cubic point groups 23 and $m\bar{3}$. An example of such insensitivity is illustrated in Fig. 4 by the statistics for the trigonal $P312$.

It should also be pointed out that within some non-symmorphic space groups the exact p.d.f.'s may differ widely, depending on the parity of the reflection indices. The statistics for two out of the four different reflection subsets for the space group $P6_1$ are displayed in Fig. 5.

A remark about the statistics of the cubic space groups nos. 207-230, including the various subsets, is in order. Exact p.d.f.'s were not formulated in a final form for these space groups since the expressions appeared rather unwieldy and indicated excessive computing effort that might be called for in their evaluation. Moreover, comparisons of histograms of $|E|$ for a $C_{14}U$ asymmetric unit with the appropriate ideal p.d.f.'s showed that they (the histograms) are either insensitive to atomic heterogeneity or display a weak tendency to hypersymmetry. It might perhaps be interesting to examine the feasibility of constructing, in such instances, reliable approximate p.d.f.'s by the Gram-Charlier correction-factor approach (*e.g.* Shmueli & Wilson, 1981; Shmueli, 1982) since the departures from ideal behaviour are here rather small.

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On Integrating the Techniques of Direct Methods with Anomalous Dispersion. II. Statistical Properties of the Two-Phase Structure Invariants

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Abstract

Results of a statistical study of probabilistic estimates of two-phase structure invariants (TPSI) for Friedel pairs in the case of single-wavelength anomalous scattering are reported. Numerical analysis of the TPSI sign, magnitude and error distributions shows that the concise formula for TPSI by probability theory [Hauptman (1982). *Acta Cryst.* **A38**, 632-641; Giacovazzo (1983). *Acta Cryst.* **A39**, 585-592] has desirable statistical properties. Computational results for the known structures of cocaine methiodide (*N*-methylcocaine iodide) and of cytochrome c_{550} and its $PtCl_4^{2-}$ derivative show that when $|E|$ values are large most of the signs of the TPSI are correctly determined - for $|E| > 1{\cdot}0$, 90% or more of the TPSI signs

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are positive as predicted - and the errors in the estimated TPSI magnitudes do not exceed ~10% for $|E| > 1{\cdot}0$ in the small-molecule case or ~50% for $|E| > 1{\cdot}5$ in the macromolecular case. These results suggest that the theory will be useful for estimating the TPSI for unknown structures.

1. Introduction

It is well known that the presence of anomalous scatterers in a macromolecular crystal structure facilitates structure determination. In part I of the present series of papers, Hauptman (1982) integrated anomalous-dispersion effects into the neighborhood concept and obtained a formula for probabilistic estimates of the Friedel-pair two-phase structure invariants (TPSI). Giacovazzo (1983) and Cascarano & Giacovazzo (1984) later obtained a similar result and suggested its practical application. The theory has not yet, however, been used in numerical computations to assess the accuracy of its estimates for the TPSI sign, magnitude and error distributions.

The TPSI relationship is shown geometrically in Fig. 1, where the phase angle of the TPSI is ψ_2, which is determined by the two normalized structure factors $E_{\mathbf{H}}$ and $E_{-\mathbf{H}}$. It is not necessary to distinguish formally the heavy-atom substructure, presumed to be known, from the light-atom substructure, presumed to be unknown. We therefore consider all atoms to be anomalous scatterers and employ the concise formulae developed by Hauptman (1982).

