

## Scattering of Small-Wavelength Neutrons by a Square-Mound-Potential Gas

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The modern theory of classical fluids, using the Born-Green-Yvon equation and a modified form of the Kirkwood superposition approximation involving powers of the particle number density  $n$ , is used to investigate the total neutron elastic scattering cross section for high-energy neutrons and heavy nuclei any pair of the latter of which interact according to the repulsive square mound potential. This potential function is defined by  $\psi(r) = \epsilon$  ( $r \leq 1$ ) and  $\psi(r) = 0$  ( $r > 1$ ), where  $\epsilon$  is a positive constant,  $r$  is the separation distance, and the particle diameter is taken as the unit of distance. If  $T$  is the absolute temperature,  $k$  the Boltzmann constant, and  $z = 1 - \exp\{-\epsilon/kT\}$ , then it is found by the present arguments for the low-density gas limit, where a number density expansion is valid, that up to the cube power of the density

$$\sigma_{\text{tot}} = 1 - (\lambda^2/2\pi)[zn + I_1(z)n^2 + I_2(z)n^3],$$

where

$$I_1(z) = -3.1416z^2 + 2.6834z^3,$$

$$(1 + 0.1563z)I_2(z) = 6.2755z^3 - 20.2741z^4 + 19.0949z^5 - 4.7807z^6,$$

and the undefined symbols have their usual meaning.

### 1. INTRODUCTION

THE expression for the total neutron-scattering cross section (including the effects of interference) by heavy nuclei (hereafter called particles) given by Placzek, Nijboer, and Van Hove,<sup>1</sup> has the asymptotic form for small wavelengths

$$\sigma_{\text{tot}} = 1 - (n\lambda^2/2\pi)K, \quad (1)$$

where

$$K = \int_0^\infty [1 - g(r)]dr. \quad (2)$$

Here,  $\sigma_{\text{tot}}$  is the total cross section with that of an isolated particle taken as the unit;  $g(r)$  is the particle radial distribution function (if necessary angle averaged);  $n$  is the particle number density ( $= N/V$  for  $N$  identical fluid particles contained in a volume  $V$ ); and  $\lambda$  is the (small) wavelength. In a recent paper<sup>2</sup> (hereafter referred to as paper I; the arguments and formulas of paper I are widely used in what follows) the present author discussed the integral (2) defining  $K$  in the low particle-density limit for the case of a gas of hard spheres, using the arguments of classical statistical mechanics in a form designed to ensure internal consistency in the theory with respect to the thermodynamic (virial) properties of the gas. In the present paper, these arguments are reconsidered for a gas whose particles interact mutually according to the repulsive square-mound force potential [defined by Eq. (8)]. The scattering cross section is now found to be dependent upon the gas temperature, which is not the case for a hard-sphere gas.

### 2. THE BASIC FORMULAS

For densities that are not too high, the radial distribution  $g(r)$  appearing in Eq. (2) can be expanded in

<sup>1</sup> G. Placzek, B. R. A. Nijboer, and L. Van Hove, Phys. Rev. **82**, 392 (1951).

<sup>2</sup> G. H. A. Cole, Phys. Rev. **126**, 383 (1962).

powers of  $n$  according to

$$g(r) = \exp\{-\psi(r)/kT\} \times [1 + a_1(r)n + a_2(r)n^2 + a_3(r)n^3 + \dots]. \quad (3)$$

Here  $k$  and  $T$  have their usual meanings;  $\psi(r)$  is the potential of the interparticle force (ultimately to be chosen as being of the square-mound type), and the coefficients  $a_i$  are as yet undefined. As in paper I, so here, the  $a_i$  are determined by making an appeal to the formulas of classical statistical mechanics; explicitly, appeal is made to the Born-Green-Yvon equation

$$\frac{\partial g(r)}{\partial r} + \frac{1}{kT} \frac{\partial \psi(r)}{\partial r} g(r) = -\frac{n}{kT} \int_0^\infty \frac{\partial \psi(r_{13})}{\partial r_{13}} g^{(3)}(r, r_{13}, r_{23}) 4\pi r_{13}^2 dr_{13}, \quad (4)$$

where  $g^{(3)}$  is the triplet distribution and  $(r, r_{13}, r_{23})$  are the three associated particle separation distances.

