucleon E_f, is accomplished by use of the general result

$$N(E) = \frac{1}{4\sqrt{E_f}} \int_{(\sqrt{E}-\sqrt{E_f})^2}^{(\sqrt{E}+\sqrt{E_f})^2} [\Phi(\varepsilon)/\sqrt{\varepsilon}]d\varepsilon , \qquad (7)$$

where E is the laboratory neutron energy.[2] Inserting Eq. (6b) and interchanging the order of integration, we obtain for the laboratory prompt fission neutron spectrum

$$N(E) = (1/3\sqrt{E_f T_m})\ [u_2^{3/2}\ E_1(u_2) - u_1^{3/2}\ E_1(u_1) + \gamma(\tfrac{3}{2}, u_2) - \gamma(\tfrac{3}{2}, u_1)] , \qquad (8)$$

where $u_1 = (\sqrt{E} - \sqrt{E_f})^2/T_m$,

$u_2 = (\sqrt{E} + \sqrt{E_f})^2/T_m$,

and $\gamma(a,x) = \int_0^x u^{a-1} \exp(-u)du$

is the incomplete gamma function. The mean laboratory neutron energy $\langle E \rangle$ is the first moment of Eq. (8) and has the value $E_f + (4/3)T_m$.

Since there are two fission fragments, each emitting approximately the same average number of neutrons,[8] but each moving with generally quite different average velocities, the transformation given by Eq. (7) must be separately applied to each fragment. This leads to

$$N(E) = \frac{1}{2}\ [N_L(E) + N_H(E)] , \qquad (9)$$

where the subscripts refer to light and heavy fragments. Equation (8) is used to evaluate each term of Eq. (9). The values of the average kinetic energy per nucleon for each fragment transformation are given by

$$E_f^L = \frac{\langle A_H \rangle}{\langle A_L \rangle} \frac{\langle E_f^{tot} \rangle}{A} \text{ and } E_f^H = \frac{\langle A_L \rangle}{\langle A_H \rangle} \frac{\langle E_f^{tot} \rangle}{A} \qquad (10)$$

where $\langle A_L \rangle$ and $\langle A_H \rangle$ are the average integer fragment atomic mass numbers as obtained from Unik et al.[5] The mean laboratory neutron energy for the spectrum given by Eq. (9) is

$$\langle E \rangle = \frac{1}{2}\ (E_f^L + E_f^H) + \frac{4}{3}\ T_m . \qquad (11)$$

The prompt fission neutron spectrum calculated from Eq. (9) for the fission of ^{235}U induced by 0.53-MeV neutrons is shown in Fig. 1. Also shown are the Watt and Maxwellian spectra[2] calculated for the same fissioning system by using temperatures T_W and T_M, respectively, constructed to yield mean energies identical to that given by Eq. (11) for the present calculation. These temperatures have the values $T_W = (8/9)T_m$ and $T_M = (1/3)(E_f^L+E_f^H) + (8/9)T_m$. In Fig. 2 the same calculated spectra are compared by forming ratios to the present calculation. The Watt spectrum is accurate to within a few percent for laboratory neutron energies between 0 and about 7 MeV and smaller than the present calculation for higher energies because the Watt temperature T_W is less than T_m. The Maxwellian spectrum is a much less accurate physical approximation, particularly at energies greater than about 5 MeV where it is most sensitive to the large value of T_M, which must account for the motion of the fission fragments as well as the center-of-mass motion of the emitted neutrons. Finally, the dependence of the present calculation upon the fissioning nucleus and the incident neutron energy is illustrated in Figs. 3 and 4. Figure 3 illustrates how the high-energy portion of the spectrum increases as the charge of the fissioning nucleus increases, for thermal-neutron-induced fission. Figure 4 illustrates a similar behavior of the spectrum as the kinetic energy of the incident neutron increases, for the fission of ^{235}U.

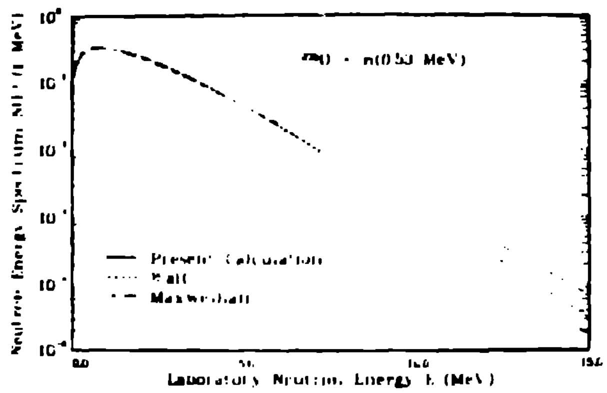

Fig. 1. Prompt fission neutron spectrum in the laboratory system for the fission of ^{235}U induced by 0.53-MeV neutrons. The solid curve gives the present spectrum calculated from Eqs. (8) and (9). The values of E_f^L, E_f^H, and T_m are, respectively, 1.062, 0.499, and 1.018 MeV. The mean laboratory energy, calculated from Eq. (11), is 2.138 MeV and is equal to the mean energy of both the calculated Watt and Maxwellian spectra which are shown for comparison.

