SCATTERING OF NEUTRONS FROM NONSPHERICAL NUCLEI

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A method for calculating the scattering of neutrons from semi-transparent nonspherical nuclei, based on the use of the exact solutions of the wave equation in spheroidal coordinates, is described.

1. INTRODUCTION

THE scattering of neutrons from nonspherical nuclei was discussed in papers by Drozdov[1] and the author.[2] In these papers it was assumed that (1) the nucleus may be considered at rest during the course of the interaction ("adiabatic approximation"), and (2) the condition $kR \gg 1$ holds (k is the wave vector of the neutron, R the nuclear radius). The papers of Zaretzkii and Shut'ko[3] and Brink[4] discuss the same question using perturbation theory, which is evidently valid only for very small deformations of the nucleus.

For comparison with experiment, the case of interest is that of arbitrary deformations and small energies of the incoming neutron. Here the condition $dR \gg 1$ will not be fulfilled, but the adiabatic approximation remains in force if the energy of the incoming neutron E_n is not too small. The criterion for the applicability of the adiabatic approximation follows from the comparison of the time of flight R/v of the neutron through the nucleus and the characteristic period of the nucleus $\omega^{-1} \approx \hbar/\epsilon$, where ϵ is the energy of the first excited rotational state ($\epsilon \approx 0.1$ Mev). Thus we obtain

$$\varepsilon kR / E_n \ll 1. \qquad (1)$$

This condition is well satisfied for heavy nuclei and neutron energies of a few Mev. A more rigorous examination shows that condition (1) is valid if the probability for exciting the second rotational level is sufficiently small. This will be the case for small deformations of the nucleus, i.e., $\Delta R/R \ll 1$.

In the present paper we compute the scattering of neutrons from a semi-transparent nonspherical even-even nucleus (the spin of the nucleus is zero) represented by a rotation ellipsoid with arbitrary eccentricity. To be specific, we consider a prolate spheroid; the results obtained can be easily used for an oblate spheroid. As in reference 1 and 2, we use the adiabatic approximation. However, we calculate the scattering amplitude not in the quasi-classical approximation, but exactly, using the known particular solutions of the wave equation in spheroidal coordinates.

2. PARTICULAR SOLUTIONS OF THE WAVE EQUATION IN SPHEROIDAL COORDINATES

To solve our problem we must first determine the scattering from a nucleus with fixed orientation. We then have to average this scattering amplitude over the orientations.[1]

We introduce the coordinate system K, with a z axis in the direction of motion of the incoming neutron, and the system K′, whose z′ axis is aligned with the symmetry axis of the nucleus. The semi-axes of the ellipsoid are a and b ($a > b$). The orientation of the nucleus is specified by the unit vector ω directed along the z′ axis.

We introduce the spheroidal coordinates μ, θ, φ, which, for the case of a prolate spheroid, are defined by the relations

$$x' = \frac{d}{2} \sinh \mu \sin \theta \cos \varphi, \quad y' = \frac{d}{2} \sinh \mu \sin \theta \sin \varphi,$$

$$z' = \frac{d}{2} \cosh \mu \cos \theta; \qquad (2)$$

d is the distance between the foci of the spheroid. The coordinate surfaces $\mu = \text{const}$ are confocal spheroids, going into spheres for large distances from the center. The surfaces $\theta = \text{const}$ are rotation hyperboloids, going into cones for large distances from the center (i.e. θ goes over into the ordinary polar angle for large distances). φ is the ordinary azimuthal angle. We also introduce the symbols $\eta = \cos\theta$, $\xi = \cosh\mu$ ($-1 \le y \le 1$, $1 \le \xi \le \infty$).

Let ξ_0 be the value of the coordinate ξ defining the nuclear boundary $[\xi_0 = (1 - b^2/a^2)^{-1/2}]$. With Feshbach, Porter, and Weisskopf[5] we shall assume that the neutron moves in the field

$$V(\xi) = \begin{cases} -V_0 - iW_0, & \xi < \xi_0 \\ 0 & , \xi > \xi_0. \end{cases} \qquad (3)$$

To find the wave function of the scattered neutron we have to solve the wave equation

$$(\Delta + k^2)\psi = 0 \text{ for } \xi > \xi_0, \; (\Delta + \varkappa^2)\psi = 0 \text{ for } \xi < \xi_0, \qquad (4)$$
$$\varkappa = k\sqrt{1 + V_0/E_n + iW_0/E_n}.$$

These solutions must then be "joined" at $\xi = \xi_0$.

