attributed to the uncertainty in the experimental angular and energy resolution. If both of these effects were included in the theoretical treatment, they would reduce the peak height and broaden the theoretical cross-section curves, particularly at the small angles at large initial energies where the cross section peaks and varies most rapidly.

The fact that the vibrational "bumps" show up in the wings of the calculation and not in the experimental data of Figs. 2–4 (this effect is evident at $1 \leqslant \beta \leqslant 2$ in Fig. 5) can be due to the following reasons: (1) The torsional barrier height that we have assumed may be too high. (2) A more exact average over molecular orientations may be required. (3) A computation accounting for energy resolution will broaden the theoretical curves and may smear out the "bumps."

At the 0.0736- and 0.102-ev back angles, where the neutron interacts more violently with the molecule, the assumption of simple harmonic vibrational modes is not adequate for the modes with low frequencies (see Figs. 3–4). This may explain the experimental data points at large α's falling above the modified Krieger-Nelkin curve in Fig. 5.

V. SUMMARY AND CONCLUSIONS

In propane the effects of discrete rotational levels are evident at only the smallest initial neutron energy and scattering angle; the rotational continuum assumption is adequate over most of the experimental range. The considerations of single vibrational state changes in the theory give better agreement with the experimental results than either the "ideal gas" or Krieger-Nelkin formulas. Discrepancies still exist in $S(\alpha,\beta)$ at large α and large β due primarily to the uncertain methyl barrier height for the three lowest energy modes, to the harmonic oscillator approximation for these modes, and to the approximate molecular orientation averaging.

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Straggling Effects on Resonant Yields

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The finite nature of energy loss processes for a charged particle in a material leads to a "ringing" effect in the thick-target yield curve. The effect is described and evaluated.

I. ORIENTATION

FOR orientation we consider a resonant nuclear reaction at an energy E_R, with width Γ, induced in a thick target by a beam of charged particles of energy E_0. We ask for the yield curve $Y(E_0)$. The cross section is supposed to be of the standard form

$$\sigma(E)=\frac{\sigma_0}{1+4(E-E_R)^2/\Gamma^2}. \tag{1}$$

The standard consideration goes as follows: for $E_0 \ll E_R$ the yield is zero, for E_0 well above E_R the particles are degraded through the resonance by their ordinary energy-loss processes, and the yield is

$$Y_0=\frac{\pi\sigma_0\Gamma N}{2(-dE/dx)_{E_R}}, \tag{2}$$

per incident particle, where N is the density of reacting targets. The transition from zero to Y_0 occurs over a range of energy Γ around E_R, given exactly by the partial integrals of (1) from zero to E_0.

We propose to discuss here an extra effect arising from the fact that the energy losses are not continuous, but occur in discrete jumps. The maximum energy loss in a single event is approximately $4m/M$ of the energy of the incident (heavy) particle, and it is the existence of beams of particles with energy resolution better than this that makes these considerations interesting. The number $4m/M$ is approximately $1/500$ for incident protons, and resolutions five times better than this are achievable.

To show that there is an interesting effect, consider first the purely fictitious case in which *all* the energy losses are in jumps β, with a probability p per unit length, so that $-dE/dx=p\beta$. Then the average distance traveled per jump is p^{-1}, and the yield is given

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by

$$Y(E_0)=\frac{N}{p}\sum_{\nu=0}^{\text{“}\infty\text{”}}\sigma(E_0-\nu\beta), \tag{3}$$

where the sum is obviously not extended to negative energies. If we *assume* that $\beta\gg\Gamma$, to dramatize the case, then only one term in (3) will contribute appreciably—the term for which the incident particle has suffered just enough energy losses to be dropped into the resonance. Thus, as E_0 is increased through E_R, the yield curve traces out the resonance formula (1) (with, in the real case, suitable modifications for Doppler width, etc.). There is then a region of low yield until, as E_0 increased through $E_R+\beta$, the pattern is repeated, etc. The *average* yield is still, however, given by (2), so that (3) represents an oscillatory behavior around the average yield, and we will show in the sequel that this feature remains in a more realistic treatment.

In the next section we consider a simplified problem that embodies most of the physics, and is easily soluble; then, in the following section, we do the real problem.

