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Cumulative Function of the Bijvoet Ratio*

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Theoretical expressions for the cumulative function of the Bijvoet ratio is worked out for a non-centrosymmetric crystal containing anomalous scatterers of the same type, as well as a large number of normal scatterers. Three cases corresponding to the number of anomalous scatterers in the unit cell being 1 and many (MN and MC cases) are considered. The theoretical results are used to obtain the percentage of reflexions for which the value of the Bijvoet ratio is greater than the specific values 0·1, 0·2, . . ., 0·6 corresponding to various values of the parameters k and σ_1^2 characterizing the anomalous scatterers.

1. Introduction

The optimum conditions for observing large Bijvoet differences in non-centrosymmetric crystals containing a single species of anomalous scatterer have been discussed by Parthasarathy (1967) (this paper will be hereafter referred to as P, 1967) from a theoretical study of the expectation value of the Bijvoet ratio (which is denoted by the symbol δ and defined as the magnitude of the ratio of the Bijvoet difference to the mean intensity of the Bijvoet pair of reflexions). The results in that paper (P, 1967) cannot however be used to predict, in the case of a given non-centrosymmetric crystal containing a known type of anomalous scatterer, the percentage of reflexions for which the Bijvoet ratio would be larger than a specific value. Before starting data collection with a given crystal, it would be useful to know *a priori* the percentage of reflexions for which the crystal will exhibit a Bijvoet ratio which is larger than any specific value. Since such a prediction can be made only from a study of the cumulative function of the Bijvoet ratio, we shall derive the cumulative function of δ for the one-atom and many-atom cases (namely, $P=1$, MN† and MC, see P, 1967 for the notation). The theoretical results are used to obtain a table showing the percentage of reflexions having a Bijvoet ratio greater than the specific values 0·1, 0·2, . . . 0·6 as a function of k (which is the ratio of the imaginary part to the total real part of the atomic scattering factor of the anomalous scatterer) and σ_1^2 (which is the fractional contribution to the local mean intensity from the anomalous scatterers in the unit cell).

The notation used in this paper is the same as that in the earlier paper (P, 1967). Here we shall not consider the two-atom case, since the cumulative function in this case turns out to be a triple integral which is somewhat tedious to evaluate for various values of δ, k and σ_1^2. Since the distribution function of the normalized Bijvoet difference (Parthasarathy & Srinivasan, 1964) and the expectation value of the Bijvoet ratio (P, 1967) for the two-atom case are close to that of the many-atom (*i.e.* $P=$ MN) case, we may expect a similar trend in the cumulative function of the Bijvoet ratio as well.

2. Derivation of the cumulative function of the Bijvoet ratio δ

Consider a non-centrosymmetric crystal containing P anomalous scatterers (all of the same type) and Q normal scatterers in the unit cell. Let $N(=P+Q)$ be the total number of atoms in the unit cell. From equation (14) of Parthasarathy (1967) we obtain the expression for the Bijvoet ratio as‡

$$\delta=4k|F'_P|\sin\theta/|F'_N|\,. \tag{1}$$

Since δ is defined to be a positive quantity, θ in (1) can be taken to be confined to the range $0\le\theta\le\pi$ where we always have $|\sin\theta|=\sin\theta$. Since it is convenient to use the normalized variables $y_P(=|F'_P|/\langle|F'_P|^2\rangle^{1/2})$ and $y_N(=|F'_N|/\langle|F'_N|^2\rangle^{1/2})$, we can rewrite (1) as

$$\begin{aligned}\delta&=4k\sigma_1 y_P\sin\theta/y_N\,,\\&=4kv\,,\quad\text{say}\,,\end{aligned} \tag{2}$$

where we have defined the variable v to be

$$v=\sigma_1 y_P\sin\theta/y_N\,,\quad 0\le\theta\le\pi\,. \tag{3}$$

It is found to be convenient to first work out the cumulative function of v and then deduce that of δ from it.

It is clear from (3) that the cumulative function of v can be worked out from a knowledge of the joint

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† The many-atom case in which the group of anomalous scatterers form a non-centrosymmetric group will be denoted by *MN* in this paper instead of *MA* in view of the comments of Rogers (1965).

‡ In obtaining (1), $|F''_P|^2$ has been neglected in comparison with $|F'_N|^2$ in the expression for the mean intensity of the Bijvoet pair of reflexions. This approximation is found to be necessary in order to reduce the complexity of the theory. It may also be noted that the range of δ as defined in equation (1) is 0 to ∞ while actually the maximum possible value of Bijvoet ratio is 2 (see Zachariasen, 1965). This change in the range of δ also arises because of the above approximation.

