ing letter. In general, when more than one sublattice has appreciable ionic polarization, considerations similar to those used to obtain the local field must be used to obtain the elastic restoring forces on an ion. The ionic polarization equations should be

$$\mathbf{E}_k=\Sigma_l\beta_{kl}\mathbf{P}_l, \qquad (5)$$

where the local field $\mathbf{E}_k$ includes the electronic contribution and where the β_{kl} are related to the noncoulomb forces within the crystal.

* This research has been assisted in part by the ONR.

Ferroelectricity *versus* Antiferroelectricity in Barium Titanate*

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(Received August 21, 1951)

SLATER'S recent treatment of $BaTiO_3$[1] has shown that the probable origin of the ferroelectricity of $BaTiO_3$ and similar substances of perovskite structure is the strong dipole-dipole interaction within lines of O and Ti ions parallel to the spontaneous polarization. Slater found that the value of the ionic polarizability necessary for spontaneous polarization of the Ti ion alone is 0.947×10^{-24} cc. This value was checked here (see row 1, Table I).

Qualitative considerations suggest that the dipole-dipole interactions in $BaTiO_3$ might be stronger in an antiferroelectric state[2] than in the observed ferroelectric state, just as in the simple cubic structure. Consequently a treatment of $BaTiO_3$ similar to that of Slater was carried out for an antiferroelectric state to determine the ionic polarizability necessary for spontaneous antiparallel polarization.

The O ion on the y-z face of the unit cell will be designated as O_x and similarly for O_y and O_z as shown in Fig. 1(A). The antiferroelectric state considered is one with polarization in a Z_5 array (in the notation of Luttinger and Tisza[3]), Fig. 1(B), on the Ti and O_z sublattices, and with no polarization on the O_x, O_y, and Ba sublattices. For convenience, the Ti and O_z ions will be referred to as 1 and 2, respectively. The only nonzero field constants for this arrangement are $f_{11}=f_{22}=5.351$ and $f_{12}=33.118$. The value of f_{12} was calculated by the Ewald method. The electronic polarizabilities used were those given by Slater.[1] The edge of the unit cell was taken as 4.00A.

Calculations were made assuming that Ti or O_z alone contributes ionic polarization. The local fields at the original lattice points were used, as has been customary. However, as pointed out elsewhere in this issue,[4] the local fields at the displaced lattice points should have been used. The calculations were repeated using the local fields given by Eqs. (4) and (5) of reference 4. For the ferroelectric arrangement $g_2=47.013$, enhancing the local field at the O_z ion considerably. On the other hand, $g_1=f_{11}=4\pi/3$. Hence the calculated polarizability is the same for Ti with both methods. For the antiferroelectric arrangements $g_2=66.236$ and $g_1=16.559$, enhancing the local field at both ions. The results of the calculations are given in Table I.

In general, the greater the local field and the greater the electronic polarizability of the ion contributing most to the local field, the smaller the ionic polarizability required for spontaneous polarization. When the local fields at the original lattice points are used, the results for ferro- and antiferroelectricity are the same for Ti. For O_z less ionic polarizability is required for antiferroelectricity and hence antiferroelectricity is favored. In the actual crystal, however, both ions may contribute ionic polarization.[5] Since Ti requires less polarizability than O_z in both arrangements, one would expect the Ti ion to contribute most of the ionic polarization. Hence, one cannot interpret decisively the favoring of ferroelectricity in $BaTiO_3$ with simple dipole-dipole interactions alone if the local fields are taken at the original lattice points. When the local fields at the actual lattice points of the ions are used, antiferroelectricity is favored for the Ti and the O_z ions both. Thus even if one uses local fields at the actual lattice points, one still cannot explain the favoring of ferroelectricity in $BaTiO_3$ with the simple dipole-dipole interaction model.

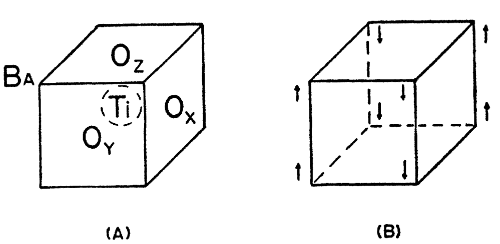

FIG. 1. (A) Unit cell of $BaTiO_3$. (B) Z_5 array.

TABLE I. Ionic polarizability required for spontaneous polarization.

