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A Joint Probability Distribution of Seven Structure Factors

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It is assumed that a crystal structure in $P1$ is fixed and that the random variables (vectors) $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$, subject to $\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0$, are uniformly and independently distributed in reciprocal space. Then the seven structure factors $E_\mathbf{h}, E_\mathbf{k}, E_\mathbf{l}, E_\mathbf{m}, E_{\mathbf{h}+\mathbf{k}}, E_{\mathbf{k}+\mathbf{l}}, E_{\mathbf{l}+\mathbf{h}}$, as functions of the primitive random variables $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$, are themselves random variables, and their joint probability distribution is found. This distribution plays the central role in the theory and estimation of the cosine invariants $\cos(\varphi_\mathbf{h}+\varphi_\mathbf{k}+\varphi_\mathbf{l}+\varphi_\mathbf{m})$.

1. Introduction

Probability distributions were introduced into X-ray crystallography by Wilson (1949). A few years later, the concept of the joint distribution of two or more structure factors was introduced (Hauptman & Karle, 1953) and its importance as a method for phase determination demonstrated. In this early work, and in most of the work which followed (*e.g.* Klug, 1958), one or more reciprocal vectors were supposed to be fixed and the atomic coordinates were assumed to be independent random variables which were uniformly distributed. The structure factors, as functions of the atomic coordinates, are then random variables themselves, and it was on this basis that their probability distributions were derived. Some time later (Hauptman & Karle, 1958; Karle & Hauptman, 1958) the crystal structure was assumed to be fixed, as well as one or more reciprocal vectors $\mathbf{h}_1, \mathbf{h}_2, \ldots$, and a single vector $\mathbf{k}$ was assumed to be a random variable, uniformly distributed throughout reciprocal space. The structure factors, as functions of the primitive random variable $\mathbf{k}$, are again random variables, and their probability distributions could again then be found. It was emphasized that the former distributions, based on atomic coordinates as the independent random variables, are conceptually quite distinct from the latter in which it is assumed that the primitive random variable is the reciprocal vector $\mathbf{k}$. It is of course the latter distributions which are more important in the applications since one is usually confronted with a fixed, but unknown, crystal structure; and a set of structure-factor magnitudes sampled from reciprocal space is also available. For this reason only the latter kind of distribution is considered here.

In the recent past Tsoucaris (1970), employing the central limit theorem, derived improved distributions for any number of structure factors. More recently Hauptman (1971, 1972), using new techniques to perform the necessary integrations, obtained still more accurate distributions, at least for the case of two and three structure factors. In the present paper these latter techniques are generalized to include the case that the number of primitive random variables (reciprocal vectors) is greater than one. The importance of this generalization is that it permits the study of the joint probability distributions of arbitrary sets of structure factors, their mutual correlations and their combined action in affecting the value of a structure invariant.

It has become increasingly clear in recent years that the cosine invariants and seminvariants play the central role in direct phase determination in that they link the observed magnitudes with the desired phases of the structure factors. Thus the individual phases are uniquely determined by the values of the cosine invariants and seminvariants (Hauptman, Fisher, Hancock & Norton, 1969) and the latter, in turn, depend essentially on the values of a relatively few appropriately chosen structure-factor magnitudes (Hauptman, 1974*a,b*). [In order to insure that magnitudes determine unique values for the cosines it is necessary to assume that no homometric solutions, other than enantiomorphs, exist,* and this assumption is made throughout. However, bimodal distributions, when used as estimators for the invariants, may have the potential for sorting out homometric solutions, and this possibility is briefly discussed in the accompanying paper (Hauptman, 1975).] It has also become clear that the nature of the dependence of these cosines on the selected magnitudes is related in an important way to the mutual correlations of the magnitudes, and the latter depend in turn on appropriately chosen probability distributions of several structure factors. Thus a major aim in writing the present paper is to show, by working out in some detail the important case of seven structure factors, how the required probability distributions are to be obtained. Another goal in deriving this particular distribution is that it is the cornerstone on which the theory of the four-phase structure invariants, $\varphi_\mathbf{h}+\varphi_\mathbf{k}+\varphi_\mathbf{l}+\varphi_\mathbf{m}$, is properly based. In recent work (Hauptman, 1974*a,b*) the theory of these invariants, based on a probability distribution of three structure factors, was initiated. However, the more satisfactory theory described here, which takes into