II. A SIMPLIFIED MODEL

Let us schematize the actual spectrum of energy losses by superimposing upon our discrete losses β, with probability p per unit length, a continuous loss rate α. Thus

$$-dE/dx=\alpha+p\beta. \tag{4}$$

We need to ask ourselves for the total track length per unit energy in the target, at energy E, of a particle incident at energy E_0. Call this $l(E_0,E)$, so that

$$Y(E_0)=N\int_0^{E_0}\sigma(E)l(E_0,E)dE, \tag{5}$$

and the case given at the end of the last section corresponds to a sum of a series of δ functions for l. For $\Gamma/E_0\ll1$, we can observe that l is a rapidly varying function only of the differences E_0-E, and a slowly varying function of E_0.

We start with the usual observation that, for $E_0<E$, $l(E_0-E)=0$. Then consider the region $E+\beta>E_0>E$, for which no catastrophic energy loss β is permitted. The likelihood that the particle will go the distance $(E_0-E)/\alpha$ necessary for this energy change without a catastrophic loss is

$$p_0=e^{-p[(E_0-E)/\alpha]}, \tag{6}$$

and the value of l in this region is

$$l(\Delta E)=\frac{1}{\alpha}e^{-x\Delta E/\beta},\quad 0<\Delta E<\beta, \tag{7}$$

where $\Delta E\equiv E_0-E$, and $x\equiv p\beta/\alpha$ is the ratio of mean catastrophic to mean noncatastrophic energy loss.

Simple combinatorics now lead to the general expression

$$l(\Delta E)=\frac{1}{\alpha}\sum_{\nu=0}^{n-1}\left(\frac{\Delta E}{\beta}-\nu\right)^{\nu}\frac{x^{\nu}}{\nu!}e^{-x[\Delta E/\beta-\nu]},\; n-1<\frac{\Delta E}{\beta}<n, \tag{8}$$

where the νth term corresponds to the likelihood of ν catastrophic energy losses in the degradation from E_0 to E. Some representative values are

$$\begin{aligned}\alpha l(0)&=1,\\ gl(\beta)&=e^{-x},\\ \alpha l(2\beta)&=e^{-x}[x+e^{-x}]>e^{-x},\end{aligned} \tag{9}$$

and it is indeed easy to show that there is a maximum between β and 2β. Thus, the oscillatory behavior is represented here too, though in a somewhat washed out form.

The asymptotic value of $l(\Delta E)$ is given by

$$l(\Delta E)\rightarrow\frac{1}{\alpha}[1+x]^{-1}=\frac{1}{\alpha+p\beta};\quad \Delta E\rightarrow\infty, \tag{10}$$

which, in view of (4), is the expected value. Relative to the asymptotic value, we see that the first peak is higher by a factor $1+x$, and the first minimum is lower by a factor $(1+x)e^{-x}$.

To get an estimate of the magnitudes involved here (which will turn out to not be very far off) consider the specific case of 1-Mev protons in aluminum, and a resonance 400 ev wide. The maximum energy loss is, then, 2 kev. It would seem reasonable to choose something like 800 ev as our definition of a "catastrophic" energy loss, since this would have a good chance of jumping the resonance without inducing a reaction. For these parameters x turns out to be about 0.20, if we try to make the ratio of catastrophic to continuous energy loss the same as in the real situation. Then the first maximum is about 20% high, and the first minimum about 2% low, which are typical numbers.

It is to be emphasized that this model serves no purpose other than to acquaint us with the physics of the problem. In the next section we do the calculation correctly.

III. THE REAL STRAGGLING PROBLEM

The essential point about the real problem is that the probability of an energy loss between T and $T+\Delta T$ is well represented by

$$p(T)\propto\Delta T/T^2. \tag{11}$$

The maximum energy loss $T_{\max}$ is ϵE, where $\epsilon=4mM/(M+m)^2\approx4m/M$, and it is a good approximation to suppose that there is a minimum energy loss $T_{\min}=\delta E$, given by $I^2/\epsilon E$, where I is a mean ionization energy of the atom. Thus, the fraction of total energy loss due

collisions in which more than T_0 is lost at a time is

$$f(T_0)=\frac{\ln(T_{\max}/T_0)}{\ln(T_{\max}/T_{\min})}. \tag{12}$$

Since the denominator in (12), which we will henceforth call L, is normally in the region between five and ten, $f(T_0)$ is not vanishingly small, and that is the reason for the magnitude of the effect discussed here. Equation (12) was the basis for the estimate of x given at the end of the last section.