Type of array	Local field	Ion displaced	Polarizability cc
1. ferroelectric (f.e.)	at original position	Ti	0.947×10^{-24}
2. antiferroelectric (a.f.e.)	at original position	Ti	0.947
3. f.e.	at original position	O_z	3.01
4. a.f.e.	at original position	O_z	5.06
5. f.e.	at displaced position	Ti	0.947
6. a.f.e.	at displaced position	Ti	0.787
7. f.e.	at displaced position	O_z	0.646
8. a.f.e.	at displaced position	O_z	0.626

I wish to thank Professor Charles Kittel for having suggested this problem and for many informative and stimulating discussions.

* This research has been assisted in part by the ONR.
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Angular Correlation in Magnetic Fields

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(Received September 4, 1951)

THE angular correlation of two successively emitted nuclear particles can be influenced by magnetic fields (e.g., from the electron shell, from neighboring atoms, or from an external source). In order to calculate a general expression, we start with the formula of Goertzel[1] for the emission probability W of two particles with directional vectors $\mathbf{k}_1$ and $\mathbf{k}_2$.

$$W(\mathbf{k}_1,\mathbf{k}_2)=S_1S_2\sum_{lmm'p}(A_l|H_1|B_m)(B_m|H_2|C_p)^*\times(A_l|H_1|B_{m'})^*(B_{m'}|H_2|C_p)\frac{1}{1-i\omega_{BB'}\tau}. \qquad (1)$$

A_l, B_m, C_p are the wave functions of the atom (nucleus+shell) for the 3 states of the cascade. H_1, H_2 designate the hamiltonians responsible for the emission of the first and second particles, respectively. $\omega_{BB'}$ is the energy splitting of the two levels B_m, $B_{m'}$, divided by $\hbar$. τ is the mean life of the intermediate state. We can now modify Goertzel's expression (1) by choosing an arbitrary z-axis. Introducing solid harmonics $Y_k^r(\mathbf{k})$ we get instead of (1)

$$W(\mathbf{k}_1,\mathbf{k}_2)=\sum_{r,k}G_k^rA_k\frac{1}{2k+1}Y_k^r(\mathbf{k}_1)Y_k^r(\mathbf{k}_2)^*. \qquad (2)$$

As is seen later, the coefficients a_k are independent of the magnetic field. The whole influence of the magnetic field is in fact contained in the attenuation factor G_k^r. This attenuation factor can be calculated for the two special cases of a weak and strong field.

(a) "Weak field" ($I-J$ coupling unbroken)

$$G_k^r=(2k+1)\sum_{F,F'}(2F+1)|W(I_BJkF|F'I_B)|^2\sum_{m,m'}|C_{F'm'kr}{}^{Fm}|^2\times\frac{1}{1-i\omega_{Fm,F'm'}\tau}. \quad (3)$$

I_B and J stand for the angular momentum of the intermediate state and the electronic shell, respectively; F is the total angular momentum of the atom; W and C are Racah and Clebsch-Gordon coefficients, respectively.[2] For the case of vanishing external magnetic field (3) reduces to

$$G_k^r=\sum_{FF'}(2F+1)(2F'+1)|W(I_BJkF|F'I_B)|^2\frac{1}{1+(\omega_{FF'}\tau)^2}. \quad (3a)$$

We have discussed this expression in a previous letter.[3]

(b) "Strong field" ($I-J$ coupling broken)

$$G_k^r=(2k+1)\sum_{m,m'}|C_{I_Bm'kr}{}^{I_Bm}|^2(1-i\omega_{mm'}\tau). \quad (4)$$

If the magnetic moment J of the shell is zero, we obtain

$$\omega_{mm'}=r\omega=r\mu H/I_B\hbar=rg\mu_kH/\hbar \quad (5)$$

(μ, g = magnetic moment and g factor of the intermediate nuclear level; μ_k = nuclear magneton). Then the sum in (4) can be evaluated:

$$G_k^r=1/(1-ir\omega\tau). \quad (6)$$

If we take the external magnetic field H perpendicular to the plane of the two quanta, Eq. (2) becomes particularly simple and useful for application:

$$W(\vartheta,H)=\Sigma_r[b_r/(1-ir\omega\tau)]e^{ir\phi} \quad (7)$$

where ϑ is the angle between the two quanta. The magnetic field induces an attenuation and a phase shift. For $\omega\tau\ll1$, this results essentially in a rotation of the symmetry axes through the classical precession angle $\phi=\omega\tau$. If the two counters cannot distinguish between the two particles, the attenuation factor becomes real:

$$G_k^r=\frac{1}{2}\left\{\frac{1}{1-ir\omega\tau}+\frac{1}{1+ir\omega\tau}\right\}=\frac{1}{1+(r\omega\tau)^2}. \quad (8)$$

Therefore a measurement of G_k^r with equally sensitive counters gives only the magnitude, but not the sign, of the nuclear g factor.