Equation (4) is closed [i.e. arranged to involve only the single unknown function  $g(r)$ ] by assuming the validity of the superposition expression for  $g^{(3)}$  involving a number density expansion, viz,

$$g^{(3)}(r, r_{13}, r_{23}) = g_K^{(3)}(r, r_{13}, r_{23}) [1 + X_1 n + X_2 n^2 + \dots], \quad (5a)$$

where

$$g_K^{(3)}(r, r_{13}, r_{23}) = g(r)g(r_{13})g(r_{23}). \quad (5b)$$

The coefficients  $X_i$  are, in general, functions of the triplet of distances  $(r, r_{13}, r_{23})$  and also of the quantity  $\psi(r)/kT$ . The coefficients  $a_i$  in (3) are to be derived by solving the differential equation which results when (5a) and (3) are inserted into (4). This procedure can be used only if the functions  $X_i$  are already known. As explained in paper I, these functions are chosen to ensure simple internal consistency for the calculated fluid thermodynamic properties. Specifically, it is required that the

virial expansion for the gas pressure in powers of  $n$  be the same whether calculated from the virial theorem, where the expression for the pressure is

$$p = nkT - \frac{n^2}{6} \int_0^\infty \frac{\partial \psi(r)}{\partial r} g(r) 4\pi r^2 dr, \quad (6a)$$

or from fluctuation theory which leads to the formula

$$kT \frac{\partial n}{\partial p} \Big|_T = 1 + 4\pi n \int_0^\infty [g(r) - 1] r^2 dr. \quad (6b)$$

One simplification will be introduced for mathematical reasons, viz., that the  $X_i$  are independent of the separation distances ( $r, r_{13}, r_{23}$ ), although they are dependent upon the ratio  $\psi/kT$ . This simplification has been found to work well thermodynamically for the case of a hard-sphere gas,<sup>2,3</sup> and also for the square-mound-potential function<sup>4</sup> at least as far as the fourth virial coefficient. The general formulas for the  $X_i$  under this simplifying approximation and applicable to any interparticle potential function have been given in paper I [see Eqs. (14a), (14b), and (14c)]. The expression for  $X_1$ , which is used later in this paper, was shown in paper I, Sec. 4, to be given by the expression

$$(4B^2 + C)X_1 = D_e^K - D_v^K, \quad (7)$$

where  $B$  and  $C$  are the second and third virial coefficients appearing in the expansion of the gas pressure in powers of  $n$ ;  $D_e^K$  is the fourth virial coefficient which results from Eqs. (3), (4), (5b), and (6b), while  $D_v^K$  is the fourth virial coefficient resulting from Eqs. (3), (4), (5b), and (6a). The expression (7) for  $X_1$  is deduced<sup>2-4</sup> by requiring Eqs. (3), (4), (5a), together with either (6a) or (6b), to each lead to a single consistent value for  $D$ . The detailed expressions for  $B$  and  $C$  are given in reference 3, Eqs. (8) and (9), while those for  $D_e$  and  $D_v$  are given in paper I, Eqs. (8).

### 3. FUNCTIONS $a_1(r)$ AND $a_2^K(r)$

The superposition approximation (5b), which is the form taken by (5a) for the special case  $X_i=0$ , is the form first suggested by Kirkwood<sup>5</sup> long ago. The coefficients appearing in (3) which are derived from (4) using the Kirkwood approximation (5b) are denoted by a superscript  $K$  wherever they differ from the corresponding coefficients which result when the approximation (5a) is used in place of (5b). It was seen in paper I that the coefficients  $a_i$  appropriate to the full superposition expression (5a) can be calculated if the analogous coefficients  $a_i^K$  are known, provided also that the functions  $X_i$  are known. Assuming that  $X_i = X_i(\psi/kT)$  is a significant approximation, then reference to paper I, Eqs. (9), and (13), and to Eq. (7) above shows that the

value of the coefficient  $X_1$  now follows simply from a knowledge of the functions  $a_1(r)$  and  $a_2^K(r)$ . Consequently, a detailed knowledge of the solutions of the various equations under the Kirkwood approximation (5b) is necessary before any improvement on the present lines can be attempted.