probability density function (abbreviated as pdf) of y_N, y_P and θ by making use of the theory of transformation of variables. The quantity θ in (3) is not a convenient one for this purpose, since $\sin\theta$ is a double-valued function in the range 0 to π. However, since the function $\sin\theta$ is symmetrical about $\theta=\pi/2$, δ has the same value for $\theta=\theta_0$ and $\theta=\pi-\theta_0$, where we define θ_0 to be an acute angle. It is therefore obvious that we can restrict the range of the argument of the sine function to 0 to $\pi/2$, provided we properly take into account the actual probabilities of occurrence for the two events, namely $\theta=\theta_0$ and $\theta=\pi-\theta_0$ for which the values of δ are the same. In this context it is found to be convenient to define a new variable θ_0 as

$$\theta_0=\begin{cases}\theta & \text{if } 0\le\theta\le\pi/2\,,\\ \pi-\theta & \text{if } \pi/2<\theta\le\pi\,.\end{cases} \quad (4)$$

In terms of the variable θ_0, we can rewrite (3) as

$$v=\sigma_1 y_P \sin\theta_0/y_N\,,\quad 0\le\theta_0\le\pi/2\,. \quad (5)$$

Derivation of the cumulative function of v

The conditional joint pdf of y_N and θ for a given y_P can be obtained from equation (6) of Parthasarathy (1967) as

$$P(y_N\theta;,y_P)=(2y_N/\pi\sigma_2^2)\exp\left[-(y_N^2+\sigma_1^2y_P^2-2\sigma_1y_Ny_P\cos\theta)/\sigma_2^2\right]\,. \quad (6)$$

The joint pdf of y_N, y_P and θ will therefore be given by

$$P(y_N,\theta,y_P)=(2y_N/\pi\sigma_2^2)\times\exp\left[-(y_N^2+\sigma_1^2y_P^2-2\sigma_1y_Ny_P\cos\theta)/\sigma_2^2\right]P(y_P)\,, \quad (7)$$

where $P(y_P)$ is the pdf of y_P. We know that

$$P(y_P)=\begin{cases}\delta(y_P-1) & \text{for } P=1\,, & (8a)\\ 2y_P\exp(-y_P^2) & \text{for } P=\text{MN}\,, & (8b)\\ \sqrt{2/\pi}\exp(-y_P^2/2) & \text{for } P=\text{MC}\,. & (8c)\end{cases}$$

The joint pdf of y_N, y_P and θ_0 can be obtained from (4) and (7) as

$$\begin{aligned}P(y_N,y_P,\theta_0)&=P(y_N,y_P,\theta=\theta_0)+P(y_N,y_P,\theta=\pi-\theta_0)\\&=(4y_N/\pi\sigma_2^2)\exp\left[-(y_N^2+\sigma_1^2y_P^2)/\sigma_2^2\right]\\&\quad\times\cosh(2\sigma_1y_Ny_P\cos\theta_0/\sigma_2^2)P(y_P)\,.\end{aligned} \quad (9)$$

From (5) and (9) the joint pdf of v, y_N and θ_0 can be obtained as

$$\begin{aligned}P(v,y_N,\theta_0)&=(4y_N^2/\pi\sigma_1\sigma_2^2\sin\theta_0)\\&\quad\times\exp\left[-(v^2/\sin^2\theta_0+1)y_N^2/\sigma_2^2\right]\\&\quad\times\cosh(2y_N^2v\cot\theta_0/\sigma_2^2)P(vy_N/\sigma_1\sin\theta_0)\,.\end{aligned} \quad (10)$$

The cumulative function of v will therefore be given by

$$N(v)=\int_0^v\int_0^{\pi/2}\int_0^\infty P(v,y_N,\theta_0)\mathrm{d}y_N\mathrm{d}\theta_0\mathrm{d}v\,. \quad (11)$$

Since the quantity v occurring in the integrand of (11) is a dummy variable of integration, it can in fact be replaced by any other symbol, say u. Since the quantity v appearing as the upper limit in the integral in (11) is a fixed quantity as far as the integrations are concerned, the order of integrations in (11) is immaterial.

One-atom case ($P=1$)

Making use of (8*a*) in (10) and the property that $\delta(ax)=\delta(x)/a$ we obtain the joint pdf of v, y_N and θ_0 as

$$\begin{aligned}P(v,y_N,\theta_0)&=\left(\frac{4y_N^2}{\pi\sigma_2^2v}\right)\exp\left[-(1+v^2/\sin^2\theta_0)y_N^2/\sigma_2^2\right]\\&\quad\times\cosh\left(\frac{2y_N^2v\cot\theta_0}{\sigma_2^2}\right)\delta\left(y_N-\frac{\sigma_1\sin\theta_0}{v}\right).\end{aligned} \quad (12)$$

Substituting (12) in (11) and carrying out the integrations, we obtain the cumulative function of v as (see Appendix *A*)

$$N(v)=\frac{1}{\pi}\int_0^{\pi/2}\exp(-\sigma_1^2\sin^2\theta_0/\sigma_2^2)[\exp(-f_+^2)+\exp(-f_-^2)+\frac{\sqrt{\pi}\sigma_1\cos\theta_0}{\sigma_2}\{\text{erf}(f_+)-\text{erf}(f_-)\}]\mathrm{d}\theta_0\,, \quad (13)$$

where we have used the simplifying notation that

$$f_\pm=\frac{\sigma_1}{\sigma_2}\left(\frac{\sin\theta_0}{v}\pm\cos\theta_0\right). \quad (14)$$

The integral in (13) is to be evaluated by a numerical method.