For $\omega\tau\gg1$, for both strong and weak fields, the relationship is simplified to a minimum correlation:

$$G_k^r=\delta_{0r}. \quad (9)$$

In this case the angular correlation is symmetric about the axis of the magnetic field. If then the direction of one particle coincides with that of the magnetic field, the angular correlation remains uninfluenced.

$$W=\Sigma_k a_kP_k(\cos\vartheta). \quad (10)$$

Thus the a_k of Eq. (2) are seen to be the coefficients of Legendre polynomials in the case of an unperturbed correlation.

I wish to thank Professor W. Pauli, Professor V. Weisskopf, Dr. A. S. Bishop, Dr. H. Frauenfelder, and Dr. M. R. Schafroth for many helpful discussions.

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The Determination of the Magnetic Moment of an Excited Nuclear Level (Cd^{111}, 247 kev)

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THE possibility of determining the g factor of the intermediate nuclear state on a $\gamma-\gamma$-cascade by measuring the influence of a magnetic field on the angular correlation has recently been discussed by several authors.[1,2] Using an external magnetic field on a source of $In^{111}\to Cd^{111}$, we have now established experimentally the existence of this effect, and have determined the magnitude and sign of the magnetic moment of the intermediate nuclear level.

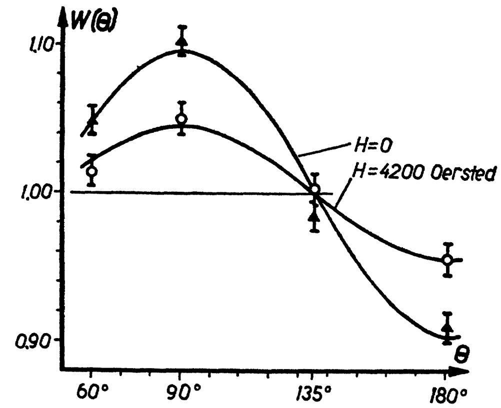

FIG. 1. Angular correlation, $W(\theta)=1+b_2'\cos2\theta$, of Cd^{111}. Magnetic field perpendicular to the plane of the two γ-rays.

The $\gamma-\gamma$-cascade of Cd^{111} is well known;[3] the measured angular correlation in sources of maximum anisotropy[4,5] follows closely the function[6]

$$W(\theta)=1+A_2\cos^2\theta \quad \text{with} \quad A_2=-0.20\pm0.01. \quad (1)$$

The intermediate level is assumed to be a $d_{\frac{5}{2}}$ state[3] and has a half-life of about 8.5×10^{-8} sec.

The general relationships for the influence of an external magnetic field upon the angular correlation of two successive nuclear radiations has been calculated by Alder.[7] For the case in which a magnetic field H is perpendicular to the plane of the two successive γ-rays, and each counter is sensitive to only one γ-ray, Alder finds the correlation function to be given by

$$W(\theta,H)=\Sigma_r[b_r/(1-ir\omega\tau)]e^{ir\theta}, \quad (2)$$

where θ is the angle between the two γ-rays, τ is the mean life of the intermediate state, and $\omega=gH\mu_k/\hbar$ is the classical precessional velocity of the nucleus in the magnetic field H.

In the case of Cd^{111}, the correlation function in the absence of a magnetic field can be well fitted by the function (1); the highest term in the development (2) thus is $r=2$. Equation (2) then becomes

$$W(\theta,H)=1+\frac{b_2}{1+(2\omega\tau)^2}\{\cos2\theta\mp2\omega\tau\sin2\theta\}, \quad (3)$$

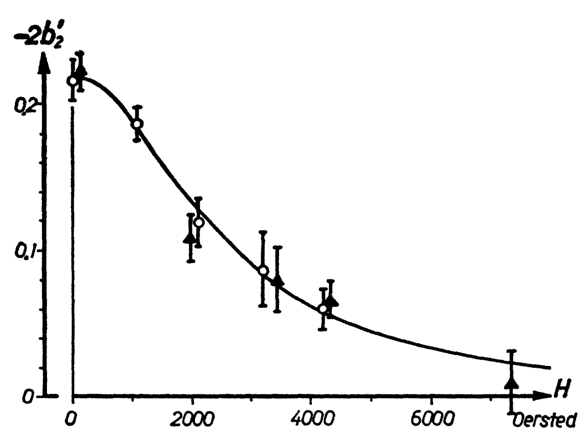

FIG. 2. Anisotropy b_2' as a function of the magnetic field strength H.