* This fact was pointed out to the author by Dr David Sayre to whom due acknowledgement is made.

account all mutual correlations among the seven related structure-factor magnitudes and their concerted influence on the value of the cosine invariant $\cos(\varphi_h+\varphi_k+\varphi_l+\varphi_m)$, leads to a better estimate for the value of the cosine and requires the distribution of the seven structure factors derived here.

2. Joint probability distribution of the seven structure factors E_h, E_k, E_l, E_m, E_{h+k}, E_{k+l}, E_{l+h}

Suppose that a crystal structure, consisting of N identical atoms in the space group $P1$, is fixed. In much the same way that the Cartesian plane may be defined as the collection of all ordered pairs (x,y) of real numbers x,y, so now the fourfold Cartesian product $\mathbf{S}\times\mathbf{S}\times\mathbf{S}\times\mathbf{S}$ of reciprocal space $\mathbf{S}$ is defined to be the collection of all ordered quadruples $(\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m})$, where $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$ are reciprocal vectors. Suppose next that the ordered quadruple of reciprocal vectors $(\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m})$ is a random variable (vector) which is uniformly distributed over the subset of $\mathbf{S}\times\mathbf{S}\times\mathbf{S}\times\mathbf{S}$ for which

$$\mathbf{h}+\mathbf{k}+\mathbf{l}+\mathbf{m}=0. \tag{2.1}$$

It should be observed that, in view of (2.1), the random variables $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$, the components of the ordered quadruple $(\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m})$, are not independently distributed in reciprocal space. Then the seven normalized structure factors $E_\mathbf{h},E_\mathbf{k},E_\mathbf{l},E_\mathbf{m},E_{\mathbf{h}+\mathbf{k}},E_{\mathbf{k}+\mathbf{l}},E_{\mathbf{l}+\mathbf{h}}$, as functions of the primitive random variables $\mathbf{h},\mathbf{k},\mathbf{l},\mathbf{m}$, are themselves random variables. [Note that, in view of (2.1), $E_{\mathbf{h}+\mathbf{m}},E_{\mathbf{k}+\mathbf{m}},E_{\mathbf{l}+\mathbf{m}}$ are the complex conjugates of $E_{\mathbf{k}+\mathbf{l}},E_{\mathbf{l}+\mathbf{h}},E_{\mathbf{h}+\mathbf{k}}$ respectively, so that nothing is gained by adding these three to the initial set of seven.] Denote by

$$P=P(R_1,R_2,R_3,R_4,R_{12},R_{23},R_{31};\ \Phi_1,\Phi_2,\Phi_3,\Phi_4,\Phi_{12},\Phi_{23},\Phi_{31}) \tag{2.2}$$

the joint probability distribution of the magnitudes $|E_\mathbf{h}|,|E_\mathbf{k}|,|E_\mathbf{l}|,|E_\mathbf{m}|,|E_{\mathbf{h}+\mathbf{k}}|,|E_{\mathbf{k}+\mathbf{l}}|,|E_{\mathbf{l}+\mathbf{h}}|$ and the phases $\varphi_\mathbf{h},\varphi_\mathbf{k},\varphi_\mathbf{l},\varphi_\mathbf{m},\varphi_{\mathbf{h}+\mathbf{k}},\varphi_{\mathbf{k}+\mathbf{l}},\varphi_{\mathbf{l}+\mathbf{h}}$ of the seven structure factors $E_\mathbf{h},E_\mathbf{k},E_\mathbf{l},E_\mathbf{m},E_{\mathbf{h}+\mathbf{k}},E_{\mathbf{k}+\mathbf{l}},E_{\mathbf{l}+\mathbf{h}}$. Then, following Karle & Hauptman (1958), P is given by the fourteenfold integral,