For our treatment of the straggling problem, we refer to previous work,[1] which we will not reproduce here, and we will take the notation bodily from that work. We consider the distribution function $f(E,x)$ for the number of particles of energy E at a depth x inside the material, and are interested only in very small energy changes $E_0-E\ll E_0$. Indeed, the number we want is the total track length at E

$$l(E_0,E)=\int_0^\infty f(E,x)dx. \tag{13}$$

We recall that the integral equation for f is

$$\frac{\partial f(E,x)}{\partial x}=c\int_\delta^\epsilon \frac{d\eta}{\eta^2}\left\{\frac{f[E(1+\eta)]}{1+\eta}-f(E)\right\}, \tag{14}$$

where we have neglected the distinction[1] between ϵ and ϵ_1, and have treated δ and c as constants. Both of the latter are justified because we are confining ourselves to small energy changes. We assume

$$f(E,0)=\delta(E-E_0), \tag{15}$$

and integrate (14) from 0 to ∞, on x, obtaining

$$-f(E,0)=-\delta(E-E_0)=c\int_\delta^\epsilon \frac{d\eta}{\eta^2}\left\{\frac{l[E(1+\eta)]}{1+\eta}-l(E)\right\}. \tag{16}$$

We will henceforth drop the argument E_0, where there is no ambiguity involved.

The standard trick is now to make a Mellin transformation on $l(E)$, through

$$l(E)=\int_C \frac{d\lambda}{2\pi i}\nu(\lambda)E^{-\lambda}, \tag{17}$$

so that

$$\nu(\lambda)=\int_0^\infty l(E)E^{\lambda-1}dE, \tag{18}$$

where the integral in (17) is parallel to the imaginary axis, to the right of all singularities of $\nu(\lambda)$, and the integral in (18) need only be taken up to E_0. Substitution into (16) then yields

$$\nu(\lambda)=E_0^{\lambda-1}/cA(\lambda), \tag{19}$$

where

$$A(\lambda)\equiv\int_\delta^\epsilon \frac{d\eta}{\eta^2}[1-(1+\eta)^{-\lambda}], \tag{20}$$

and this is an integral whose properties we will have to study in detail. We have, finally,

$$l(E)=\frac{1}{cE_0}\int \frac{d\lambda}{2\pi i}\frac{(E_0/E)^\lambda}{A(\lambda)}. \tag{21}$$

We will see later that the zero of $A(\lambda)$ at $\lambda=0$ gives the asymptotic yield for the reaction, so that

$$l(E)\rightarrow 1/cE_0A'(0), \quad E_0-E\gg\epsilon E_0, \tag{22}$$

where

$$A'(0)=\int_\delta^\epsilon \frac{d\eta}{\eta^2}\ln(1+\eta)\approx\ln(\epsilon/\delta)\equiv L. \tag{23}$$

It is convenient to normalize the yield to unity well above the threshold, and to measure energy in units of ϵE_0. We therefore define a new variable α, by $E_0\equiv E(1+\alpha\epsilon)$, and a new yield function $y(\alpha)$, so that

$$y(\alpha)=A'(0)\int \frac{d\lambda}{2\pi i}\frac{(1+\alpha\epsilon)^\lambda}{A(\lambda)}, \tag{24}$$

and now $y(\infty)=1$, and $y(\alpha)=0$ for $\alpha<0$. Also, since $\epsilon\ll1$ for heavy incident particles, $(1+\alpha\epsilon)^\lambda$ can be replaced by $e^{\alpha\lambda\epsilon}$, for $\lambda\epsilon^2\ll1$, since $\alpha=O(1)$.

We turn to a discussion of $A(\lambda)$, and can again write

$$\begin{aligned}A(\lambda)&\approx\int_\delta^\epsilon \frac{d\eta}{\eta^2}[1-e^{-\lambda\eta}]\\ &\approx\lambda L+\lambda\int_0^{\lambda\epsilon}\frac{d\sigma}{\alpha^2}[1-\sigma-e^{-\sigma}],\end{aligned} \tag{25}$$

since $\delta\ll\epsilon$, and thus matters only in the term involving L. Thus

$$y(\alpha)\approx\int_C \frac{dz}{2\pi iz}\frac{e^{z\alpha}}{B(z)}, \tag{26}$$

where $z\equiv\lambda\epsilon$,

$$B(z)=1+\frac{1}{L}\int_0^z \frac{d\sigma}{\sigma^2}[1-\sigma-e^{-\sigma}], \tag{27}$$

and the contour is again to the right of all singularities in the z plane.