Many-atom case ($P=$MN)

From (8*b*) and (10) we obtain the joint pdf of v, y_N and θ_0 as

$$P(v,y_N,\theta_0)=\frac{8}{\pi}\frac{vy_N^3\,\text{cosec}^2\,\theta_0}{\sigma_1^2\sigma_2^2}\times\exp\left[-\frac{y_N^2}{\sigma_2^2}\left(1+\frac{v^2}{\sigma_1^2\sin^2\theta_0}\right)\right]\cosh(2vy_N^2\cot\theta_0/\sigma_2^2)\,. \quad (15)$$

Making use of (15) in (11) the cumulative function of v can be shown to be (see Appendix *B*)

$$N(v)=v/(v^2+\sigma_1^2\sigma_2^2)^{1/2}. \quad (16)$$

Many-atom case ($P=$MC)

Making use of (8*c*) in (10) we obtain the joint pdf of v, y_N and θ_0 as

$$P(v,y_N,\theta_0)=\frac{4\sqrt{2}}{\pi^{3/2}\sigma_1\sigma_2^2}\frac{y_N^2}{\sin\theta_0}\times\exp\left[-\frac{y_N^2}{\sigma_2^2}\left(1+\frac{gv^2}{\sin^2\theta_0}\right)\right]\cosh(2y_N^2v\cot\theta_0/\sigma_2^2)\,, \quad (17)$$

where we have used the simplifying notation that

$$g=(1+\sigma_1^2)/2\sigma_1^2\,. \quad (18)$$

Substituting (17) in (11) and carrying out the integrations we can obtain the cumulative function of v as (see Appendix C).

$$N(v)=\frac{\sigma_2}{\pi\sqrt{2}\sigma_1}\int_0^{\pi/2}[F_+(\theta_0)+F_-(\theta_0)]\mathrm{d}\theta_0\,, \qquad (19)$$

where we have used the simplifying notation that

$$F_\pm(\theta_0)=\frac{gv\pm\cos\theta_0\sin\theta_0}{(g-\cos^2\theta_0)[\sin^2\theta_0\pm 2v\cos\theta_0\sin\theta_0+gv^2]^{1/2}}\,. \qquad (20)$$

The integral in (19) is to be evaluated by a numerical method.

3. Discussion of the theoretical results

It is possible to make use of (9) to obtain the pdf of the normalized Bijvoet difference x (Parthasarathy & Srinivasan, 1964) and the expectation value of the Bijvoet ratio δ (P, 1967). Since this method is only an alternate procedure for arriving at the earlier results, the details are not given here.

From (2) it is clear that (k being a constant for a given crystal)

$$P(\delta\le\delta_0)=P(v\le\delta_0/4k)\,. \qquad (21)$$

If we denote the cumulative functions of δ and v by $N_\delta(\delta)$ and $N_v(v)$ respectively, we can rewrite (21) as

$$N_\delta(\delta_0)=N_v(\delta_0/4k)\,. \qquad (22)$$

Thus, by evaluating the cumulative function of v at $v=\delta_0/4k$ we can obtain the value of the cumulative function of δ at $\delta=\delta_0$.The function $N_\delta(\delta_0)$ has been evaluated in this way for various values of the parameters k and σ_1^2 by making use of the expressions for $N_v(v_0)$ as obtained in (13), (16) and (19). From this, the percentage of reflexions for which the Bijvoet ratio is larger than any given value, say δ_0 can be obtained as

$$P(\delta\ge\delta_0)=1-N_\delta(\delta_0)\,. \qquad (23)$$

The values of $P(\delta\ge\delta_0)$ for $\delta_0=0{\cdot}1, 0{\cdot}2, \ldots 0{\cdot}6$ have been obtained for various values of the parameters $k(=0{\cdot}04, 0{\cdot}06, \ldots, 0{\cdot}3)$ and $\sigma_1^2(=0{\cdot}1, 0{\cdot}2, \ldots, 0{\cdot}9)$ and the results are given in Table 1. It is seen from (16) that the function $N_v(v_0)$ for the many-atom ($P=$ MN) case is symmetrical about $\sigma_1^2=0{\cdot}5$ and hence in this particular case it would be sufficient to tabulate the values of $P(\delta\ge\delta_0)$ in the range $\sigma_1^2\le 0{\cdot}5$. For example, the function $N_v(v_0)$ for the $P=$ MN case has the same value for $\sigma_1^2=0{\cdot}4$ and 0·6. It may be noted here that in order to make use of this Table in the case of an actual crystal, it is necessary to employ values of k and σ_1^2 which are averaged over the whole range of $\sin\theta/\lambda$ (for which data is being collected), since the quantities k and σ_1^2 in general vary with ($\sin\theta/\lambda$).

From a study of Table 1 we arrive at the same conclusions as in the earlier paper (P, 1967), namely, (i) that large Bijvoet ratios would be observed when the value of σ_1^2 is close to 0·5, (ii) that the cumulative function of δ is more sensitive to the variation in k than in σ_1^2 and (iii) that the optimum conditions for observing large Bijvoet differences are $\sigma_1^2\simeq 0{\cdot}5$ and k large.