The probabilistic estimate of the TPSI for one crystal with anomalous scatterers at one wavelength as obtained by Hauptman (1982) is

$$\psi_2 = \varphi_{\mathbf{H}} + \varphi_{-\mathbf{H}} \approx -\xi. \tag{1.1}$$

The quantity ξ is calculated by means of

$$\tan \xi = -S_{\mathbf{H}}/C_{\mathbf{H}}. \tag{1.2}$$

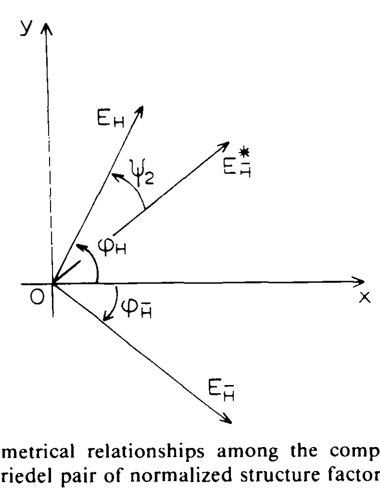

Fig. 1. Geometrical relationships among the components of a Friedel pair of normalized structure factors.

$$C_{\mathbf{H}} = (1/\alpha_{\mathbf{H}}) \sum_{j=1}^{N} |f_{j\mathbf{H}}|^2 \cos 2\delta_{j\mathbf{H}}, \tag{1.3}$$

$$S_{\mathbf{H}} = (1/\alpha_{\mathbf{H}}) \sum_{j=1}^{N} |f_{j\mathbf{H}}|^2 \sin 2\delta_{j\mathbf{H}}, \tag{1.4}$$

$$\alpha_{\mathbf{H}} = \sum_{j=1}^{N} |f_{j\mathbf{H}}|^2, \tag{1.5}$$

where N is the number of atoms in the unit cell and the atomic scattering factor,

$$f_{j\mathbf{H}} = f^0_{j\mathbf{H}} + f'_j + if''_j,$$

is expressed as

$$f_{j\mathbf{H}} = |f_{j\mathbf{H}}| \exp(i\delta_{j\mathbf{H}}) \tag{1.6}$$

with

$$|f_{j\mathbf{H}}| = [(f^0_{j\mathbf{H}} + f'_j)^2 + (f''_j)^2]^{1/2}$$

and

$$\delta_{j\mathbf{H}} = \tan^{-1}[f''_j/(f^0_{j\mathbf{H}} + f'_j)].$$

The TPSI estimate (1.1) is good provided that the variance of the distribution [see (4.1) below] is small.

In paper I, Hauptman (1982) pointed out that for a given chemical composition ξ depends only on $|\mathbf{H}|$ [or $(\sin\theta)/\lambda$] and is independent of the magnitudes $|E_{\mathbf{H}}|$ and $|E_{-\mathbf{H}}|$ of the Friedel pair. This implies that the TPSI ψ_2 depends much more strongly on the chemical composition of the crystal than on its structure. Fortier, Fraser & Moore (1986) noted 'This result is unexpected since the ability to estimate uniquely the value of ψ_2 is in fact equivalent to the resolution of the phase ambiguity from the magnitudes $|E_{\mathbf{H}}|$ and $|E_{-\mathbf{H}}|$ alone'.

The problem seems to be that the probabilistic estimates of ψ_2 by (1.1) are positive, but in practice some ψ_2 may be negative. Recent results on the sign distribution of the TPSI (Guo, 1990) show that there is a strong tendency towards positive sign when the $|E|$ magnitudes are large. It is, therefore, very worthwhile to investigate the statistical properties of the probabilistic estimates of the TPSI by numerical computation for some typical cases.

The probabilistic selection of positive sign for the TPSI is analogous to the standard practice of breaking the twofold ambiguity of anomalous-dispersion phasing by selecting phase angles closest to the phase angles of a known substructure of the strong anomalous scatterers, since they are usually also the heavy atoms in the structure (Srinivasan & Parthasarathy, 1976, and references cited therein). The important difference is that the probabilistic estimates of the TPSI can be obtained without prior knowledge of the heavy-atom substructure.