Equations (26) and (27) are our final result, and there remains only the discussion of how best to evaluate them. We defer this question to the Appendix, and observe here only that $B(z)$ has an infinity of complex zeros which, combined with the exponential in (26), lead to the damped oscillatory behavior of the yield curve, as expected. Further, (2) or the generalization

[1] H. W. Lewis, Phys. Rev. **85**, 20 (1952).

thereof for a resonance of nonstandard shape, remains valid for the asymptotic yield, so that (26) is referred to (2) as normalization. Thus, the usual width–cross-section products for resonant reactions are correctly inferred from the thick-target yield curves, and this consideration does not affect the standard procedure.

IV. CONCLUSIONS

We conclude that the discreteness of the energy loss processes for a charged particle in a solid induces a "ringing" in the thick-target yield curve for a sharply resonant reaction. The criterion for its observation is that the combined energy resolution of the experimental system (including the natural and Doppler widths of the resonance) should be much less than the maximum energy loss for the particle. We have confined ourselves here to nuclear reactions induced by heavy charged particles, although one can think of applying the same considerations to, for example, electron-induced atomic reactions, or neutron resonances in a moderating material.[2] The effect has, in fact, recently been observed on the $Al^{27}(p,\gamma)Si^{28}$ reaction,[3] and is in reasonable agreement with our results.

Finally we note that the effect here described depends specifically on the finiteness of the energy losses, and is, in particular, not obtainable from Fokker-Planck or other diffusion-type treatments of the straggling.

APPENDIX. EVALUATION OF (26) AND (27)

The best two ways of evaluating (26) are by summing over the zeros of $B(z)$ and by integrating up the imaginary axis. We treat these in order.

In the first case, one has to find the zeroes z_n of $B(z)$, preferably by expanding the integrand in (27) in power series. Then

$$B(z)=1+\frac{1}{L}\sum_{\nu=1}^{\infty}\frac{z^{\nu}}{\nu(\nu+1)!}, \tag{28}$$

and the zeros are found in polar coordinates. The first zeros, for $L=5.3$ (1-Mev proton in aluminum) are at $z_1=-5.43+5.52i$, $z_2=-6.53+12.30i$, etc. The zeros occur, of course, in complex conjugate pairs, in the second and third quadrants. Summing only over the ones in the third quadrant, we have

$$y(\alpha)=1+2L\,\mathrm{Re}\sum_{n=1}^{\infty}\frac{z_n e^{\alpha z_n}}{1-z_n-e^{-z_n}}, \tag{29}$$

where the series converges because of the increasing negative real parts of the z_n.

The second procedure, better adapted to computing machines because it is explicit, consists of integrating up the imaginary axis, taking care only to treat the principal part at the origin correctly. The result is

$$y(\alpha)=\frac{1}{2}+\frac{1}{\pi}\int_0^{\infty}\frac{d\rho}{\rho|c(\rho)|}\sin[\alpha\rho+\phi(\rho)], \tag{30}$$

where $\phi(\rho)\equiv\arg c(\rho)$, and

$$\mathrm{Re}c=1-\frac{1}{L}\int_0^{\rho}\frac{\sigma-\sin\sigma}{\sigma^2}d\sigma, \tag{31}$$

$$\mathrm{Im}c=\frac{1}{L}\int_0^{\rho}\frac{1-\cos\sigma}{\sigma^2}d\sigma. \tag{32}$$

$c(\rho)$ is an auxiliary function, to be computed once and for all, after which (30) has to be integrated numerically once for each point α.

Indeed, the function $c(\rho)$ can be expressed in terms of standard sine and cosine integrals, through

$$L\,\mathrm{Re}c=L+1-\sin\rho/\rho-\ln(\rho\gamma)+\mathrm{Ci}(\rho), \tag{33}$$

$$L\,\mathrm{Im}c=\mathrm{Si}(\rho)-(1-\cos\rho)/\rho, \tag{34}$$

where $\ln\gamma$ is Euler's constant $0.577\cdots$, and

$$\mathrm{Ci}(\rho)=-\int_{\rho}^{\infty}\frac{\cos\sigma}{\sigma}d\sigma, \tag{35}$$

$$\mathrm{Si}(\rho)=\int_0^{\rho}\frac{\sin\sigma}{\sigma}d\sigma=\frac{\pi}{2}-\int_{\rho}^{\infty}\frac{\sin\sigma}{\sigma}d\sigma. \tag{36}$$

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[2] I am indebted to M. L. Goldberger for this comment.

[3] W. L. Walters, D. G. Costello, J. G. Skofronick, D. W. Palmer, W. E. Kane, and R. G. Herb, Phys. Rev. Letters 7, 284 (1961).