The theoretical results have been tested by making use of the calculated Bijvoet ratios for a few crystal structures and the details of these structures are given in Table 2. One of these structures (*i.e.* 4) corresponds to the two-atom case (*i.e.* $P=2$) and the others (*i.e.* 1, 2 and 3) correspond to the four-atom case ($P=4$). Though the exact theoretical expressions for the cumulative function for the two-atom and four-atom cases

Table 1. *Cumulative function of the Bijvoet ratio as a function of k and σ_1^2*

ONE ATOM CASE (P = 1)

DELTA = 0.10

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.08	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.10	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.12	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.14	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.16	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.18	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.20	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.22	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.24	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.26	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	67.0
0.28	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	69.2
0.30	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	71.1

DELTA = 0.20

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.2
0.06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.1
0.08	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	3.1
0.10	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	6.3
0.12	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	10.5
0.14	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	15.1
0.16	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	19.9
0.18	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	24.6
0.20	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	29.0
0.22	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	33.2
0.24	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	37.0
0.26	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	40.6
0.28	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	43.8
0.30	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	46.7

DELTA = 0.30

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.1
0.06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.2
0.08	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.7
0.10	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.6
0.12	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	3.1
0.14	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	5.1
0.16	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	7.6
0.18	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	10.5
0.20	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	13.5
0.22	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.24	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	19.9
0.26	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	23.0
0.28	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	26.1
0.30	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	29.0

DELTA = 0.40

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.0
0.06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.1
0.08	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.2
0.10	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.5
0.12	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.1
0.14	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.9
0.16	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	3.1
0.18	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	4.6
0.20	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	6.3
0.22	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	8.3
0.24	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	10.5
0.26	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	12.8
0.28	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	15.1
0.30	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	17.5

DELTA = 0.50

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.0
0.06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.0
0.08	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.1
0.10	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.2
0.12	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.5
0.14	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.8
0.16	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	1.4
0.18	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	2.2
0.20	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	3.1
0.22	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	4.3
0.24	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	5.6
0.26	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	7.1
0.28	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	8.7
0.30	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	10.5

DELTA = 0.60

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.0
0.06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.0
0.08	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.1
0.10	2.2	4.2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.1
0.12	3.1	5.9	8.2	9.7	10.1	9.1	6.5	2.8	0.2
0.14	4.2	7.9	10.8	12.7	13.1	11.8	8.5	4.0	0.4
0.16	5.4	10.1	13.7	15.9	16.2	14.5	10.7	5.4	0.7
0.18	6.8	12.4	16.7	19.1	19.4	17.3	13.0	6.9	1.1
0.20	8.2	14.9	19.8	22.4	22.5	20.1	15.4	8.6	1.6
0.22	9.8	17.6	22.9	25.6	25.6	22.9	17.8	10.5	2.3
0.24	11.5	20.3	26.0	28.7	28.5	25.6	20.3	12.4	3.1
0.26	13.5	23.0	29.1	31.7	31.3	28.2	22.7	14.5	4.1
0.28	15.1	25.7	32.1	34.6	34.0	30.7	25.1	16.5	5.1
0.30	17.0	28.5	34.9	37.3	36.5	33.2	27.4	18.8	6.3

MANY ATOM CASE(P = NC)

DELTA = 0.10

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.06	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.08	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.10	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.12	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.14	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.16	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.18	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.20	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.22	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.24	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
0.26	59.1	66.9	70.6	72.8	74.1	74.7	74.5	73.1	68.3
0.28	61.1	68.6	72.2	74.3	75.6	76.2	76.1	74.8	70.3
0.30	62.9	70.1	73.6	75.7	76.9	77.5	77.5	76.3	72.0

DELTA = 0.20

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	2.5	4.0	4.9	5.4	5.6	5.5	5.1	4.4	3.2
0.06	5.3	8.7	10.0	10.9	11.2	11.1	10.4	9.0	6.8
0.08	8.7	13.1	15.6	17.0	17.5	17.3	16.3	14.4	11.0
0.10	12.4	18.1	21.3	23.0	23.7	23.5	22.4	20.0	15.5
0.12	16.2	23.0	26.6	28.7	29.5	29.4	28.2	25.5	20.1
0.14	20.0	27.5	31.5	33.8	34.8	34.7	33.5	30.6	24.5
0.16	23.5	31.7	35.9	38.3	39.4	39.5	38.3	35.3	28.7
0.18	26.9	35.5	39.9	42.4	43.6	43.7	42.6	39.6	32.7
0.20	30.1	38.9	43.4	45.9	47.2	47.4	46.4	43.4	36.4
0.22	33.1	42.0	46.6	49.1	50.4	50.7	49.7	46.9	39.8
0.24	35.8	44.8	49.4	52.0	53.3	53.6	52.7	50.0	42.9
0.26	38.3	47.4	51.9	54.5	55.9	56.2	55.4	52.8	45.8
0.28	40.7	49.7	54.2	56.8	58.2	58.6	57.9	55.3	48.5
0.30	42.9	51.9	56.3	58.8	60.2	60.7	60.0	57.6	50.9