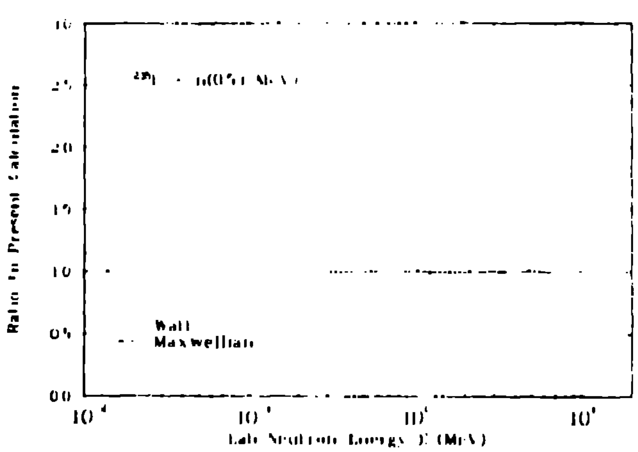

Fig. 2. Ratio of Watt spectrum and the Maxwellian spectrum to the present spectrum, corresponding to the curves shown in Fig. 1.

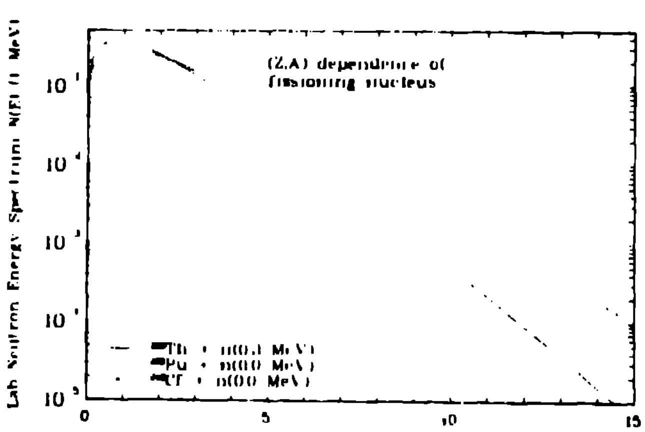

Fig. 3. Dependence of the prompt fission neutron spectrum upon the fissioning nucleus, for thermal-neutron-induced fission, as calculated from Eqs. (8) and (9).

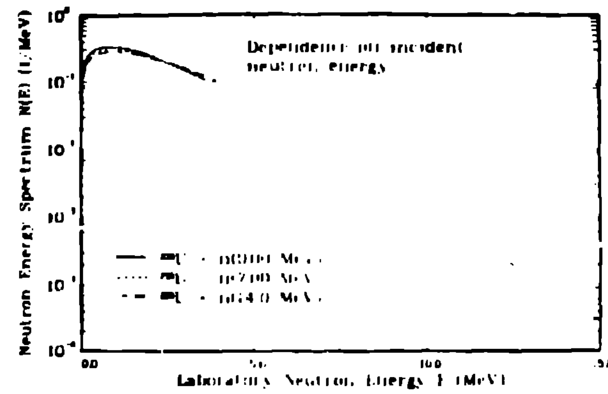

Fig. 4. Dependence of the prompt fission neutron spectrum upon the kinetic energy of the incident neutron, for the fission of ^{235}U, as calculated from Eqs. (8) and (9). The values of E_f^L and E_f^H, obtained from Eq. (10), are held fixed for all incident neutron energies. The 14-MeV spectrum is calculated for first-chance fission only.