For the present arguments the gas particles are assumed to interact according to the repulsive square-mound potential defined by

$$\psi(r) = \begin{cases} \epsilon (>0, \text{ a constant}) & \text{for } 0 \leq r \leq 1, \\ 0 & \text{for } r > 1, \end{cases} \quad (8)$$

where the particle diameter is chosen as being the unit of length. It is convenient also to introduce the function  $z$  defined by

$$z = 1 - \exp\{-\epsilon/kT\} \quad (9)$$

into the theory; the dependence of any function on  $z$  is fully equivalent to a temperature dependence. In particular, when  $T=0$ ,  $z=1$ , while when  $T=\infty$ ,  $z=0$ . For hard spheres [where in (8),  $\epsilon \rightarrow \infty$ ],  $z=1$  is the only possibility, there then being no temperature dependence.

The functions  $a_1$  and  $a_2^K$  and so on are obtained by inserting (8), (3), and (5b) into (4) and equating the coefficients for equal powers of  $n$  in the ensuing equation. The coefficient of the linear term in  $n$  is  $a_1(r)$ ; Cole<sup>4</sup> has shown that for the square-mound potential (8)

$$a_1(r) = \begin{cases} z^2 \pi \left( \frac{4}{3} - r + \frac{1}{2} r^3 \right) & \text{for } r \leq 2, \\ 0 & \text{for } r > 2. \end{cases} \quad (10)$$

The quadratic term in  $n$  gives<sup>4</sup>  $a_2^K(r)$ :

$$a_2^K(r) = \vartheta_2(r) + \omega_2(r) + \chi_2(r), \quad (11a)$$

where

$$\vartheta_2(r) = z^4 \pi^2 \left( \frac{8}{9} - \frac{4}{3} r + \frac{1}{2} r^2 + \frac{1}{9} r^3 - \frac{1}{12} r^4 + \frac{1}{288} r^6 \right) \text{ for } 0 \leq r \leq 1, \\ = 0 \text{ for } r > 1; \quad (11b)$$

$$\chi_2(r) = z^4 \pi^2 \left( -\frac{9}{35} \frac{1}{r} + \frac{29}{9} - \frac{101}{30} r + \frac{3}{4} r^2 + \frac{5}{16} r^3 - \frac{2}{15} r^4 + \frac{43}{10080} r^6 \right) \text{ for } 1 \leq r \leq 2, \\ = 0 \text{ for } r < 1 \text{ and for } r > 2; \quad (11c)$$

$$\omega_2(r) = z^3 \pi^2 \left( \frac{27}{70} \frac{1}{r} - \frac{9}{4} + \frac{9}{5} r - \frac{1}{4} r^2 - \frac{1}{6} r^3 + \frac{1}{20} r^4 - \frac{1}{1260} r^6 \right) \text{ for } 1 \leq r \leq 3, \\ = 0 \text{ for } r < 1 \text{ and for } r > 3. \quad (11d)$$

<sup>2</sup> G. H. A. Cole, J. Chem. Phys. **34**, 2016 (1961).

<sup>4</sup> G. H. A. Cole, J. Chem. Phys. **37**, 1631 (1962).

<sup>5</sup> J. G. Kirkwood, J. Chem. Phys. **3**, 300 (1935).

It is not necessary to determine any further coefficients beyond  $a_2^K$  for our present purposes. With the functions  $a_1$  and  $a_2^K$  known, the expansion (3) for  $g$  in powers of  $n$  is known up to the quadratic term under the Kirkwood superposition approximation.