DELTA = 0.30

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	1.1	1.9	2.3	2.5	2.6	2.6	2.4	2.0	1.5
0.06	2.5	4.0	4.9	5.4	5.6	5.5	5.1	4.4	3.2
0.08	4.3	6.7	8.2	9.0	9.2	9.1	8.5	7.4	5.5
0.10	6.4	9.8	11.8	12.9	13.3	13.1	12.3	10.8	8.1
0.12	8.7	13.1	15.6	17.0	17.5	17.3	16.3	14.4	11.0
0.14	11.1	16.5	19.4	21.0	21.7	21.5	20.4	18.2	14.0
0.16	13.7	19.8	23.1	25.0	25.7	25.6	24.4	21.9	17.0
0.18	16.2	23.0	26.6	28.7	29.5	29.4	28.2	25.5	20.1
0.20	18.7	26.0	30.0	32.1	33.1	33.0	31.8	28.9	23.1
0.22	21.2	29.0	33.1	35.3	36.4	36.4	35.2	32.2	25.9
0.24	23.5	31.7	35.9	38.3	39.4	39.5	38.3	35.3	28.7
0.26	25.8	34.3	38.6	41.1	42.2	42.3	41.2	38.2	31.4
0.28	28.0	36.7	41.1	43.6	44.8	45.0	43.9	40.9	34.0
0.30	30.1	38.9	43.4	45.9	47.2	47.4	46.4	43.4	36.4

DELTA = 0.40

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	0.8	1.1	1.3	1.5	1.5	1.5	1.4	1.2	0.9
0.06	1.4	2.3	2.9	3.2	3.3	3.2	3.0	2.5	1.8
0.08	2.5	4.0	4.9	5.4	5.6	5.5	5.1	4.4	3.2
0.10	3.8	6.0	7.3	8.0	8.3	8.1	7.6	6.6	4.9
0.12	5.3	8.7	10.0	10.9	11.2	11.1	10.4	9.0	6.8
0.14	6.9	10.6	12.8	13.9	14.4	14.1	13.3	11.7	8.8
0.16	8.7	13.1	15.6	17.0	17.5	17.3	16.3	14.4	11.0
0.18	10.5	15.6	18.5	20.0	20.7	20.5	19.4	17.2	13.2
0.20	12.4	18.1	21.3	23.0	23.7	23.5	22.4	20.0	15.5
0.22	14.3	20.6	24.0	25.9	26.7	26.5	25.4	22.8	17.8
0.24	16.2	23.0	26.6	28.7	29.5	29.4	28.2	25.5	20.1
0.26	18.1	25.3	29.2	31.3	32.2	32.1	30.9	28.1	22.3
0.28	20.0	27.5	31.5	33.8	34.8	34.7	33.5	30.6	24.5
0.30	21.8	29.7	33.8	36.1	37.2	37.2	36.0	33.0	26.7

DELTA = 0.50

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	0.4	0.7	0.9	0.9	1.0	0.9	0.9	0.7	0.6
0.06	0.9	1.5	1.9	2.1	2.1	2.1	1.9	1.7	1.2
0.08	1.6	2.6	3.3	3.6	3.7	3.6	3.3	2.9	2.1
0.10	2.5	4.0	4.9	5.4	5.6	5.5	5.1	4.4	3.2
0.12	3.5	5.6	6.8	7.5	7.7	7.6	7.0	6.1	4.6
0.14	4.7	7.3	8.9	9.7	10.0	9.9	9.2	8.0	6.0
0.16	5.9	9.2	11.1	12.1	12.5	12.3	11.5	10.1	7.6
0.18	7.3	11.1	13.3	14.5	15.0	14.8	13.9	12.2	9.3
0.20	8.7	13.1	15.6	17.0	17.5	17.3	16.3	14.4	11.0
0.22	10.1	15.1	17.9	19.4	20.0	19.8	18.8	16.7	12.8
0.24	11.6	17.1	20.1	21.8	22.5	22.3	21.2	18.9	14.6
0.26	13.2	19.1	22.4	24.1	24.9	24.8	23.6	21.2	16.4
0.28	14.7	21.1	24.6	26.5	27.3	27.1	25.9	23.3	18.3
0.30	16.2	23.0	26.6	28.7	29.5	29.4	28.2	25.5	20.1