The solutions of the wave equation in spheroidal coordinates have been investigated in detail in reference 6. With the notation somewhat changed,* these results lead essentially to the following.

The wave equation has a set of particular solutions each characterized by the quantum numbers l and m. These numbers can take on the same values as the quantum numbers of the orbital angular momentum and its projection. The particular solution ψ_{lm} has the form

$$\psi_{lm} = R_{lm}(c, \xi) J_{lm}(c, \mathbf{n}), \; c = \frac{1}{2}kd = \sqrt{1 - (b/a)^2}\,(a/b)^{1/3}kR \qquad (5)$$

(R is the radius of a spherical nucleus with the same volume, n is a unit vector specified by the "angle" θ and the angle φ).

The "angular" part of the solution is defined thus:

$$J_{lm}(c, \mathbf{n}) = \sum_n s^l_{nm}(c) Y_{nm}(\mathbf{n}),$$
$$s^l_{nm}(c) = \Big[\sum_n |b^l_{nm}|^2\Big]^{-1/2} b^l_{nm}(c), \qquad (6)$$
$$b^l_{nm}(c) = \left[\frac{2n+1}{2}\cdot\frac{(n-|m|)!}{(n+|m|)!}\right]^{-1/2} d^{l-|m|}_{n-|m|}(c),$$
$$s^l_{nm}(0) = \delta_{nl}.$$

The functions $J_{lm}(c, \mathbf{n})$ are orthonormal, therefore

$$\sum_n s^{l'*}_{nm}(c)\, s^l_{nm}(c) = \delta_{ll'}. \qquad (7)$$

The quantities d:: which appear in the expression for the coefficients s^l_{nm} have been determined in reference 6, where they are tabulated for $l < 3$. The summation in (6) goes only over either even or odd indices, and starts with a value n equal to m or m + 1, depending on whether l is even or odd.

*In particular, the number l used here, and the number l used in reference 6, are related by $l_{[6]} = l - |m|$.

The "radial" functions R_{lm} are of two kinds: (1) the regular function $R^{(1)}_{lm}$, which for large ξ has the form

$$R^{(1)}_{lm}(c,\xi) \approx \frac{\sin(c\xi - l\pi/2)}{c\xi} \approx \frac{\sin(kr - l\pi/2)}{kr} \qquad (8)$$

[here we use the fact that $c\xi = kr$ for large r, as is easily seen from (2)]; (2) the function is irregular at $\xi = 1$, having for large distances the form

$$R^{(2)}_{lm}(c,\xi) \approx -\frac{\cos(c\xi - l\pi/2)}{c\xi} \approx -\frac{\cos(kr - l\pi/2)}{kr}. \qquad (9)$$

Reference 6 gives a method for developing these functions as expansions in Bessel functions.

We expand the plane wave in terms of these solutions:

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \exp\{ic[\cosh\mu\cos\theta\cos\theta' + \sinh\mu\sin\theta\sin\theta'\cos(\varphi - \varphi')]\} \qquad (10)$$
$$= \sum_{lm} A_{lm} J^*_{lm}(c,\mathbf{q})\, J_{lm}(c,\mathbf{n})\, R^{(1)}_{lm}(c,\cosh\mu),$$

where $\mathbf{q} = \mathbf{k}/k$, and θ', φ' are the angles of vector $\mathbf{q}$ in the K' system. It is immediately seen from symmetry considerations that the expansion coefficients (10) contain the quantities $J^*_{lm}(c, \mathbf{q})$. The coefficients A_{lm} can be obtained by observing that for large distances $\sinh\mu \approx \cosh\mu = \xi$, hence

$$e^{i\mathbf{k}\cdot\mathbf{r}} \approx \exp\{ic\xi[\cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi - \varphi')]\} = e^{ic\xi\mathbf{q}\cdot\mathbf{n}}$$
$$\approx \sum_{lm} 4\pi i^l \frac{\sin(c\xi - l\pi/2)}{c\xi} Y^*_{lm}(\mathbf{q}) Y_{lm}(\mathbf{n}). \qquad (11)$$

Equating (11) and (10) for large ξ, multiplying both sides by $J^*_{lm}(c, \mathbf{n})\, J_{lm}(c, \mathbf{q})$, and integrating over the solid angles corresponding to $\mathbf{q}$ and $\mathbf{n}$, we obtain $A_{lm} = 4\pi i^l$

