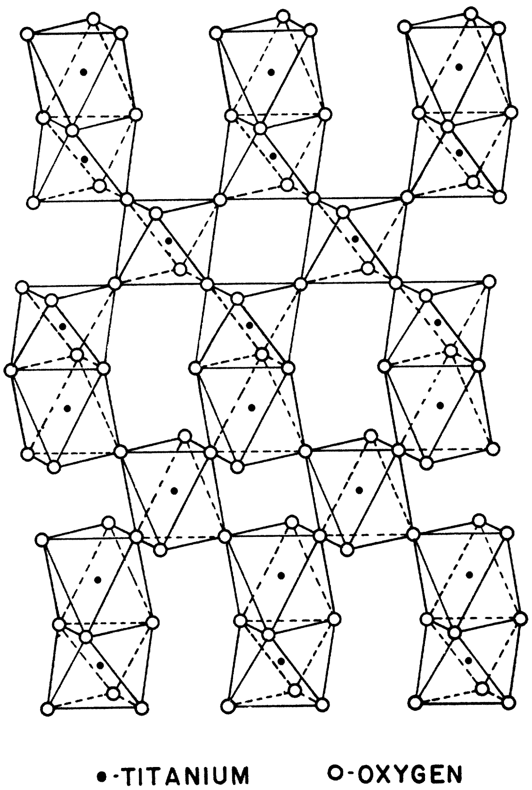

FIG. 1. Schematic idealized representation of the oxygen octahedra in hexagonal barium titanate.

Experimentally, hexagonal $BaTiO_3$ has been found to be nonferroelectric. I have applied the Lorentz local field correction to the hexagonal modification to ascertain if it leads reasonably to the conclusion that the hexagonal modification should be nonferroelectric.

To simplify the calculation a little, the crystal structure was idealized, somewhat. The O octahedra were all taken as equal regular octahedra with the Ti ions at the centers and with dimensions the same as the octahedra of the cubic modification.[3] The directions of the O octahedron chains were taken as mutually perpendicular. The resulting dimensions of the unit cell of the idealized hexagonal structure are $a'=5.68$A, $c'=13.9$A, and $c'/a'=2.45$, compared with the actual dimensions of $a=5.735$A, $c=14.05$A, and $c/a=2.450$.

At the site of each O and Ti ion, the local field was calculated due to the polarization of all the other O and Ti ions contained with a cylinder of infinite length with axis parallel to the c axis and of radius equal to $a'/\sqrt{3}=0.58a'$ circumscribed about the particular site as a center. As in Slater's paper, it was assumed that only the Ti ions undergo ionic polarization. The field due to the polarization of the Ba ions, P_{Ba}, was approximated as the ordinary Lorentz correction of $4\pi P_{Ba}/3$. Ignoring the effect of the material outside of the cylinders, is equivalent to approximating the surrounding material as being uniformly polarized.

The calculation indicated a necessary value of 1.6×10^{-24} cm^3 for the ionic polarizability of the Ti to produce ferroelectricity in the hexagonal modification. This is appreciably greater than the necessary value of 0.9×10^{-24} cm^3 calculated for the cubic modification and presumably just barely attained there at the ferroelectric Curie point temperature of 120°C. Therefore, subject to the assumption that only the Ti ions undergo ionic polarization, it may reasonably be expected that hexagonal $BaTiO_3$ should be nonferroelectric. This is consistent with the experimental finding.

Physically, the absence of ferroelectricity in hexagonal $BaTiO_3$ may be traced to (1) the existence of short finite chains of alternating Ti and O ions instead of infinite chains, and the noncollinearity of successive chains, (2) the absence of a highly polarizable O ion between the two Ti ions at the neighboring ends of successive chains, and (3) the larger distance between these Ti ions as compared with the Ti−O distance.

I should like to thank Professor C. Kittel for proposing this problem and for making helpful suggestions.

[1] J. C. Slater, Phys. Rev. **78**, 748 (1950).
[2] R. D. Burbank and H. T. Evans, Jr., Acta Cryst. 1, 330 (1948).
[3] Helen D. Megaw, Proc. Roy. Soc. (London) **189A**, 261 (1947).

Note on the Bose-Einstein Integral Functions*

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EXPANSIONS of the Bose-Einstein integral functions

$$F(\sigma,\alpha)\equiv[1/\Gamma(\sigma)]\int_0^\infty (x^{\sigma-1}/e^{x+\alpha}-1)dx \quad (1)$$

in powers of α, which would correspond to well-known developments of the Fermi-Dirac integral functions,[1] are desirable for discussing the behavior of the $F(\sigma,\alpha)$ for small α. However, the power series for the Bose-Einstein functions seems not to be generally known.