DELTA = 0.60

k \ σ_1^2	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.04	0.3	0.5	0.6	0.7	0.7	0.7	0.6	0.5	0.4
0.06	0.6	1.1	1.3	1.5	1.5	1.5	1.4	1.2	0.9
0.08	1.1	1.9	2.3	2.5	2.6	2.6	2.4	2.0	1.5
0.10	1.8	2.9	3.5	3.9	4.0	3.9	3.6	3.1	2.3
0.12	2.5	4.0	4.9	5.4	5.6	5.5	5.1	4.4	3.2
0.14	3.3	5.3	6.5	7.1	7.3	7.2	6.7	5.8	4.3
0.16	4.3	6.7	8.2	9.0	9.2	9.1	8.5	7.4	5.5
0.18	5.3	8.2	10.0	10.9	11.2	11.1	10.4	9.0	6.8
0.20	6.4	9.8	11.8	12.9	13.3	13.1	12.3	10.8	8.1
0.22	7.5	11.5	13.7	14.9	15.4	15.2	14.3	12.6	9.5
0.24	8.7	13.1	15.6	17.0	17.5	17.3	16.3	14.4	11.0
0.26	9.9	14.8	17.5	19.0	19.6	19.4	18.4	16.3	12.5
0.28	11.1	16.5	19.4	21.0	21.7	21.5	20.4	18.2	14.0
0.30	12.4	18.1	21.3	23.0	23.7	23.5	22.4	20.0	15.5

MANY-ATOM CASE (P = MN)

DELTA = 0.10

k \ σ_1^2	0.1 / 0.9	0.2 / 0.8	0.3 / 0.7	0.4 / 0.6	0.5
0.04	9.8	15.8	19.4	21.3	21.9
0.06	18.8	27.9	32.7	35.2	36.0
0.08	27.9	38.4	43.7	46.2	47.0
0.10	36.0	47.0	52.1	54.5	55.3
0.12	43.0	53.8	58.6	60.9	61.5
0.14	48.9	59.2	63.7	65.8	66.4
0.16	53.8	63.6	67.7	69.6	70.2
0.18	58.0	67.2	71.0	72.7	73.2
0.20	61.5	70.2	73.7	75.3	75.7
0.22	64.6	72.7	75.9	77.4	77.8
0.24	67.2	74.8	77.8	79.2	79.6
0.26	69.5	76.6	79.5	80.7	81.1
0.28	71.5	78.2	80.9	82.1	82.4
0.30	73.2	79.5	82.1	83.2	83.6

DELTA = 0.30

k \ σ_1^2	0.1 / 0.9	0.2 / 0.8	0.3 / 0.7	0.4 / 0.6	0.5
0.04	1.3	2.2	2.9	3.2	3.4
0.06	2.8	4.8	6.1	6.9	7.2
0.08	4.8	8.0	10.2	11.4	11.8
0.10	7.2	11.8	14.7	16.3	16.8
0.12	9.8	15.8	19.4	21.3	21.9
0.14	12.7	19.9	24.0	26.2	26.9
0.16	15.8	23.9	28.5	30.9	31.6
0.18	18.8	27.9	32.7	35.2	36.0
0.20	21.9	31.6	36.7	39.2	40.0
0.22	24.9	35.1	40.3	42.9	43.7
0.24	27.9	38.4	43.7	46.2	47.0
0.26	30.7	41.5	46.7	49.3	50.0
0.28	33.4	44.4	49.5	52.0	52.8
0.30	36.0	47.0	52.1	54.5	55.3

DELTA = 0.50

k \ σ_1^2	0.1 / 0.9	0.2 / 0.8	0.3 / 0.7	0.4 / 0.6	0.5
0.04	0.5	0.8	1.1	1.2	1.3
0.06	1.0	1.8	2.3	2.7	2.8
0.08	1.8	3.1	4.0	4.4	4.8
0.10	2.8	4.8	6.1	6.9	7.2
0.12	3.9	6.6	8.5	9.5	9.8
0.14	5.2	8.7	11.0	12.3	12.7
0.16	6.6	11.0	13.7	15.3	15.8
0.18	8.2	13.3	16.5	18.3	18.8
0.20	9.8	15.8	19.4	21.3	21.9
0.22	11.6	18.2	22.2	24.3	24.9
0.24	13.3	20.7	24.9	27.2	27.9
0.26	15.2	23.1	27.6	30.0	30.7
0.28	17.0	25.5	30.2	32.6	33.4
0.30	18.8	27.9	32.7	35.2	36.0

DELTA = 0.20

k \ σ_1^2	0.1 / 0.9	0.2 / 0.8	0.3 / 0.7	0.4 / 0.6	0.5
0.04	2.8	4.8	6.1	6.9	7.2
0.06	5.9	9.8	12.4	13.8	14.3
0.08	9.8	15.8	19.4	21.3	21.9
0.10	14.3	21.9	26.3	28.6	29.3
0.12	18.8	27.9	32.7	35.2	36.0
0.14	23.4	33.4	38.5	41.1	41.9
0.16	27.9	38.4	43.7	46.2	47.0
0.18	32.1	43.0	48.2	50.7	51.4
0.20	36.0	47.0	52.1	54.5	55.3
0.22	39.6	50.6	55.6	57.9	58.6
0.24	43.0	53.8	58.6	60.9	61.5
0.26	46.0	56.7	61.3	63.5	64.1
0.28	48.9	59.2	63.7	65.8	66.4
0.30	51.4	61.5	65.8	67.8	68.4