3. SCATTERING AMPLITUDE

The general solution of the wave equation (4) in the exterior region $(\xi > \xi_0)$ can be written in the form

$$\psi^{(e)} = \sum_{lm} B_{lm} J_{lm}(c,\mathbf{n})\, R_{lm}(c,\xi), \qquad (12)$$

where B_{lm} is a coefficient depending on $\mathbf{q}$, and R_{lm} has the form

$$R_{lm}(c, \xi) = \cos\delta_{lm} R^{(1)}_{lm}(c,\xi) - \sin\delta_{lm} R^{(2)}_{lm}(c,\xi). \qquad (13)$$

Imposing the usual requirement

$$\psi^{(e)} \approx e^{i\mathbf{k}\cdot\mathbf{r}} + f(\mathbf{q},\mathbf{n})\, e^{ikr}/r \text{ for } r \to \infty, \qquad (14)$$

we find

$$B_{lm} = 4\pi i^l e^{i\delta_{lm}} J^*_{lm}(c,\mathbf{q}); \tag{15}$$

the scattering amplitude is

$$f(\mathbf{q},\mathbf{n}) = \frac{2\pi}{ik} \sum_{lm} J^*_{lm}(c,\mathbf{q}) \; [e^{2i\delta_{lm}} - 1] \, J_{lm}(c,\mathbf{n}). \tag{16}$$

To find the scattering phase δ_{lm} it is necessary to investigate the solution of (4) in the interior region ($\xi < \xi_0$). In this case the general solution will contain only the regular functions $R^{(1)}_{lm}$, and it will be of the form

$$\psi^{(i)} = \sum_{lm} C_{lm} J_{lm}(p, \mathbf{n}) \, R^{(1)}_{lm}(p, \xi), \tag{17}$$

where $p = \kappa d/2$. This solution has to be "joined" with the solution (12) at $\xi = \xi_0$. This "joining" is complicated by the fact that the functions $J_{lm}(p, \mathbf{n})$ and $J_{lm}(c, \mathbf{n})$ represent two different complete systems of functions. They can be reduced to one system by expanding, say, $J_{lm}(c, \mathbf{n})$ in terms of $J_{lm}(p, \mathbf{n})$:

$$J_{l'm}(c, \mathbf{n}) = \sum_{l} u^m_{ll'}(c, p) \, J_{lm}(p, \mathbf{n}), \tag{18}$$

where

$$u^m_{ll'}(c, p) = \int J^*_{lm}(p, \mathbf{n}) \, J_{l'm}(c, \mathbf{n}) \, d\mathbf{n} = \sum_{n} s^{l*}_{nm}(p) \, s^{l'}_{nm}(c). \tag{19}$$

Evidently $u^m_{ll'} = 0$ if the numbers l and l' have opposite parity.

Now

$$\psi^{(e)} = \sum_{lm} J_{lm}(p, \mathbf{n}) \sum_{l'} B_{l'm} u^m_{ll'}(c, p) \, R_{l'm}(c,\xi). \tag{20}$$

Equating the functions $\psi^{(i)}$ and $\psi^{(e)}$ and their derivatives at $\xi = \xi_0$, we obtain a system of equations for the phases

$$C_{lm} R^{(1)}_{lm}(p, \xi_0) = \sum_{l'} B_{l'm} u^m_{ll'}(c, p) \, R_{l'm}(c, \xi_0),$$

$$C_{lm} R^{(1)'}_{lm}(p, \xi_0) = \sum_{l'} B_{l'm} u^m_{ll'}(c, p) \, R'_{l'm}(c, \xi_0); \tag{21}$$

$$(l = 0, 1, 2, \ldots).$$

Here the prime denotes the derivative with respect to ξ_0. Dividing the second equation by the first and using

$$x_{lm} = \frac{1}{2}(1 - e^{2i\delta_{lm}}) \, J^*_{lm}(c, \mathbf{q}),$$

$$T_{lm} = R^{(1)'}_{lm}(p, \xi_0) / R^{(1)}_{lm}(p, \xi_0),$$

we obtain

$$\sum_{l'} M^m_{ll'} x_{l'm} = N_{lm}, \; (l = 0, 1, 2, \ldots), \tag{22}$$

where

$$M^m_{ll'} = i^{l'} u^m_{ll'} [R^{(1)'}_{l'm}(c, \xi_0) + i R^{(2)'}_{l'm}(c, \xi_0)$$
$$- T_{lm}(R^{(1)}_{l'm}(c, \xi_0) + i R^{(2)}_{l'm}(c, \xi_0))], \tag{23}$$

$$N_{lm} = \sum_{l'} i^{l'} u^m_{ll'} [R^{(1)'}_{l'm}(c, \xi_0) - T_{lm} R^{(1)}_{l'm}(c, \xi_0)] \, J^*_{l'm}(c, \mathbf{q}). \tag{24}$$