Table 1. *Statistical averages and probabilistic estimates for cocaine methiodide*

λ	$\|E\|_{\min}$	N_p	$\psi_2>0$ (%)	$\langle\psi_2\rangle$ (°)	$\langle-\xi\rangle$ (°)	$\langle\varepsilon\rangle/\langle\psi_2\rangle$ (%)	$\langle\psi_2\rangle/\langle-\xi\rangle$
Cr *Kα*	0·1	1976	96·7	53·03	53·28	33·9	0·995
	1·2	454	100·0	52·07	53·19	14·0	0·979
	1·5	185	100·0	49·91	52·38	11·9	0·953
Cu *Kα*	0·1	1966	98·0	25·56	25·04	29·7	1·021
	1·2	464	100·0	24·57	24·99	12·7	0·983
	1·5	194	100·0	23·82	24·87	10·9	0·958
Mo *Kα*	0·1	1968	97·7	6·92	6·76	29·5	1·025
	1·2	466	100·0	6·61	6·74	13·1	0·980
	1·5	199	100·0	6·42	6·71	11·3	0·957

Table 2. *Statistical averages and probabilistic estimates for the* $PtCl_4^{2-}$ *derivative and the native protein cytochrome* c_{550}

Crystal	λ	$\|E\|_{\min}$	N_p	$\psi_2>0$ (%)	$\langle\psi_2\rangle$ (°)	$\langle-\xi\rangle$ (°)	$\langle\varepsilon\rangle/\langle\psi_2\rangle$ (%)	$\langle\psi_2\rangle/\langle-\xi\rangle$
$PtCl_4^{2-}$	Cr *Kα*	0·3	10 000	80·2	6·50	5·92	>100	1·10
		1·2	2403	91·0	6·09	5·79	53	1·05
		1·5	1044	93·0	5·78	5·65	46	1·02
$PtCl_4^{2-}$	Cu *Kα*	0·3	10 000	79·1	3·71	3·38	>100	1·10
		1·2	2394	90·5	3·49	3·30	57	1·06
		1·5	1046	92·8	3·29	3·22	49	1·02
Native	Cr *Kα*	0·3	10 000	81·1	1·81	1·70	99	1·06
		1·2	2377	92·6	1·71	1·66	52	1·03
		1·5	979	95·5	1·67	1·61	43	1·04
Native	Cu *Kα*	0·3	10 000	68·8	1·26	1·15	>100	1·10
		1·2	2382	77·6	1·15	1·12	>100	1·03
		1·5	980	80·2	1·09	1·08	86	1·01

2. Statistical properties

Known structures of small-molecule and macromolecular crystals were used to calculate normalized structure-factor magnitudes $|E_{\mathbf{H}}|$ and $|E_{-\mathbf{H}}|$, phase angles $\varphi_{\mathbf{H}}$ and $\varphi_{-\mathbf{H}}$ and the true values of $\psi_2=\varphi_{\mathbf{H}}+\varphi_{-\mathbf{H}}$. The probabilistic estimates $-\xi$ were calculated from (1.2) to (1.6). Atomic scattering factors were taken from Cromer & Waber (1974) and Cromer (1974). All calculations were done on a VAX 8600 computer in double precision (about 15 significant digits). Several test calculations were repeated in single precision and they showed that double precision was not a necessary refinement.

2.1. *A small-molecule example*

A suitable example is cocaine methiodide, $C_{18}H_{24}NO_4^+.I^-$, which crystallizes in $P2_12_12_1$ with $Z=4$ (Shen, Ruble & Hite, 1975). The computations were done for $N_p=2000$ Friedel pairs with $|E|>0·1$ at wavelengths of Cr *Kα*, Cu *Kα* and Mo *Kα*. The values $\langle\psi_2\rangle=\langle\varphi_{\mathbf{H}}+\varphi_{-\mathbf{H}}\rangle$, $\langle-\xi\rangle$ and $\langle\varepsilon\rangle$ averaged over the N_p data pairs are listed in Table 1. The quantity $\langle\varepsilon\rangle$ is defined to be the average absolute error,

$$\langle\varepsilon\rangle=(1/N_p)\sum_{i=1}^{N_p}|\psi_{2i}+\xi_i|. \qquad (2.1)$$

The relative error $\langle\varepsilon\rangle/\langle\psi_2\rangle$ is given as a percentage, and the table column headed $\psi_2>0$ gives the percentage of ψ_2 with positive sign.