DELTA = 0.40

k \ σ_1^2	0.1 / 0.9	0.2 / 0.8	0.3 / 0.7	0.4 / 0.6	0.5
0.04	0.7	1.3	1.6	1.9	1.9
0.06	1.6	2.8	3.6	4.1	4.2
0.08	2.8	4.8	6.1	6.9	7.2
0.10	4.2	7.2	9.1	10.2	10.6
0.12	5.9	9.8	12.4	13.8	14.3
0.14	7.8	12.7	15.8	17.5	18.1
0.16	9.8	15.8	19.4	21.3	21.9
0.18	12.0	18.8	22.9	25.0	25.7
0.20	14.3	21.9	26.3	28.6	29.3
0.22	16.5	24.9	29.6	32.0	32.7
0.24	18.8	27.9	32.7	35.2	36.0
0.26	21.1	30.7	35.7	38.2	39.0
0.28	23.4	33.4	38.5	41.1	41.9
0.30	25.7	36.0	41.2	43.7	44.5

DELTA = 0.60

k \ σ_1^2	0.1 / 0.9	0.2 / 0.8	0.3 / 0.7	0.4 / 0.6	0.5
0.04	0.3	0.6	0.7	0.8	0.9
0.06	0.7	1.3	1.6	1.9	1.9
0.08	1.3	2.2	2.9	3.2	3.4
0.10	1.9	3.4	4.4	4.9	5.1
0.12	2.8	4.8	6.1	6.9	7.2
0.14	3.7	6.3	8.1	9.1	9.4
0.16	4.8	8.0	10.2	11.4	11.8
0.18	5.9	9.8	12.4	13.8	14.3
0.20	7.2	11.8	14.7	16.3	16.8
0.22	8.5	13.7	17.0	18.8	19.4
0.24	9.8	15.8	19.4	21.3	21.9
0.26	11.3	17.8	21.7	23.8	24.4
0.28	12.7	19.9	24.0	26.2	26.9
0.30	14.3	21.9	26.3	28.6	29.3

have not been obtained yet, it is expected that the cumulative function of δ for these cases would follow closely that of the many-atom (P=MN) case. The theoretical curves for these structures have therefore been obtained by making use of the results for the P=MN case and are shown by the solid line in Fig. 1. The experimental distributions for the various cases are shown by crosses (×). The origins for the curves of the structures (2), (3) and (4) have been shifted along the y axis to 0·3, 0·6 and 0·9 respectively in order to show all four distribution curves in the same figure. It is seen from Fig. 1 that the agreement between theory and experiment is fairly good showing that even when the number of anomalous scatterers in the unit cell is not large in the strict sense, we can make use of the results of the many atom (P=MN) case for the cases P=2 and 4 to obtain useful results.

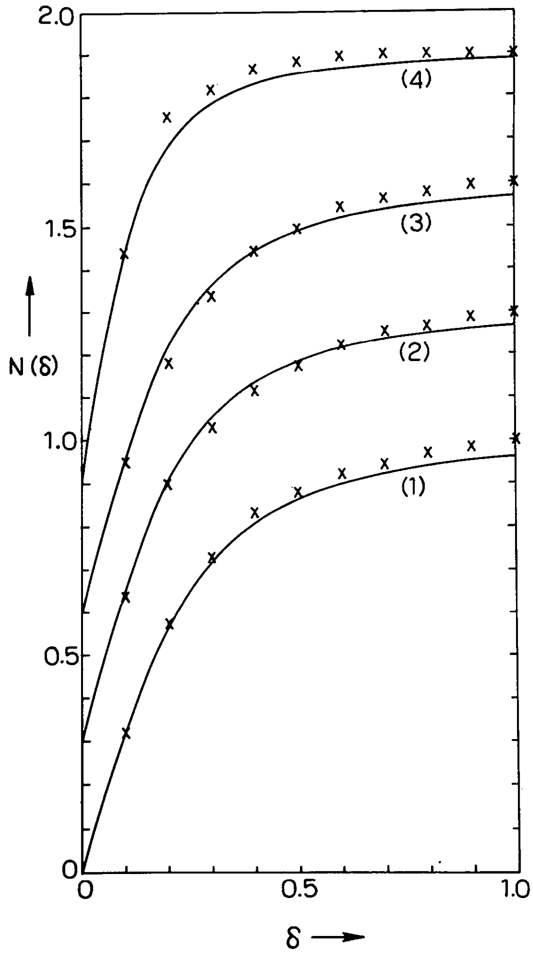

Fig. 1. Verification of the theoretical cumulative function of δ in the case of the structures in Table 2. The number near each curve corresponds to the number in the first column of Table 2.