The system (22) can be solved in the following manner. We set $x_{lm} = 0$ for $l \geq l_0$, where l_0 is a sufficiently large number. Then the system becomes finite, and the number of equations will be equal to the number of variables. We denote the solutions of this system by $x^{(0)}_{lm}$. The next step is to set $x_{lm} = 0$ for $l \geq l_0 + 2$, and obtain the next approximation, the solutions $x^{(2)}_{lm}$. A detailed analysis shows that, for small neutron energies and small deformations of the nucleus ($\Delta R/R \ll 1$), such a process converges very rapidly. In practice, for small deformations, one can set equal to zero all the phases that are sufficiently small for the spherical nucleus. For small neutron energies this leads to a solution of a system with two or three unknowns. Thus, for example, for heavy nuclei and $E_n \approx 1$ Mev the phases with $l = 4$ are already very small. In this case we obtain for x_{00} and x_{20} the system

$$M^0_{00} x_{00} + M^0_{02} x_{20} = N_{00}, \; M^0_{20} x_{00} + M^0_{22} x_{20} = N_{20}. \tag{25}$$

Analogous systems are obtained for the quantities x_{10}, x_{30} and x_{11}, x_{31}, and the quantities x_{21}, x_{22}, x_{32}, x_{33} are determined by first-degree equations. Thus, in particular,

$$x_{21} = N_{21} / M^1_{22}. \tag{26}$$

In the resulting solution of system (22) the quantities x_{lm} will, of course, be expressed in the form

$$x_{lm} = \sum_{\lambda} x^{\lambda}_{lm} J^*_{\lambda m}(c, \mathbf{q}). \tag{27}$$

Here λ runs through values of the same parity as that of l. For $E_n \sim 1$ Mev and $\Delta R/R \ll 1$ these sums will contain only one or two terms.

Now the scattering amplitude takes the form

$$f(\mathbf{q}, \mathbf{n}) = \frac{4\pi i}{k} \sum_{lm\lambda} x^{\lambda}_{lm} J^*_{\lambda m}(c, \mathbf{q}) \, J_{lm}(c, \mathbf{n}) \tag{28}$$

4. CROSS SECTIONS

We proceed to calculate the various cross sections connected with the scattering of neutrons from nonspherical nuclei

The integral cross section σ_s (the cross section for the excitation of all rotational levels, including the elastic scattering) is given by the expression (cf. reference 1):

$$\sigma_s = \frac{1}{4\pi}\int d\omega \int d\mathbf{n}\,|f(\mathbf{q},\ \mathbf{n})|^2. \tag{29}$$

Integration over $\mathbf{n}$ gives

$$\int d\mathbf{n}\,|f(\mathbf{q},\ \mathbf{n})|^2 = \frac{16\pi^2}{k^2}\sum_{lm\lambda\lambda'} x^{\lambda}_{lm}(x^{\lambda'}_{lm})^* J^*_{\lambda m}(c,\ \mathbf{q})\,J_{\lambda' m}(c,\ \mathbf{q}). \tag{30}$$

Since the azimuthal angle of vector $\mathbf{q}$ drops out, one can change the integration over ω in (29) to an integration over $\mathbf{q}$, i.e. instead of averaging over the orientations of the nucleus we average over the directions of the incoming neutron. The result is

$$\sigma_s = \frac{4\pi}{k^2}\sum_{lm\lambda}|x^{\lambda}_{lm}|^2. \tag{31}$$

The total cross section σ_t for all processes is expressed by the imaginary part of the scattering amplitude in the forward direction, averaged over the orientations of the nucleus:

$$\sigma_t = \frac{1}{k}\,\mathrm{Im}\int d\omega f(\mathbf{q},\ \mathbf{q}). \tag{32}$$

From this we obtain

$$\sigma_t = \frac{4\pi}{k^2}\sum_{lm}\mathrm{Re}\,(x^{l}_{lm}). \tag{33}$$

The capture cross section σ_c is equal to the difference of σ_t and σ_s:

$$\sigma_c = \frac{4\pi}{k^2}\sum_{lm\lambda}[\mathrm{Re}\,(x^{\lambda}_{lm}\delta_{l\lambda}) - |x^{\lambda}_{lm}|^2]. \tag{34}$$

In the calculation of the differential cross sections it is necessary to go from the system K′ to the system K. We note that the symbol $Y_{lm}(\mathbf{a})$ has a definite meaning only if we define a definite coordinate system to which the unit vector $\mathbf{a}$ is referred. The vector $\mathbf{a}$ will carry a prime if it is referred to the system K′, and will be without prime if referred to system K.