Table 1 shows three things: First, although the estimate $-\xi$ might not be accurate for some particular Friedel pair, it is statistically very accurate for a sufficiently large sample of Friedel pairs. This is shown by the close agreement between the average estimates $\langle-\xi\rangle$ and the true averages $\langle\psi_2\rangle$. Second, as shown by the percentage of ψ_2 with positive sign, the TPSI do tend strongly to be positive and this tendency is stronger the larger the $|E|$ values. Indeed, for $|E|>1$ nearly all the ψ_2 are positive. Third, the larger the $|E|$ values, the more reliable the estimates $\langle-\xi\rangle$. The relative errors $\langle\varepsilon\rangle/\langle\psi_2\rangle$ become very small for $|E|>1$.

2.2. *A macromolecular example*

The protein cytochrome c_{550}, $C_{637}FeN_{170}O_{20}S_6$ (H atoms not included in the calculation of the $|E|$ magnitudes), crystallizes in space group $P2_12_12_1$ with $Z=4$ and gives a single-site $PtCl_4^{2-}$ derivative (Timkovich & Dickerson, 1973, 1976). Table 2 summarizes results of calculations, analogous to those described in the preceding section, performed for the native and derivative proteins for $N_p=10\,000$ Friedel pairs with $|E|>0·3$ at Cr *Kα* and Cu *Kα* wavelengths. (The wavelength of Mo *Kα* is impractically short for macromolecular crystals.)

The same three statistical principles evidenced in Table 1 are supported by Table 2: For a statistically large sample of Friedel pairs, the true average $\langle\psi_2\rangle$ is close to the estimate $\langle-\xi\rangle$; there is a strong tendency to the positive sign; and the reliability of the estimated TPSI increases with increasing $|E|$. Not surprisingly, owing to the large number of light atoms in the protein structures and the consequent relative weakness of the anomalous scattering intensities, the relative errors $\langle\varepsilon\rangle/\langle\psi_2\rangle$ are substantially larger for the macromolecule than for the small-molecule calculations. Table 2 also indicates the effects of choice of wavelength and heavy-atom derivative: the average relative errors are smaller for the Cr wavelength and the $PtCl_4^{2-}$ derivative.