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APPENDIX *A*

Integrating (12) with respect to y_N we obtain the joint pdf of v and θ_0 as

$$P(v,\theta_0)=\frac{4\sigma_1^2\sin^2\theta_0}{\pi\sigma_2^2v^3}\exp\left[-\frac{\sigma_1^2}{\sigma_2^2}\left(1+\frac{\sin^2\theta_0}{v^2}\right)\right]\times\cosh\left(\frac{2\sigma_1^2\sin\theta_0\cos\theta_0}{\sigma_2^2 v}\right). \quad (A1)$$

The probability that $v\le v_0$ will therefore be given by

$$N(v_0)=\int_0^{v_0}\int_0^{\pi/2}P(v,\theta_0)\mathrm{d}v\mathrm{d}\theta_0\,. \quad (A2)$$

Making use of (A1) in (A2) and then substituting $u=1/v$ we obtain

$$N(v_0)=\frac{4\sigma_1^2}{\pi\sigma_2^2}\int_0^{\pi/2}\sin^2\theta_0\int_{1/v_0}^{\infty}\exp\left[-\frac{\sigma_1^2}{\sigma_2^2}(1+u^2\sin^2\theta_0)\right]\times\cosh\left(\frac{2\sigma_1^2u\cos\theta_0\sin\theta_0}{\sigma_2^2}\right)u\mathrm{d}u\,. \quad (A3)$$

It is easy to show that

$$\int_c^{\infty}\exp(-ax^2)\cosh(bx)x\mathrm{d}x$$

$$=\frac{1}{4a}\left[2\exp(-ac^2)\cosh(bc)+\frac{\sqrt{\pi}}{2}\frac{b}{\sqrt{a}}\exp(b^2/4a)\times\{\mathrm{erf}(\sqrt{a}c+b/2\sqrt{a})-\mathrm{erf}(\sqrt{a}c-b/2\sqrt{a})\}\right]. \quad (A4)$$

Table 2. *Details of the crystal structures used for verifying the theoretical results*

Number	Crystal	Reference	Space group	Number of P atoms in the unit cell	$\langle\sigma_1^2\rangle$	$\langle k\rangle$
1.	Methyl melaleucate iodoacetate	Hall & Maslen (1965)	$P2_12_12_1$	4	0·79	0·18
2.	Davallol iodoacetate	Yow-Lam Oh & Maslen (1966)	$P2_12_12_1$	4	0·84	0·18
3.	Beyerol monoethylidene iodoacetate	O'Connell & Maslen (1966)	$P2_12_12_1$	4	0·85	0·18
4.	L-α-γ-Diaminobutyric acid hydrochloride	Naganathan & Venkatesan (1971)	$P2_1$	2	0·55	0·08

Making use of ($A4$) we can simplify ($A3$) to obtain

$$N(v_0)=\frac{1}{\pi}\int_0^{\pi/2}\exp\left(-\sigma_1^2\sin^2\theta_0/\sigma_2^2\right)\times\left[\exp\left(-f_+^2\right)+\exp\left(-f_-^2\right)+\frac{\sqrt{\pi}\sigma_1\cos\theta_0}{\sigma_2}\left\{\operatorname{erf}(f_+)-\operatorname{erf}(f_-)\right\}\right]d\theta_0\,,\quad (A5)$$

where we have used the simplifying notation of (14) and the result that

$$\cosh(x)=[\exp(x)+\exp(-x)]/2\,.$$

APPENDIX *B*

Integrating (15) with respect to θ_0, we obtain the joint pdf of v and y_N as

$$P(v,y_N)=\frac{4}{\sqrt{\pi}}\frac{y_N^2}{\sigma_1\sigma_2}\exp\left[-y_N^2(v^2+\sigma_1^2\sigma_2^2)/\sigma_1^2\sigma_2^2\right],\quad (B1)$$

where we have made use of the substitution $\cot\theta_0=\sqrt{t}$ and then the equation (39) on p. 166 of Erdelyi (1954). Carrying out the integration over y_N by making use of equation (15) on p. 313 of Erdelyi (1954) we obtain the pdf of v to be

$$P(v)=\sigma_1^2\sigma_2^2/(v^2+\sigma_1^2\sigma_2^2)^{3/2}.\quad (B2)$$

The probability that $v\le v_0$ will therefore be given by

$$N(v_0)=\int_0^{v_0}\frac{\sigma_1^2\sigma_2^2dv}{(v^2+\sigma_1^2\sigma_2^2)^{3/2}}=v_0/(v_0^2+\sigma_1^2\sigma_2^2)^{1/2}.\quad (B3)$$

APPENDIX *C*

Integrating (17) with respect to y_N by making use of the substitution $t=y_N^2$ and the equation (19) on p. 164 of Erdelyi (1954) we obtain the joint pdf of v and θ_0 as

$$P(v,\theta_0)=\frac{\sigma_2\sin^2\theta_0}{\pi\sqrt{2}\sigma_1}\left[\frac{1}{(\sin^2\theta_0+2v\sin\theta_0\cos\theta_0+gv^2)^{3/2}}+\frac{1}{(\sin^2\theta_0-2v\sin\theta_0\cos\theta_0+gv^2)^{3/2}}\right].\quad (C1)$$

The probability that $v\le v_0$ will therefore be given by

$$N(v_0)=\int_0^{v_0}\int_0^{\pi/2}P(v,\theta_0)dvd\theta_0\,.\quad (C2)$$

Carrying out the integration over v first by making use of equation (167) on p. 26 of Peirce & Foster (1966) we obtain

$$N(v_0)=\frac{\sigma_2}{\pi\sqrt{2}\sigma_1}\int_0^{\pi/2}[F_+(\theta_0)+F_-(\theta_0)]d\theta_0\,,\quad (C3)$$

where we have used the simplifying notation of (20).

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