The cross section for the process in which the neutron is inelastically scattered into the direction $\mathbf{n}$, and the nucleus goes from the ground state ($I = 0$) into the rotational state with angular momentum I and momentum projection M, is defined by the expression

$$\sigma_{IM}(\mathbf{n}) = \frac{1}{4\pi}\left|\int Y^*_{IM}(\omega)\,f(\mathbf{q}',\ \mathbf{n}')\,d\omega\right|^2. \tag{35}$$

On substituting (28) for the amplitude, the computation of the integral in this expression reduces to the calculation of the integrals

$$Q^{IM}_{nn'm} = (-1)^m\int d\omega Y^*_{IM}(\omega)\,Y^*_{nm}(\mathbf{q}')\,Y^*_{n'-m}(\mathbf{n}'). \tag{36}$$

In going from the system K to the system K′ for an arbitrary vector $\mathbf{a}$ we obtain

$$Y_{lm}(\mathbf{a}) = \sum_{m'} D^{(l)}_{mm'}(\omega)\,Y_{lm'}(\mathbf{a}'), \tag{37}$$

where $D^{(l)}_{mm'}$ is an element of the irreducible representation of the rotation group of order $2l + 1$. For the inverse transformation we have, owing to the unitarity of the matrices $D^{(l)}$,

$$Y_{lm}(\mathbf{a}') = \sum_{m'} D^{(l)*}_{m'm}(\omega)\,Y_{lm'}(\mathbf{a}). \tag{38}$$

Applying this formula to the vectors $\mathbf{q}$ and $\mathbf{n}$, and noting that $Y^*_{nm'}(\mathbf{q}) = \sqrt{(2n+1)/4\pi}\,\delta_{m'0}$, we obtain

$$Q^{IM}_{nn'm} = (-1)^m\sqrt{\frac{2n+1}{4\pi}} \times \sum_{\mu} Y^*_{n'\mu}(\mathbf{n})\int d\omega Y^*_{IM}(\omega)\,D^{(n)}_{0m}(\omega)\,D^{(n')}_{\mu -m}(\omega). \tag{39}$$

Using the well-known Wigner theorem,[7] we have

$$D^{(n)}_{0m}D^{(n')}_{\mu -m} = \sum_{L}(nn'0\mu\,|\,nn'L\mu)\,(nn'm-m\,|\,nn'L0)\,D^{(L)}_{\mu 0}, \tag{40}$$

where $(nn'0\mu\,|\,nn'L\mu)$ and $(nn'm-m\,|\,nn'L0)$ are Clebsch-Gordan coefficients. Moreover, we have

$$D^{(L)}_{\mu 0}(\omega) = \sqrt{\frac{4\pi}{2L+1}}\,Y_{L\mu}(\omega). \tag{41}$$

Substituting (40) into (39) and using (41), we obtain finally

$$\sigma_{IM}(\mathbf{n}) = \frac{1}{2I+1}\frac{4\pi}{k^2}\left|\sum_{lm\lambda nn'}(-1)^m\sqrt{2n+1}\,(nn'0M\,|\,nn'IM) \times (nn'm-m\,|\,nn'I0)\,s^{\lambda}_{nm}s^{l}_{n'm}x^{\lambda}_{lm}Y_{n'M}(\mathbf{n})\right|^2. \tag{42}$$

The cross section (42) is obviously independent of the azimuthal angle.