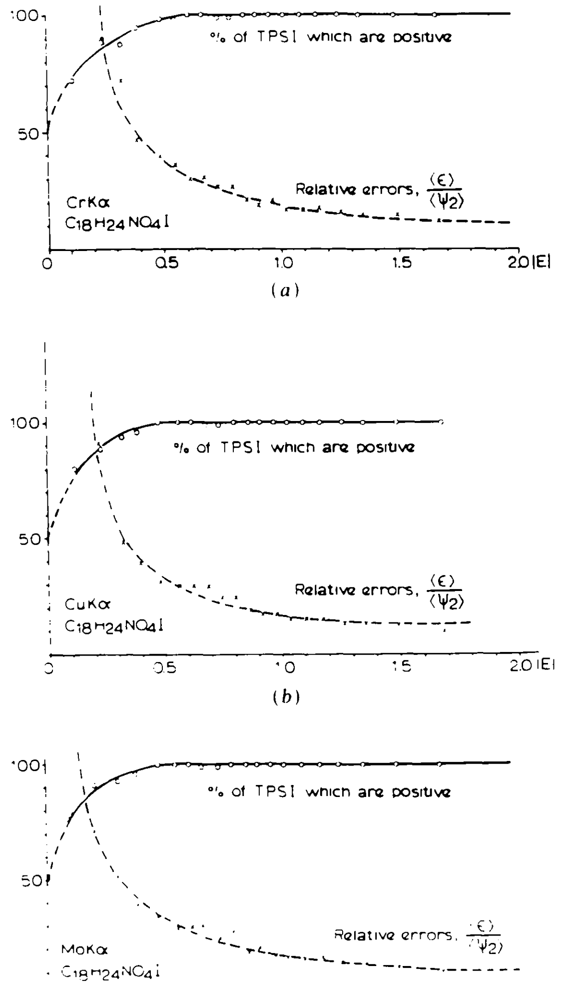

Fig. 2. Sign and error distributions for Friedel-pair two-phase structure invariants for cocaine methiodide for (*a*) Cr $K\alpha$, (*b*) Cu $K\alpha$ and (*c*) Mo $K\alpha$ radiations. The abscissa is the geometric mean magnitude $|E|=(|E_{\mathbf{H}}||E_{-\mathbf{H}}|)^{1/2}$.

3. Empirical distributions of TPSI signs, magnitudes and errors

The results very briefly summarized in Tables 1 and 2 are shown in more detail in Figs. 2 to 6, which show that the error distribution is quite symmetrical and the average signed error,

$$\langle\eta\rangle=(1/N_p)\sum_{i=1}^{N_p}(\psi_{2i}+\xi_i), \tag{3.1}$$

is always close to zero.

Fig. 2 shows that, for the small-molecule case, the near certainty of the positive sign for the TPSI and minimal error in the estimated values of the TPSI hold very well when $|E|>1$ and reasonably well even down to $|E|>0{\cdot}5$, independently of wavelength in the Cr $K\alpha$ to Mo $K\alpha$ range.

For Figs. 3 and 4 the data were ranked on the true value $\psi_2=\varphi_{\mathbf{H}}+\varphi_{-\mathbf{H}}$ and then averages $\langle\psi_2\rangle$, $\langle-\xi\rangle$ and $\langle\varepsilon\rangle$ were computed for ranked groups of 100 Friedel pairs. For the data with $|E|>0{\cdot}1$, the averages $\langle\psi_2\rangle$ *vs* $\langle-\xi\rangle$ follow an ideal diagonal distribution quite closely, well within the error limits $\pm\langle\varepsilon\rangle$ (Fig. 3). The diagonal trend is almost perfect for $|E|>1{\cdot}2$ (Fig. 4).

For a macromolecule, stronger intensity data are required for positive TPSI sign and minimal error for the TPSI estimates. Fig. 5(*a*) indicates that for the cytochrome c_{550} $PtCl_4^{2-}$ derivative the number of sign errors and the size of the TPSI errors begin to increase substantially for $|E|<1{\cdot}5$, but Figs. 5(*b*) and (*c*) show that for the $N_p=2400$ Friedel pairs with $|E|>1{\cdot}2$ the diagonal distribution holds very well. Fig. 6 shows that for the native cytochrome c_{550}, the Cr $K\alpha$ data are better behaved than the Cu $K\alpha$ data, because of the significantly stronger anomalous scattering at the Cr wavelength.

4. Error analysis from the TPSI probability distribution

Following Hauptman (1982), the variance of the TPSI estimate is

$$\mathrm{var}(\Psi_2)=\int_{\Psi_{2m}-\pi}^{\Psi_{2m}+\pi}(\Psi_2-\Psi_{2m})^2P(\Psi_2||E_{\mathbf{H}}|,|E_{-\mathbf{H}}|)\,\mathrm{d}\Psi_2, \tag{4.1}$$

where $\Psi_2=\Psi_{2m}$ at the maximum of the conditional probability distribution of the TPSI $\varphi_{\mathbf{H}}+\varphi_{-\mathbf{H}}$ given the two magnitudes $|E_{\mathbf{H}}|$ and $|E_{-\mathbf{H}}|$. The conditional probability density is

$$P(\Psi_2||E_{\mathbf{H}}|,|E_{-\mathbf{H}}|)=(1/K)\exp[C\cos(\Psi_2+\xi)], \tag{4.2}$$