Energy-Dependent Compound-Nucleus Cross Section

In this section we calculate the prompt fission neutron spectrum in the case of an energy-dependent cross section for the inverse process of compound-nucleus formation. We obtain this cross section using the optical model. The calculation proceeds exactly as in the previous section except that the integrations must now be performed by numerical methods. The complete expression for the numerical integration is obtained by combining Eqs. (1), (3), and (6a) into Eq. (7) which yields the double integral

$$N(E) = \frac{1}{4\sqrt{E_f}} \int_{(\sqrt{E}-\sqrt{E_f})^2}^{(\sqrt{E}+\sqrt{E_f})^2} \sqrt{\varepsilon}\, \sigma_c(\varepsilon) \left[\int_0^{T_m} (2T/T_m^2) \times c(T) \exp(-\varepsilon/T)\, dT \right] d\varepsilon \qquad (12)$$

where the normalization integral c(T) is given by

$$c(T) = \{\int_0^\infty \nu\, \sigma_c(\nu) \exp(-\nu/T) d\nu\}^{-1} .$$

Gauss-Laguerre and Gauss-Legendre quadrature of order 32 are used to evaluate the three integrals appearing in Eq. (12). We represent the optical-model compound-nucleus formation cross section by a cubic-spline fit to a calculated array of 75 points extending from 1 keV to 30 MeV.

Following the numerical integration of Eq. (12) for E_f values and energy-dependent cross sections appropriate to each fragment, we obtain the laboratory prompt fission neutron spectrum using Eq. (9). Calculations were performed for the fission of ^{235}U induced by 0.53-MeV neutrons using three, well-known, neutron-nucleus global optical-model potentials. These are the potentials of Moldauer,[9] Wilmore and Hodgson,[10] and Becchetti and Greenlees.[11] The results are shown in Fig. 5 where the ratios of the three calculations to the constant compound-nucleus cross section calculation of Fig. 1 are plotted. The results are similar for the three potentials, namely, there is approximately a 10% enhancement at a laboratory energy of about 700 keV and a gradual decrease above 2 MeV, relative to the constant cross section calculation. These structure changes are due to the gradual decrease of $\sigma_c(\varepsilon)$ with energy and the relative maxima and minima of $\sigma_c(\varepsilon)$ below the 1-MeV region.

Comparisons with Experimental Data

We compare our results to experimentally determined prompt fission neutron spectra in Figs. 6 and 7 for, respectively, the fission of ^{235}U induced by 0.53-MeV neutrons[12] and the spontaneous fission of ^{252}Cf.[13] Calculations using the constant compound-nucleus cross section agree reasonably well with this data although they are slightly high in various portions of the tail region. In both figures a clear preference exists for the energy-dependent compound-nucleus cross section calculation shown for the case of the Wilmore-Hodgson optical potential. This is evident in the high-energy region as well as in the 1-MeV region where the data appear to support the existence of enhanced structure. However, our energy-dependent calculation is unable to reproduce the magnitude of this structure in the case of ^{252}Cf(sf).

Conclusions

A new calculation of the prompt fission neutron spectrum has been presented. The calculation demonstrates the importance of accounting for the physical effects of the residual nuclear temperature distribution and the energy-dependence of the cross section for the inverse process of compound-nucleus formation. The calculation predicts clear dependencies upon fissioning nuclear species and incident neutron energy. Fission neutron spectra can now be calculated in regions devoid of experimental spectrum measurements.

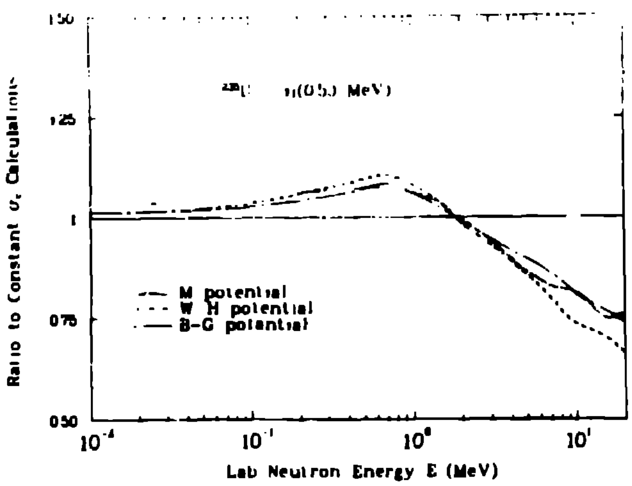

Fig. 5. Ratio of the prompt fission neutron spectra calculated with energy-dependent compound-nucleus cross sections to that calculated using the constant compound-nucleus cross section shown in Fig. 1, for the fission of ^{235}U induced by 0.53-MeV neutrons. The dotted curve is for the potential of Moldauer, the dashed curve is for the potential of Wilmore and Hodgson, and the dot-dashed curve is for the potential of Becchetti and Greenlees. The E_f^L and E_f^H values are the same for all four of the calculations.