The $F(\sigma,\alpha)$ defined in Eq. (1) can be continued analytically for complex σ by an integral, say $G(\sigma,\alpha)$, which is analytic over the entire σ-plane and for all positive α, save for the singularity at $\sigma=1$ when $\alpha=0$, by a procedure similar to that of McDougall and Stoner.[1] Here, however, we seek only a continuation for all σ and *small* positive α, and shall follow a simpler treatment. By the use of Mellin transforms[2] one can express the Bose functions in terms of power series whose functional behavior for small α is translucent, and which are, for those σ of greatest interest, particularly well suited to numerical computation when $\alpha<1$.

In deriving the result it is sufficient to consider the case $\alpha>0$, $\sigma>1$, and $\sigma\neq$integer. The Mellin transform of $F(\sigma,\alpha)$ is then

$$\mathfrak{F}(\sigma,s)=\int_0^\infty F(\sigma,\alpha)\alpha^{s-1}d\alpha=\int_0^\infty \sum_{n=1}^{\infty}\frac{e^{-n\alpha}}{n^\sigma}\alpha^{s-1}d\alpha =\Gamma(s)\zeta(s+\sigma), \quad (2)$$

where $\zeta(s+\sigma)$ is the ordinary Riemann zeta-function. The inverse transformation then gives:

$$F(\sigma,\alpha)=(1/2\pi i)\int_{c-i\infty}^{c+i\infty}\mathfrak{F}(\sigma,s)\alpha^{-s}ds =(1/2\pi i)\int_{c-i\infty}^{c+i\infty}\alpha^{-s}\Gamma(s)\zeta(s+\sigma)ds,\quad c>0. \quad (3)$$

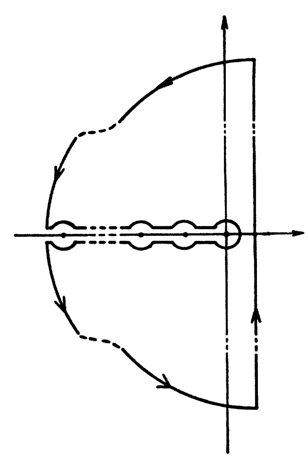

FIG. 1. Contour for evaluating the Mellin integral of Eq. (3).

For $|\alpha|<2\pi$, the contour of Fig. 1, which is indented at the (simple) poles of the integrand, can be used. (The cut along the negative axis of reals makes possible immediate use of the Stirling asymptotic expansion of $\log\Gamma(s)$[3] to show that the integrand vanishes on the arcs as the contour recedes to infinity.) The function $\zeta(s+\sigma)$ has a simple pole at $s=1-\sigma$ with residue $+1$, and $\Gamma(s)$ has simple poles at $s=-n$ with residues $(-1)^n/n!$ Consequently, we have

$$F(\sigma,\alpha)=\Gamma(1-\sigma)\alpha^{\sigma-1}+\sum_{n=0}^{\infty}\frac{(-)^n}{n!}\zeta(\sigma-n)\alpha^n. \qquad (4)$$

This is patently an analytic function of σ if $\sigma\leqslant 0$ and for all non-integral σ.

If now $\sigma=m$, a positive integer, although $\Gamma(1-\sigma)\alpha^{\sigma-1}$ and one term of the series in Eq. (4) become infinite separately, their sum remains finite. We have

$$F(m,\alpha)=\lim_{\sigma\to m}\left\{\Gamma(1-\sigma)\alpha^{\sigma-1}+\frac{(-)^{m-1}}{(m-1)!}\zeta(\sigma-m+1)\alpha^{m-1}\right\}$$
$$+\sum_{n=m-1}^{\infty}\frac{(-)^n}{n!}\zeta(\sigma-n)\alpha^n=\frac{(-)^{m-1}}{\Gamma(m)}\left\{C+\frac{\Gamma'(m)}{\Gamma(m)}-\log\alpha\right\}\alpha^{m-1}$$
$$+\sum_{n=m-1}^{\infty}\frac{(-)^n}{n!}\zeta(\sigma-n)\alpha^n,$$

where C is Euler's constant. Therefore, by the principle of analytic continuation, Eq. (4) holds for *all* σ. The series converges absolutely if $|\alpha|\leqslant 2\pi$.

Equation (4) readily yields the differentiation property of the Bose functions:

$$\partial^n F(\sigma,\alpha)/\partial\alpha^n=(-)^n F(\sigma-n,\alpha).$$

When $\alpha\to 0$, it is seen that $F(\sigma,\alpha)$ diverges as $\alpha^{-|\sigma-1|}$ if $\sigma<1$, and as $\log(1/\alpha)$ if $\sigma=1$, and of course converges toward $\zeta(\sigma)$ if $\sigma>1$. If $1<\sigma\leqslant 2$, then $F(\sigma,\alpha)$ has an infinite slope at the origin although the function itself remains finite. Clearly, the origin $\alpha=0$ is a branch point for all the $F(\sigma,\alpha)$.