where

$$K=2\pi I_0(C), \tag{4.3}$$

$$C=2|E_{\mathbf{H}}||E_{-\mathbf{H}}|X/(1-X^2) \tag{4.4}$$

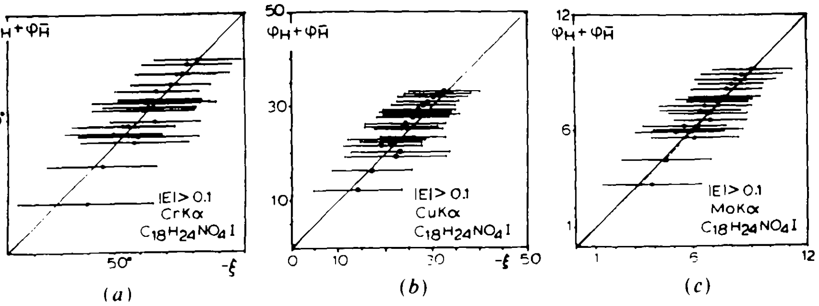

Fig. 3. Ranked group-averaged true $\psi_2 = \varphi_H + \varphi_{-H}$ *vs* estimated $-\xi$ for cocaine methiodide Friedel pairs with $|E| > 0{\cdot}1$ for (*a*) Cr $K\alpha$, (*b*) Cu $K\alpha$ and (*c*) Mo $K\alpha$ radiations. The error bars bracket $\pm\langle\varepsilon\rangle$.

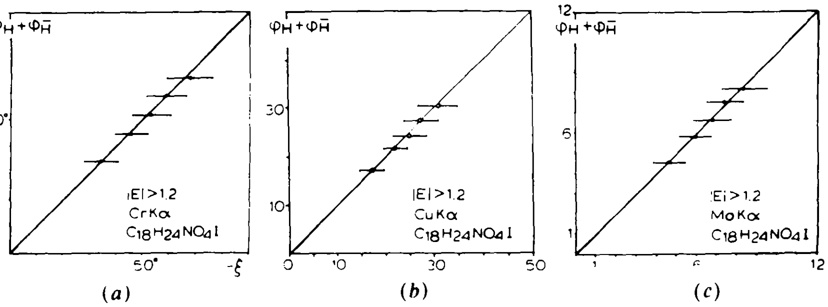

Fig. 4. As Fig. 3 but with $|E| > 1{\cdot}2$.

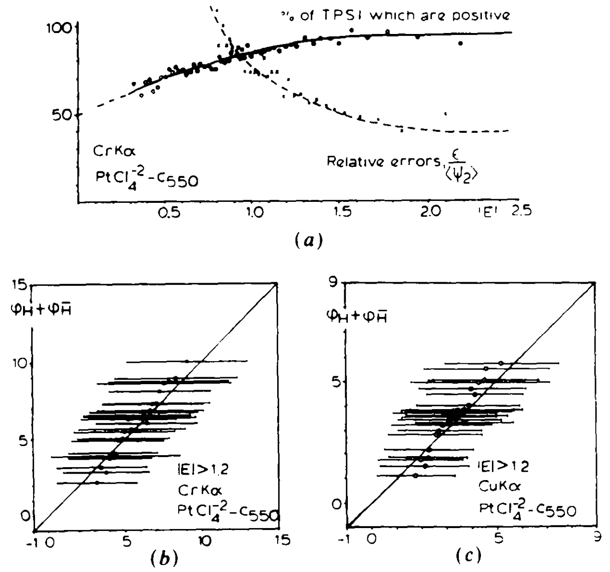

Fig. 5. (*a*) Sign and error distributions for cytochrome c_{550} $PtCl_4^{2-}$ Friedel-pair two-phase structure invariants with $|E| = (|E_H||E_{-H}|)^{1/2} > 0{\cdot}3$ for Cr $K\alpha$. (*b*) Ranked group-averaged true $\psi_2 = \varphi_H + \varphi_{-H}$ *vs* estimated $-\xi$ for cytochrome c_{550} $PtCl_4^{2-}$ Friedel pairs with $|E| > 1{\cdot}2$ for Cr $K\alpha$ radiation. (*c*) Same as (*b*) for Cu $K\alpha$ radiation.