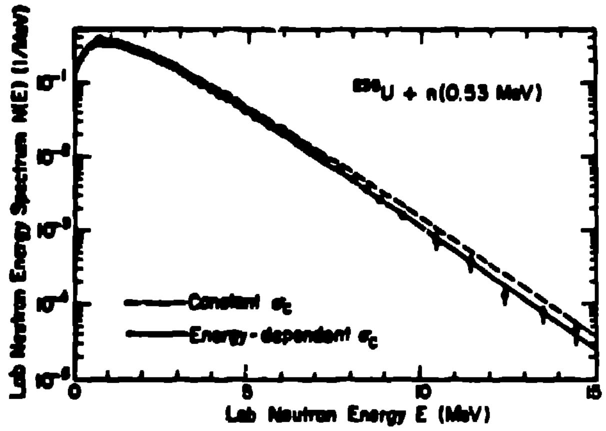

Fig. 6. Prompt fission neutron spectrum for the fission of ^{235}U induced by 0.53-MeV neutrons. The dashed curve gives the constant cross section calculation identical to that of Fig. 1 and the solid curve depicts the energy-dependent cross section calculation using the optical potential of Wilmore and Hodgson. In both cases the same values of E_f^L and E_f^H have been employed. The experimental data are those of Johansson and Holmquist.

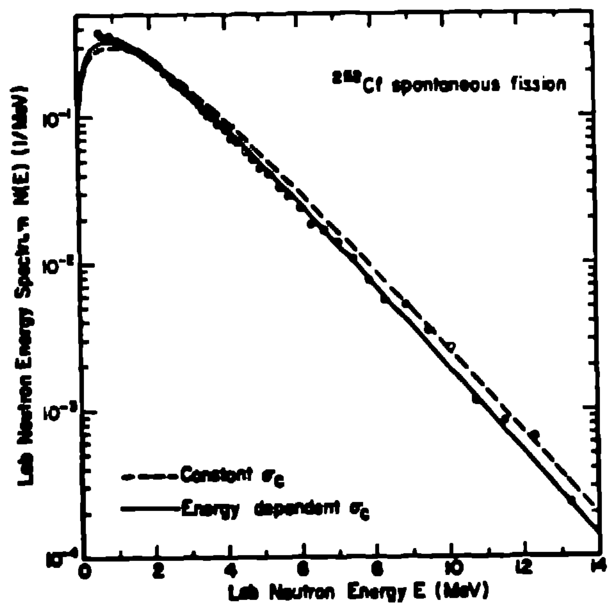

Fig. 7. Prompt fission neutron spectrum for the spontaneous fission of ^{252}Cf. The dashed curve gives the constant cross section calculation where the values of E_f^L, E_f^H, and T_m are, respectively, 0.984, 0.553, and 1.209 MeV. The solid curve depicts the energy-dependent cross section calculation using the optical potential of Wilmore and Hodgson. In both cases the same values of E_f^L and E_f^H have been employed. The experimental data are those of Boldeman, et al.

References

1. V. Weisskopf, Phys. Rev. 52, 295 (1937).
2. J. Terrell, Phys. Rev. 113, 527 (1959).

3. A. H. Wapstra and K. Bos, Atomic Data Nucl. Data Tables 19, 177 (1977).

4. W. D. Myers, Droplet Model of Atomic Nuclei (IFI/Plenum Data Co., New York, 1977).

5. J. P. Unik, J. E. Gindler, L. E. Glendenin, K. F. Flynn, A. Gorski, and R. K. Sjoblom, in Proceedings of the Third IAEA Symposium on the Physics and Chemistry of Fission, Rochester, New York, USA, 1973 (IAEA, Vienna, 1974), Vol. II, p. 19.

6. V. E. Viola, Jr., Nucl. Data A 1, 391 (1966).

7. S. S. Kapoor, R. Ramanna, and P. N. Rama Rao, Phys. Rev. 131, 283 (1963).

8. J. Terrell, Phys. Rev. 127, 880 (1962).

9. P. A. Moldauer, Nucl. Phys. 47, 65 (1963).

10. D. Wilmore and P. E. Hodgson, Nucl. Phys. 55, 673 (1964).

11. F. D. Becchetti and G. W. Greenlees, Phys. Rev. 182, 1190 (1969).

12. P. I. Johansson and B. Holmquist, Nucl. Sci. Eng. 62, 695 (1977).

13. J. W. Boldeman, D. Dulley, and R. J. Cawley, Trans. Am. Nucl. Soc. 32, 733 (1979).