#### 4. THE FUNCTION $X_1$

The function  $X_1$  is to be determined from the expression (7) for the potential function (8). The second, third, and fourth virial coefficients can be determined under the Kirkwood superposition approximation (5b) with our present knowledge of  $a_1$  and  $a_2^K$ , as is clear from paper I and reference 3. Then  $X_1$  can be determined and the modified consistent expression for  $g(r)$  constructed. In this way, the integral (2) defining  $K$  is evaluated.

If a subscript  $v$  denotes the virial coefficients derived from the Eq. (6a) while the subscript  $c$  denotes the coefficients derived from Eq. (6b), then for  $B$  it follows from the well-known expression [see reference 3, Eqs. (8a) and (9b)] that for the potential function (8):

$$B = B_v = B_c = zb, \quad (12)$$

where  $b$  is four times the volume of each molecule. For  $C$  [see reference 3, Eqs. (8b) and (8c)] it follows, using (10) above, that

$$C = C_v = C_c = (5/8)z^3b^2. \quad (13)$$

These two values are exact and there is no need to make reference to the Kirkwood approximation explicitly through a superscript. This is not the case for  $D$  where the theory involving the Kirkwood superposition approximation (5b) leads to two different values. From Eqs. (8a) of paper I and the expressions (11) for  $a_2^K$  it follows that

$$D_v^K = [- (34/35)z^4 + (5361/4480)z^5]b^3, \quad (14a)$$

$$D_c^K = [- (68/105)z^3 + (193/256)z^4 + (6347/26880)z^5]b^3. \quad (14b)$$

The insertion of the expressions (12), (13), (14a), and (14b) into (7) yields for  $X_1(z)$  the following expression

$$\begin{aligned} (1 + (5/32)z)X_1(z) \\ = [- (68/105)z + (15459/8960)z^2 \\ - (25819/26880)z^3]b. \end{aligned} \quad (15)$$

It should be remembered that any distance dependence of  $X_1$  is excluded in the derivation of (7); the temperature does, however, appear through the factor  $z$  defined by (9).

The modified expression for  $a_2$  can now be constructed using the arguments of paper I. Explicitly, from Eqs. (9a) and (13a) of paper I we have now

$$a_2(r) = a_2^K(r) + X_1(z)a_1(r), \quad (16)$$

where  $a_2^K$  is given by Eqs. (11),  $X_1(z)$  by (15), and  $a_1$  by (10).

It is of interest to note that the particular expression (15) for  $X_1$  leads to the formula for the modified consistent fourth virial coefficient  $D^M$

$$(1 + (5/32)z)D^M = [- (289/210)z^4 + (151291/71680)z^5 \\ - (35555/86016)z^6]b^3,$$

which is in very close agreement with the corresponding expression given by Hiroike<sup>6</sup> using entirely different arguments. Unfortunately, Hiroike's arguments do not lead explicitly to an expression for  $a_2(r)$  so that his approach cannot be used as a check on our scattering expressions which are derived later.

One immediate test of the formulas derived so far can be made easily when it is remembered that the substitution  $z=1$  in the formulas above reduces them to the form appropriate to a hard-sphere gas. It is seen from paper I and reference 3 that all our formulas satisfy this requirement.

#### 5. DENSITY EXPANSION FOR $K$

Knowing the expansion (3) of  $g$  in powers of  $n$  [from the expressions (10), (11), (15), and (16)], the integral  $K$ , Eq. (2), is readily expressed as a power series in  $n$ . Thus

$$K = z + I_1(z)n + I_2(z)n^2 + \dots, \quad (17a)$$

where

$$I_1(z) = (z-1) \int_0^1 a_1(r)dr - \int_1^\infty a_1(r)dr, \quad (17b)$$

$$I_2(z) = (z-1) \int_0^1 a_2(r)dr - \int_1^\infty a_2(r)dr, \quad (17c)$$

and so on. Here  $a_2(r)$  is given by (16). These expressions reduce to those appropriate to hard spheres [see paper I, Eqs. (19)] in the limit  $z=1$ .

#### 6. NUMERICAL RESULTS

The theory has now developed to the stage of yielding numerical values. The function  $I_1(z)$  readily follows from (17b) and (10). Thus, it is found that

$$I_1(z) = -3.1416z^2 + 2.6834z^3. \quad (18)$$

When  $z=1$  (hard-sphere gas),  $I_1 = -0.4581$ , which is the value previously found in paper I.