$$P=\frac{R_1R_2R_3R_4R_{12}R_{23}R_{31}}{(2\pi)^{14}}\int_{\varrho_1,\varrho_2,\varrho_3,\varrho_4,\varrho_{12},\varrho_{23},\varrho_{31}=0}^{\infty}$$
$$\times\int_{\theta_1,\theta_2,\theta_3,\theta_4,\theta_{12},\theta_{23},\theta_{31}=0}^{2\pi}\varrho_1\varrho_2\varrho_3\varrho_4\varrho_{12}\varrho_{23}\varrho_{31}$$
$$\times\exp\{-i[R_1\varrho_1\cos(\theta_1-\Phi_1)+R_2\varrho_2\cos(\theta_2-\Phi_2)$$
$$+R_3\varrho_3\cos(\theta_3-\Phi_3)+R_4\varrho_4\cos(\theta_4-\Phi_4)$$
$$+R_{12}\varrho_{12}\cos(\theta_{12}-\Phi_{12})+R_{23}\varrho_{23}\cos(\theta_{23}-\Phi_{23})$$
$$+R_{31}\varrho_{31}\cos(\theta_{31}-\Phi_{31})]\}\prod_{\lambda=1}^{N}g_\lambda$$
$$\times d\varrho_1d\varrho_2d\varrho_3d\varrho_4d\varrho_{12}d\varrho_{23}d\varrho_{31}$$
$$\times d\theta_1d\theta_2d\theta_3d\theta_4d\theta_{12}d\theta_{23}d\theta_{31} \tag{2.3}$$

where

$$g_\lambda=g(\mathbf{r}_\lambda;\varrho_1,\varrho_2,\varrho_3,\varrho_4,\varrho_{12},\varrho_{23},\varrho_{31};\ \theta_1,\theta_2,\theta_3,\theta_4,\theta_{12},\theta_{23},\theta_{31})$$
$$=\Big\langle\exp\frac{i}{N^{1/2}}\{\varrho_1\cos(2\pi\mathbf{h}.\mathbf{r}_\lambda-\theta_1)$$
$$+\varrho_2\cos(2\pi\mathbf{k}.\mathbf{r}_\lambda-\theta_2)+\varrho_3\cos(2\pi\mathbf{l}.\mathbf{r}_\lambda-\theta_3)$$
$$+\varrho_4\cos[2\pi(\mathbf{h}+\mathbf{k}+\mathbf{l})\cdot\mathbf{r}_\lambda+\theta_4]$$
$$+\varrho_{12}\cos[2\pi(\mathbf{h}+\mathbf{k}).\mathbf{r}_\lambda-\theta_{12}]$$
$$+\varrho_{23}\cos[2\pi(\mathbf{k}+\mathbf{l}).\mathbf{r}_\lambda-\theta_{23}]$$
$$+\varrho_{31}\cos[2\pi(\mathbf{l}+\mathbf{h}).\mathbf{r}_\lambda-\theta_{31}]\}\Big\rangle_{\mathbf{h},\mathbf{k},\mathbf{l}}, \tag{2.4}$$

in which $\mathbf{r}_\lambda$ is the position vector of the atom labeled λ and the average is taken over all vectors $\mathbf{h},\mathbf{k},\mathbf{l}$ in reciprocal space. The mathematical Appendices I–IV contain, respectively, I: some preliminary formulas, II: the derivation of g_λ, III: the derivation of $\prod_{\lambda=1}^{N} g_\lambda$, and IV: a brief description of the techniques required to evaluate the fourteenfold integral (2.3). Only the final formula, the chief result of the present paper, is written down here:

$$P=\frac{R_1R_2R_3R_4R_{12}R_{23}R_{31}}{\pi^7}$$
$$\times\exp\Big\{-R_1^2-R_2^2-R_3^2-R_4^2-R_{12}^2-R_{23}^2-R_{31}^2$$
$$+\frac{2R_1R_2R_{12}}{N^{1/2}}\cos(\Phi_1+\Phi_2-\Phi_{12})$$
$$+\frac{2R_3R_4R_{12}}{N^{1/2}}\cos(\Phi_3+\Phi_4+\Phi_{12})$$
$$+\frac{2R_2R_3R_{23}}{N^{1/2}}\cos(\Phi_2+\Phi_3-\Phi_{23})$$
$$+\frac{2R_1R_4R_{23}}{N^{1/2}}\cos(\Phi_1+\Phi_4+\Phi_{23})$$
$$+\frac{2R_1R_3R_{31}}{N^{1/2}}\cos(\Phi_1+\Phi_3-\Phi_{31})$$
$$+\frac{2R_2R_4R_{31}}{N^{1/2}}\cos(\Phi_2+\Phi_4+\Phi_{31})$$
$$-\frac{2R_1R_3R_{12}R_{23}}{N}\cos(\Phi_1-\Phi_3-\Phi_{12}+\Phi_{23})$$
$$-\frac{2R_2R_4R_{12}R_{23}}{N}\cos(\Phi_2-\Phi_4-\Phi_{12}-\Phi_{23})$$
$$-\frac{2R_1R_2R_{23}R_{31}}{N}\cos(\Phi_1-\Phi_2+\Phi_{23}-\Phi_{31})$$
$$-\frac{2R_3R_4R_{23}R_{31}}{N}\cos(\Phi_3-\Phi_4-\Phi_{23}-\Phi_{31})$$

$$- \frac{2R_2R_3R_{31}R_{12}}{N} \cos (\Phi_2 - \Phi_3 + \Phi_{31} - \Phi_{12})$$
$$- \frac{2R_1R_4R_{31}R_{12}}{N} \cos (\Phi_1 - \Phi_4 - \Phi_{31} - \Phi_{12})$$
$$- \left. \frac{4R_1R_2R_3R_4}{N} \cos (\Phi_1 + \Phi_2 + \Phi_3 + \Phi_4) \right\}$$
$$\times \left\{ 1 + \mathrm{O}\left(\frac{1}{N}\right) \right\}, \tag{2.5}$$

where $\mathrm{O}(1/N)$ represents terms of order $1/N$ or higher in which the terms of order $1/N$ are independent of the Φ's. Particularly noteworthy (in view of § 3) is the numerical coefficient, -4, of the last term in the argument of the exponential function of (2·5). It should also be noted that the exponent in (2.5) is a quartic (not quadratic) polynomial in the R's with coefficients consisting of all the possible three or four phase cosine invariants which can be constructed from the seven phase variables $\Phi_1, \Phi_2, \Phi_3, \Phi_4, \Phi_{12}, \Phi_{23}, \Phi_{31}$.

3. Joint probability distribution of the four structure factors $E_{\mathbf{h}}, E_{\mathbf{k}}, E_{\mathbf{l}}, E_{\mathbf{m}}$

Under the same hypotheses as in § 2 and using similar notation and methods, one readily finds

$$P(R_1, R_2, R_3, R_4; \Phi_1, \Phi_2, \Phi_3, \Phi_4) = \frac{R_1R_2R_3R_4}{\pi^4}$$
$$\times \exp \left\{ -R_1^2 - R_2^2 - R_3^2 - R_4^2 + \frac{2R_1R_2R_3R_4}{N} \right.$$
$$\left. \times \cos (\Phi_1 + \Phi_2 + \Phi_3 + \Phi_4) \right\} \left\{ 1 + \mathrm{O}\left(\frac{1}{N}\right) \right\}, \tag{3.1}$$

where again $\mathrm{O}(1/N)$ represents terms of order $1/N$ or higher in which the terms of order $1/N$ are independent of the Φ's. The numerical coefficient, $+2$, of the last term in the exponent of (3.1) is to be compared with the corresponding coefficient, -4, of the last term in the exponent of (2.5). It follows, as shown in the accompanying paper (Hauptman, 1975), that (3.1) can lead only to a positive estimate, dependent on four magnitudes, for the cosine invariant $\cos (\varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}} + \varphi_{\mathbf{m}})$ but (2.5), dependent on the presumed known values of the seven (rather than only four) related structure-factor magnitudes, may lead to any estimate between -1 and $+1$ for the value of this cosine.