It is easily shown that for $c \to 0$ i.e., in going to a spherical nucleus, formula (42) gives for $I = 0$ the usual formula for the elastic scattering from a spherically symmetric field, while the cross sections go to zero for $I \neq 0$. Indeed, for $c = 0$, $s^{\lambda}_{nm} = \delta_{n\lambda}$, $s^{l}_{n'm} = \delta_{n'l}$, $x^{\lambda}_{lm} = x_l\delta_{l\lambda}$. For the proof we must also make use of the relation

$$\sum_{m}(-1)^m(llm-m\,|\,llI0) = [(ll00\,|\,ll00)]^{-1}\delta_{I0}. \tag{43}$$

It is also easily seen that σ_{IM} vanishes for odd I. Indeed, since the numbers n and n′ in

(42) are of the same parity (the parity of l), we have for all m and odd I

$$(nn'm - m \mid nn'I0) + (nn' - mm \mid nn'I0) = 0. \quad (44)$$

This relation is obtained by expanding the product $Y_{n,m}Y_{n',-m}$ into a Clebsch-Gordan series, and by requiring that this expansion have no odd harmonics. Using (44) and the obvious relation $x^{\lambda}_{lm} = x^{\lambda}_{l-m}$, we have the required proof. Even-even nuclei do not have states with odd I, therefore this last property allows us to sum over the complete system of spherical functions used in the derivation of (29).

Integrating (42) over the angles and summing over M, we obtain, using the orthogonality of the Clebsch-Gordan coefficients, the integral cross section for the excitation of the I-th rotational level

$$\sigma_I = \frac{4\pi}{k^2}\sum_{nn'}\Big|\sum_{l\lambda m}(-1)^m (nn'm - m \mid nn'I0)\, s^{\lambda}_{nm} s^{l}_{n'm} x^{\lambda}_{lm}\Big|^2. \quad (45)$$

The summation over I in this formula leads back to (31), if we use (7).

We have mentioned in the beginning that perturbation theory is applicable only for very small deformations of the nucleus. Indeed, the case of a spherical nucleus is obtained for $c \to 0$ and $p \to 0$, i.e., we should use as small parameters the quantities

$$c = \sqrt{1-(b/a)^2}\,(a/b)^{2/3} kR$$

$$\text{and } p = \sqrt{1-(b/a)^2}\,(a/b)^{2/3} \varkappa R.$$

From the results of Stratton et al.[6] it follows that the parameter in the spheroidal functions may be considered small if it does not exceed unity. For the applicability of perturbation theory it is therefore necessary that $|p| < 1$ (the limitation of c does not come into play, since $c < |p|$), or

$$\frac{a^2-b^2}{a^2}|\varkappa R| < \frac{1}{|\varkappa R|}, \quad \text{i.e. } \frac{\Delta R}{R}|\varkappa R| \ll 1, \quad (46)$$

since $|\kappa R| \approx 10$ for heavy nuclei. It is therefore clear that perturbation theory is of no practical use in our case.

It also follows from the foregoing that we can set $s^{\lambda}_{nm} = \delta_{n\lambda}$, $s^{l}_{n'm} = \delta_{n'l}$ in (42) and (45), if the energies and deformations are small, and $c < 1$. Then the formulas assume the simple form:

$$\sigma_{IM} = \frac{4\pi}{2I+1}\frac{1}{k^2}\Big|\sum_{lm\lambda}(-1)^m \sqrt{2\lambda+1}\,(\lambda l0M|\lambda lIM) \times (\lambda lm - m|\lambda lI0)\, x^{\lambda}_{lm} Y_{IM}(\mathbf{n})\Big|^2; \quad (47)$$

$$\sigma_I = \frac{4\pi}{k^2}\sum_{l\lambda}\Big|\sum_{m}(-1)^m (\lambda lm - m \mid \lambda lI0)\, x^{\lambda}_{lm}\Big|^2. \quad (48)$$

5. NUMERICAL CALCULATIONS AND COMPARISON WITH EXPERIMENT

In order to estimate the magnitude and the character of the effects of the nonsphericity of the nucleus, we made several computations of the scattering.

In constructing the "radial" functions and their derivatives inside the nucleus, i.e. in the numerical calculation of the quantities T_{lm}, we found it convenient not to use the method of reference 6, which is of little practical use for $p \gg 1$, but to use a method described briefly below.

The equation for the radial function $R_{lm}(p, \xi)$ will be:[6]

$$(1-\xi^2)\frac{d^2R_{lm}}{d\xi^2} - 2\xi\frac{dR_{lm}}{d\xi} + \Big(\lambda_{lm} - \frac{m^2}{1-\xi^2} - p^2\xi^2\Big)R_{lm} = 0, \quad (49)$$

where λ_{lm} is a separation constant which represents an eigenvalue arising from the requirement of regularity of the solutions of the wave equation. For $p \gg 1$, we find λ_{lm} with the help of an asymptotic formula obtained by Meixner:[8]

$$\begin{aligned}\lambda_{lm}(p) = {} & pq + m^2 - \frac{1}{8}[q^2+5] - \frac{q}{64p}[q^2 + 11 - 32m^2] \\ & - \frac{1}{1024p^2}[5(q^4+26q^2+21) - 384m^2(q^2+1)] \\ & - \frac{1}{p^3}\Big[\frac{1}{128\cdot128}(33q^5 + 1594q^3 + 5621q) \\ & - \frac{m^2}{128}(37q^3+167q) + \frac{m^4}{8}q\Big] + O(p^{-4}),\end{aligned} \quad (50)$$

where $q = 2l + 1$.