The function  $I_2(z)$  is derived from (16) and (17c). It is convenient to make the calculation by noting that

$$I_2(z) = I_2^K(z) + X_1(z)I_1(z), \quad (19a)$$

where  $I_2^K(z)$  is the value appropriate to the Kirkwood superposition approximation (5b), viz.,

$$I_2^K(z) = (z-1) \int_0^1 a_2^K(r)dr - \int_1^\infty a_2^K(r)dr. \quad (19b)$$

Using expressions (11) it follows that

$$I_2^K(z) = 2.0143z^3 - 5.5969z^4 + 3.9527z^5. \quad (20a)$$

<sup>6</sup> K. Hiroike, J. Phys. Soc. Japan 12, 327 (1957).

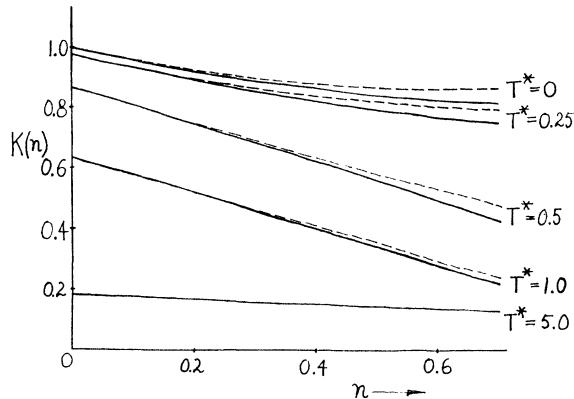


FIG. 1. Plot of the integral  $K(n)$ , defined by Eq. (2) of the text, as a function of the low number density  $n$  for a square-mound potential specified by Eq. (8) of the text. Data for several temperatures are given, the reduced temperature  $T^* = (k/\epsilon)T$ . The solid curves relate to Eq. (21) in conjunction with Eq. (20c) and the modified superposition approximation Eq. (5a). The dashed curves relate to Eq. (21) in conjunction with Eq. (20a) and the Kirkwood superposition approximation Eq. (5b).

When  $z=1$  we have  $I_2^K(z=1) = +0.3702$ , which is the Kirkwood value given previously in paper I. Further, we have

$$(1+0.1563z)X_1I_1 = 4.2611z^3 - 14.9919z^4 + 16.0167z^5 - 5.3983z^6, \quad (20b)$$

which is the correction term appropriate to the superposition approximation (5a). Adding (20a) and (20b) according to (19a) we obtain the final modified consistent value for  $I_2(z)$ ;

$$(1+0.1563z)I_2(z) = 6.2755z^3 - 20.2741z^4 + 19.0949z^5 - 4.7807z^6. \quad (20c)$$

This gives correctly  $I_2(z=1) = +0.2729$ . In the high-temperature limit  $T^* \rightarrow \infty$ , when  $z \rightarrow 0$ , all the functions  $I_1$ ,  $I_2^K$ ,  $X_1$ ,  $I_2$ ,  $B$ ,  $C$ ,  $D_v^K$ ,  $D_c^K$ , and  $D$  vanish,  $K$  itself also vanishing.

Numerical values of the quantities  $I_1$ ,  $I_2^K$ , and  $I_2$  are given in Table I for several values of the temperature. It is convenient for these purposes to introduce a reduced temperature  $T^*$  according to

$$T^* = (k/\epsilon)T.$$

Then  $T^*=0$  follows either from  $T=0$  or  $\epsilon \rightarrow \infty$ . Data for the dependence of  $K$  upon  $n$  for several temperatures, derived by using Table I in connection with Eq. (17a) are plotted in Fig. 1 in the range  $0 \leq n \leq 0.7$ . The full curves are derived using the modified expression for  $I_2(z)$ , i.e., (20c), while the dashed curves are derived from the Kirkwood expression (20a). The magnitude of  $n$  for close packing of spheres is  $\sqrt{2}$ , and  $n=0.7$  would seem to be an upper limit on the range of validity of formulas based on the expansion of relevant functions in powers of  $n$ . The difference between the values of  $K$  based on the Kirkwood approximation (5b) and those based on the modified approximation (5a) is seen from