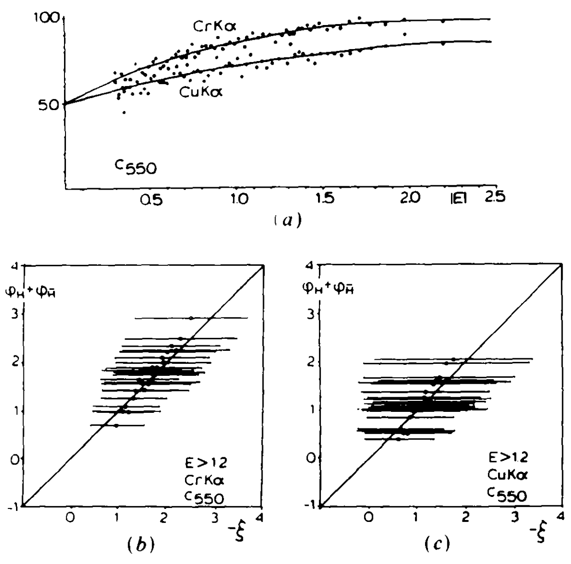

Fig. 6. (*a*) Sign distributions against $|E| = (|E_H||E_{-H}|)^{1/2}$ for native cytochrome c_{550} Friedel-pair two-phase structure invariants for Cr $K\alpha$ and Cu $K\alpha$ radiations. (*b*) Ranked group-averaged true $\psi_2 = \varphi_H + \varphi_{-H}$ *vs* estimated $-\xi$ for native c_{550} Friedel pairs with $|E| > 1{\cdot}2$ for Cr $K\alpha$ radiation. (*c*) Same as (*b*) for Cu $K\alpha$ radiation.

and, using (1.3) to (1.6),

$$X = (C_{\mathrm{H}}^2 + S_{\mathrm{H}}^2)^{1/2}. \tag{4.5}$$

The standard deviation is

$$\sigma(\Psi_2) = [\mathrm{var}\,(\Psi_2)]^{1/2} \tag{4.6}$$

and to calculate the integral in (4.1) and obtain $\sigma(\Psi_2)$ a very simple approximation is possible.

Assume that the conditional probability density (4.2), which has its maximum value P_m at Ψ_{2m}, can be fairly approximated by a rectangular distribution with width $2D$. Then from (4.2),

$$P_m = (1/K)\exp C, \tag{4.7}$$

and, using the normalization condition $2DP_m = 1$, (4.1) gives

$$\mathrm{var}\,(\Psi_2) = D^2/3 = (1/3)[\pi I_0(C)\exp(-C)]^2 \tag{4.8}$$

and

$$\sigma(\Psi_2) = (1/3)^{1/2}\pi I_0(C)\exp(-C). \tag{4.9}$$

Fig. 7 shows $\sigma(\Psi_2)$ plotted against C.

The approximate formula (4.9) helps explain the numerical results in Figs. 2, 5(a) and 6(a), which show that the relative error in the TPSI estimates decrease with increasing geometric mean magnitude $|E| = (|E_{\mathrm{H}}||E_{-\mathrm{H}}|)^{1/2}$. Equation (4.5) shows that the variable C is proportional to $|E|^2$ and (4.9) shows that $\sigma(\Psi_2)$ falls off exponentially with increasing C, which approximately parallels the $|E|$ dependence of the numerical error estimates.

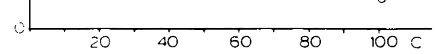

Fig. 7. Plot of $\sigma(\Psi_2)$ *vs* C. See equations (4.9), (4.4), (4.5) and (1.3) to (1.6).

5. Concluding remarks

The probabilistic estimates of the TPSI from Hauptman's (1982) formula are confirmed by applications to real structures using error-free data. Further practical analysis of the TPSI must naturally involve the individual TPSI estimates. A preliminary investigation about individual TPSI (Guo & Hauptman, 1989) shows that further work is worthwhile.

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