It is easily seen that, for $p \gg 1$ and not too large nonsphericity ($\Delta R/R \approx 0.2 - 0.3$), the motion described by Eq. (49) is quasi-classical in the neighborhood of the nuclear boundary. Therefore, applying the usual quasi-classical method, we obtain for the logarithmic derivative of the "radial" function the following expression:

$$\begin{aligned}T_{lm} = {} & \frac{R^{(1)\prime}_{ml}(p,\xi_0)}{R^{(1)}_{ml}(p,\xi_0)} = -\frac{\xi_0}{4}\frac{2\xi_0^2 - 1 - \alpha}{(\xi_0^2-\alpha)(\xi_0^2-1)} \\ & + p\sqrt{\frac{\xi_0^2-\alpha}{\xi_0^2-1}}\cot\Phi(\xi_0),\end{aligned} \quad (51)$$

$$\begin{aligned}\alpha = \frac{\lambda_{lm}}{p^2}, \quad \Phi(\xi_0) = p\Big\{ & \frac{\sqrt{\xi_0^2-\alpha}}{\xi_0}\sqrt{\xi_0^2-1} \\ & - (1-\alpha)F\Big(\arcsin\frac{1}{\xi_0}, \sqrt{\alpha}\Big) \\ & + E\Big(\arcsin\frac{1}{\xi_0}, \sqrt{\alpha}\Big)\Big\} - \frac{l\pi}{2},\end{aligned}$$

F and E are the elliptic integrals of first and second kind.

In our calculations we made the following choice of parameters:

$$E_n = 1\,\text{Mev}, \; A = 178,$$

$$R = 1.4 \; A^{1/3} \cdot 10^{-13}\,\text{cm}, \; V_0 = 42\,\text{Mev},$$

$W_0/V_0 = 0.03$, $a/b = 1.25$. This choice of parameters corresponds to the Hf nucleus (in particular, the deformation parameters are chosen to agree approximately with the results of Mottelson and Nilsson[9] and with the experimental evidence on scattering gathered by Barschall and Walt[10]). Figure 1 gives the angular distribution obtained in reference 10, as well as the summary angular distribution calculated with a nonspherical nucleus and the distribution calculated with a spherical nucleus. We see that the angular distributions for the spherical and the nonspherical nucleus differ little in the region of small angles, but are distinctly different for large angles. Here the behavior of the angular distribution for the nonspherical nucleus is visibly in better agreement with the experimental evidence that that of the angular distribution for the spherical nucleus. In the table we compare the values of σ_t, σ_c and σ_s (these are given in barns). We see that the model of a nonspherical nucleus explains the values of σ_t and, in particular, of σ_c better than the model of a spherical nucleus. However, for σ_s the value obtained with a spherical nucleus is somewhat closer to the experimental value.

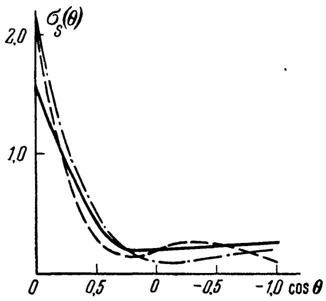

FIG. 1. Angular distribution (in barns per sterad) of neutrons scattered by the Hf nucleus. Solid curve: experiment; dash-dotted curve: a/b = 1.25; dashed curve: a/b = 1.00

The example considered shows therefore that the nonsphericity has a noticeable influence on the scattering. However, for a more definite choice we need additional experiments and more detailed calculations. In particular, it is necessary to consider the contribution from scattering accompanied by formation of the compound nucleus.