TABLE I. Containing the temperature dependencies of several functions derived by the accompanying arguments. The reduced temperature  $T^* = (k/\epsilon)T$ .  $z$  of column 2 is derived from Eq. (9);  $I_1$  of column 3 is derived from Eq. (18);  $I_2^K$  of column 4 is obtained from Eq. (20a); the modifying correction  $X_1I_1$  of column 5 comes from Eq. (20b); and the last column contains values of the final modified function  $I_2$  given by Eq. (20c). These several functions are to be used in connection with Eq. (17a) to provide the quantity  $K$ , defined by Eq. (2), in the low gas-density limit when an expansion in powers of the particle number density  $n$  is valid.

$T^*$	$z$	$I_1$	$I_2^K$	$X_1I_1$	$I_2$
0	1	-0.4581	+0.3702	-0.0973	+0.2729
0.25	0.9817	-0.4889	+0.3115	-0.1049	+0.2065
0.50	0.8647	-0.6141	+0.0841	-0.1235	-0.0394
0.75	0.7355	-0.6318	+0.0144	-0.0887	-0.0743
1.00	0.6321	-0.5775	+0.0141	-0.0412	-0.0271
2.00	0.3935	-0.32291	+0.0258	+0.0294	+0.0553
5.00	0.1813	-0.08724	+0.0067	+0.0119	+0.0186
$\infty$	0	0	0	0	0

Fig. 1 to decrease broadly as the temperature increases. In the limit  $T^* = \infty$  ( $z=0$ ) both curves become identically zero. It is seen that  $K$  decreases gradually with increasing  $n$ , and for any  $n$ ,  $K$  is smaller the greater the  $T^*$ . By virtue of Eq. (1) it follows that  $\sigma_{\text{tot}}$  itself, in consequence, increases with the temperature for a given  $n$ , reaching the limit unity as  $T^*$  becomes indefinitely large.

## 7. CONCLUSION

The total elastic-scattering cross section for high-energy neutrons and a low-density gas of heavy nuclei has been calculated using classical arguments in which the heavy nuclei are represented by particles interacting mutually according to the square-mound potential. One important feature of the theory is that the calculations are based on an internal consistency in respect to the thermodynamic (virial) properties of the gas by employing a modified form of the usual Kirkwood form of the superposition approximation.

The results of the calculations yield the total neutron elastic-scattering cross section up to terms involving  $n^3$  of the form

$$\sigma_{\text{tot}} = 1 - (\lambda^2/2\pi)[zn + I_1(z)n^2 + I_2(z)n^3], \quad (21)$$

where  $I_1(z)$  is given by (18) and  $I_2(z)$  is given by (20c). The calculation is based on the superposition approximation (5a), with the additional approximation that  $X_1$  is a function only of  $z$ . Exact information concerning  $X_1$  will doubtless show it to be a function of the three separation distances associated with the placing of three particles in space, but in the present absence of this information the assertion  $X_1 = X_1(z)$  alone is the only reasonable mathematical choice open to us. Problems of the proper normalization of  $g^{(3)}$  under this approximation are avoided by regarding the calculated  $g^{(3)}$  not as a distribution in its own right, but rather as an auxiliary function which is able to lead to significant data for the pair distribution  $g$ . The question immediately arises of the significance of this approximation,

and of the arguments set out above. If  $X_1(r, r_{13}, r_{23}, z)$  were known exactly, then these arguments would be exact. However, no exact values of  $I_2$  appropriate to the square-mound potential are known so that any direct test of the success of our assumption that  $X_1$  is a function of  $z$  alone is not, at present, possible. Indirect evidence in support of our present arguments is, then, valuable and can be sought in two directions.