The series in Eq. (4) converges quite rapidly in the neighborhood of $\alpha=0$ for positive σ which are not too large. For example, with an accuracy of at least 1 percent when $\alpha\leqslant 1$, we have

$$F(\tfrac{1}{2},\alpha)=1.77\alpha^{-\frac{1}{2}}-1.46+0.208\alpha-0.0128\alpha^2,$$
$$F(\tfrac{3}{2},\alpha)=-3.54\alpha^{\frac{1}{2}}+2.61+1.46\alpha-0.104\alpha^2+0.00425\alpha^3,$$
$$F(5/2,\alpha)=2.36\alpha^{\frac{3}{2}}+1.34-2.61\alpha-0.730\alpha^2+0.0347\alpha^3.$$

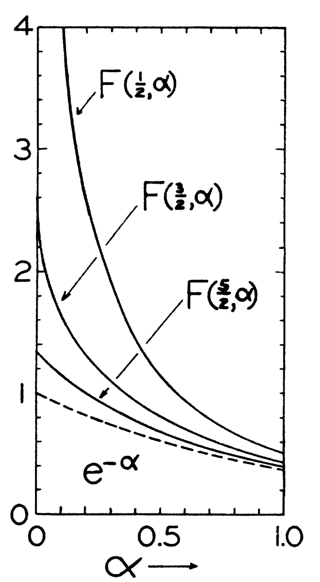

FIG. 2. The Bose-Einstein integral functions $F(\frac{1}{2},\alpha)$, $F(\frac{3}{2},\alpha)$, and $F(5/2,\alpha)$ for the range $0\leqslant\alpha\leqslant 1$.

These functions, together with $e^{-\alpha}$, are shown graphically in Fig. 2 for the range $\alpha\leqslant 1$. For $\alpha>1$, the $F(\sigma,\alpha)$ are conveniently evaluated by the familiar series of exponentials.

The author wishes to thank Professor F. London for his interest in this work.

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[1] J. McDougall and E. Stoner, Trans. Roy. Soc. (London) **A237**, 67 (1938).
[2] E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals* (Oxford University Press, London, 1948), pp. 7 ff., 190 ff. G. G. MacFarlane, Phil. Mag. **40**, 188 (1949).
[3] E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, London, 1947), p. 276.

Radioactive Decay of I^{131}

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THE principal radiations emitted in the disintegration of I^{131} have been organized into schemes by Metzger and Deutsch (M.D.)[1] and by Kern, Mitchell, and Zaffarano (K.M.Z.).[2] These are shown in Fig. 1, and it will be seen that they include essentially the same features and differ only in the soft beta-ray branch. However, a number of less prominent features remain to be accounted for. Brosi *et al.*[3] have found that a small fraction of the disintegrations lead to the 12-day metastable level of Xe^{131}; a gamma-ray of an energy approximately 720 kev occurring in about 5 percent of disintegrations has been discovered by Cavanagh[4], and subsequently reported by Cork *et al.*[5], and by Zeldes *et al.*;[6] Cork[5] has produced a convincing photographic spectrum showing K and L conversion lines due to a 177-kev gamma; Zeldes[6] has produced evidence of a weak 810-kev beta-ray. All these radiations, except the 810-kev beta-ray, have been assembled by Cork[5] into a scheme which must, however, be very far from the truth. As the authors point out, there are wide anomalies in the intensities. For instance, in one branch the 600-kev beta-ray which arises from 85 percent of the disintegrations is shown followed by the 723-kev gamma-ray (5 percent) leading to the metastable level (1 percent). Moreover, the scheme places both the 637- and the 364-kev gamma-rays in the soft beta-branch, although M.D. have shown that only the first of these is associated with the soft beta-ray, the other being in the 600-kev beta-

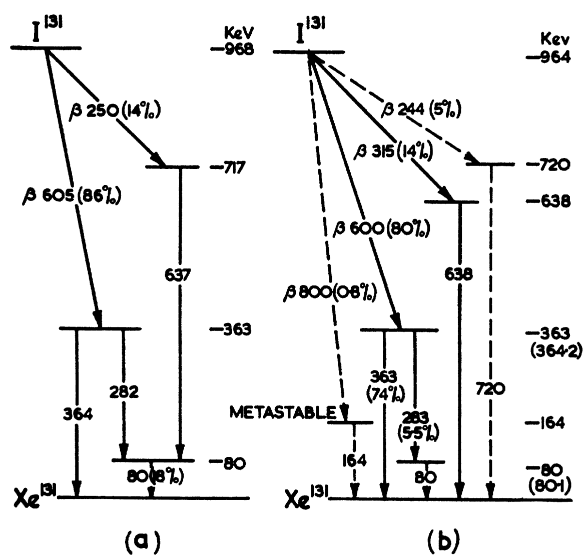

FIG. 1. Decay schemes for I^{131}: (a) Kern, Mitchell, and Zaffarano (K.M.Z.); (b) Metzger and Deutsch (M.D.) with proposed additional branches (dotted).