We clearly get a more immediate comparison of theory and experiment if we take account of the excitation of rotational levels by the neutrons. We see from the table that $\sigma_2/\sigma_s \approx 0.1$, i.e., the cross section for inelastic scattering with the excitation of the first rotational level is as large as 10% of the elastic scattering cross section. Moreover, it is seen from Fig. 2 that the inelastic scattering goes mainly into large angles, whereas the elastic scattering is concentrated into the small angles. Therefore, for large angles the probability for inelastic scattering is only 2 to 3 times smaller than the probability for elastic scattering into the same angle. For large angles we have thus favorable conditions under which to explore experimentally the excitation of rotational levels by neutrons. Unfortunately, the corresponding experiments have so far not been made. A calculation using for the deformation parameter the value $a/b = 1.1$ gave $\sigma_2/\sigma_s \approx 0.03$, i.e., the cross section for the excitation of the first rotational level increases approximately linearly with the deformation.

	σ_t	σ_c	σ_s	σ_2
Spherical nucleus	5.85	1.06	4.79	—
Non-spherical nucleus	6.70	2.47	4.23	0.42
Experiment	7.20	2.10	5.10	—

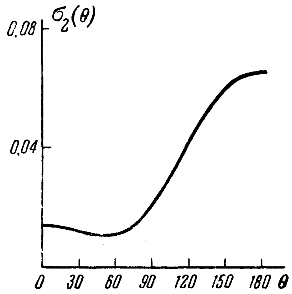

FIG. 2. Angular distribution (in barns per sterad) of neutrons scattered inelastically by the Hf nucleus with the simultaneous excitation of the first rotational level.

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PARAMAGNETIC LATTICE RELAXATION IN HYDRATED SALTS OF DIVALENT COPPER

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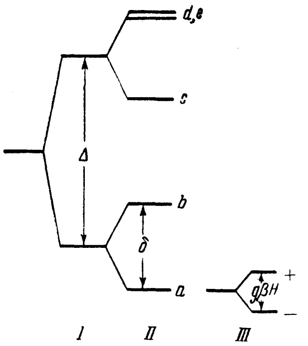
A theoretical calculation of the spin-lattice relaxation time in hydrated salts of divalent copper is carried out. The anisotropy of the relaxation time experimentally observed in $CuSO_4 \cdot 5H_2O$ crystals can be explained by taking into account the anisotropy of the spin-orbit interaction in the Cu^{++} ion due to partially covalent nature of the copper ion bonds in the crystal.

1. INTRODUCTION

HYDRATED salts of divalent copper form a group of paramagnets whose magnetic properties are comparatively well known: detailed examinations of the static susceptibility and paramagnetic resonance spectra have been carried out for a number of these salts, and experimental data on the spin-lattice relaxation are on hand. We shall dwell below on those results that have been utilized for our calculations.

In the crystals of hydrated copper salts the water molecules that surround a magnetic ion form, at the point where the magnetic ion is located, an electric field of cubic symmetry on which is superimposed a comparatively weak field of lower symmetry (tetragonal, trigonal, or rhombic). We shall now examine the Tutton's copper salts and the hydrated copper sulfate $CuSO_4 \cdot 5H_2O$. The unit cells of the crystals of the above salts contain two Cu^{++} ions each. The internal field is of tetragonal, almost cubic, symmetry. The angle between the tetragonal axes is 82° for two magnetic ions of a unit cell of the crystal.[1,2]

The basic state of the Cu^{++} ion is the ^2D state. The ground orbital level of the Cu^{++} ion is split up into a triplet and a doublet by the cubical field, the doublet lying lower. The orbital doublet is split up into two single levels by the tetragonal field. Since the spin is $S = 1/2$, the lower level is



Scheme of the successive splitting of the ground level of a Cu^{++} ion under the influence of: I – an electric field of cubic symmetry; II – tetragonal symmetry; III – levels of the electron spin in the external magnetic field.

a Kramer doublet whose degeneracy is removed by the external magnetic field (see diagram). Optical examinations have shown that the magnitude Δ of the splitting due by the cubical component of the field is 12,300 cm^{-1} (references 1, 3, 4). Reliable data on the magnitude δ of the splitting due to the tetragonal component of the field are lacking. Following Owen's[4] calculations, we assume δ = 1400 cm^{-1}. In accordance with the diagram, we shall designate the two possible spin orientations in an external magnetic field H by + and − signs.

The paramagnetic-resonance spectra observed in crystals of Tutton's salts have been interpreted with g-factor values $g_{\parallel} = 2.4$ and $g_{\perp} = 2.1$ (Ref. 1).* Here $g_{\parallel}$ and $g_{\perp}$ characterize the

*More exact values of the g-factor for different Tutton's salts are given in the paper by Bleany et al.[5]