The first concerns the calculations of paper I for the temperature-independent case of hard spheres where a direct test shows that the value of  $I_2$  calculated on the assumption  $X_1 = \text{const}$  is in error by about 2%. The inherent similarity between the hard-sphere and square-mound-potential functions would make it plausible that  $I_2$  given by (20c) involves an error of a few percent. Because  $I_1$ , given by (18), is exact this would mean that  $K(n)$  computed from Eq. (21) is more accurate than our present calculated  $I_2$  itself.

The second indirect evidence suggesting a reasonable accuracy for our function  $I_2$  comes from the calculated data for the fourth virial coefficient. For hard spheres,

the value of  $D$  calculated under the assumption  $X_1 = \text{const}$  is found to be about  $\frac{1}{2}\%$  too high (see reference 3). For the present square-mound potential it has already been mentioned that the function  $D^M$  resulting from the present approach is virtually the same as the approximate function derived by Hiroike<sup>6</sup> using entirely different arguments. It is possible that both sets of data are quite wrong but, in this case, there is the problem of explaining why they are so remarkably alike.

The present arguments take the calculation of  $K$  only as far as the cube term in  $n$ , although in paper I the quartic term was also determined for hard spheres. The formulas developed above could, after rather tedious although elementary calculation, be extended to include higher powers in  $n$ . However, such an extension would, in this case, be very doubtful in the absence of a direct check on the accuracy of  $I_2$  for the square-mound potential, which is, however, available for hard spheres. The inclusion of further terms must be associated with more information about the lower members of the set of functions  $X_i$ .

## Electroelastic Properties of the Sulfides, Selenides, and Tellurides of Zinc and Cadmium\*

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A complete set of elastic, piezoelectric, and dielectric constants is presented for the sulfides, selenides, and tellurides of zinc and cadmium. The piezoelectric constants for the hexagonal crystals in this group are markedly higher than for the cubic crystals. An elementary model theory applied to these data leads to electric charges on the metal atom increasing from  $+0.066 e$  for ZnTe to  $+0.84 e$  for CdS. The elastic compliance increases regularly with increasing anion and cation weight, with no break between the cubic and hexagonal crystals. Pyroelectric constants are given for CdS and CdSe. The quality factor of elastic resonances of CdS plates is measured as function of electric conductivity.

### I. INTRODUCTION

THE binary compounds crystallizing in the tetrahedrally coordinated cubic sphalerite and hexagonal wurtzite structures are the simplest crystals lacking a center of symmetry and, hence, capable of exhibiting piezoelectric and related effects depending on polar symmetry. Compounds of the bivalent column II B metals, zinc and cadmium, and the bivalent column VI elements, sulfur, selenium, and tellurium, are stable to high temperatures and can be made sufficiently insulating to allow precise measurements of piezoelectric, elastic, and dielectric constants. Such data eventually may serve to verify a quantitative theory of piezoelectricity and elasticity in these structure

types which have been of great interest since the earliest lattice theories of crystal elasticity.<sup>1</sup> Until recently, only cubic zinc sulfide crystals of natural origin were available for such measurements, but interest in semiconducting properties of II-VI compounds has led to growth processes yielding good crystals of most of these compounds. Piezoelectric<sup>2-4</sup>

<sup>1</sup> M. Born, *Atomtheorie des Festen Zustandes* (B. G. Teubner, Leipzig, 1923); also, M. Born and M. Goepfert-Mayer, in *Handbuch der Physik*, edited by S. Flügge (Verlag Julius Springer, Berlin, 1933), pp. 623-794.

<sup>2</sup> H. Jaffe, D. Berlincourt, and L. Shiozawa, Proceedings of the Fourteenth Annual Symposium on Frequency Control, U. S. Army Research and Development Laboratory, Fort Monmouth, New Jersey, 1960 (unpublished), p. 304.

<sup>3</sup> A. R. Hutson, *Phys. Rev. Letters* 4, 505 (1960).

<sup>4</sup> T. Tanaka and S. Tanaka, *J. Phys. Soc. Japan* 15, 726 (1960). The extremely low values found by these authors may be due to electric conductivity since they use a low-frequency method.

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