4. Concluding remarks

In contrast to previously derived distributions in which only the single reciprocal vector **k** had been assumed to be the primitive random variable, here joint probability distributions of seven and four structure factors have been obtained on the basis that four reciprocal vectors **h**, **k**, **l**, **m**, subject to (2.1), are the primitive random variables. The mathematical techniques illustrated in their derivation presumably may be carried over without essential change in order to derive almost any conceivable distribution involving an arbitrary set of structure factors and dependent on an arbitrary number of primitive random variables. It is anticipated that suitably chosen distributions will serve as the starting point from which estimates for the cosine invariants, in terms of an arbitrary number of structure-factor magnitudes, may be obtained. In fact the distributions derived here already begin to serve this purpose. As shown in the following paper (Hauptman, 1975), (2.5) leads directly to the conditional distribution of the structure invariant $\varphi = \varphi_{\mathbf{h}} + \varphi_{\mathbf{k}} + \varphi_{\mathbf{l}} + \varphi_{\mathbf{m}}$ from which an estimate for $\cos \varphi$, dependent on the seven magnitudes $|E_{\mathbf{h}}|, |E_{\mathbf{k}}|, |E_{\mathbf{l}}|, |E_{\mathbf{m}}|, |E_{\mathbf{h}+\mathbf{k}}|, |E_{\mathbf{k}+\mathbf{l}}|, |E_{\mathbf{l}+\mathbf{m}}|$, may be found. Since these particular cosines have already proved to be useful in the applications (*e.g.* DeTitta, Edmonds, Langs & Hauptman, 1974; Einspahr, Gartland, Freeman & Schenk, 1974) it is anticipated that the improved theory based on (2.5) will find early application.

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APPENDIX I

Some preliminary formulas

From elementary trigonometry

$$\sum_{\mu} A_{\mu} \exp \{i(\varphi + \alpha_{\mu})\} = X \exp \{i(\varphi + \xi)\}, \tag{I.1}$$

where X and ξ are determined by

$$X = \left\{ \sum_{\mu,\nu} A_{\mu}A_{\nu} \cos (\alpha_{\mu} - \alpha_{\nu}) \right\}^{1/2}, \tag{I.2}$$
$$X \exp (i\xi) = \sum_{\mu} A_{\mu} \exp (i\alpha_{\mu}) . \tag{I.3}$$

Referring to Watson (1958, pp. 20, 21), infer that

$$\frac{1}{2\pi} \int_0^{2\pi} \exp (iz \cos \varphi) \cos m\varphi \mathrm{d}\varphi = i^m J_m(z) , \tag{I.4}$$

where $J_m(z)$ is the Bessel function of order m, so that the right side of (I.4) may be interpreted as the average value of the integrand on the left provided that φ is assumed to be a random variable which is uniformly distributed in the interval $(0, 2\pi)$. Evidently also,

$$\int_0^{2\pi} \exp (iz \cos \varphi) \sin m\varphi \mathrm{d}\varphi = 0 . \tag{I.5}$$

The addition theorem for Bessel functions may be written (Watson, 1958, p. 359)

$$J_{\nu} \left((Z^2 + z^2 + 2Zz \cos \varphi)^{1/2} \right) \left(\frac{Z + z \exp (-i\varphi)}{Z + z \exp (i\varphi)} \right)^{1/2\nu}$$
$$= \sum_{m=-\infty}^{\infty} (-1)^m J_{\nu+m}(Z) J_m(z) \exp (im\varphi). \tag{I.6}$$

The Taylor expansion of the Bessel function may be written (Watson, 1958, p. 40)

$$J_m(z)=\frac{(\frac{1}{2}z)^m}{\Gamma(m+1)}\left\{1-\frac{(\frac{1}{2}z)^2}{1\,.\,(m+1)}+\frac{(\frac{1}{2}z)^4}{1\,.\,2\,.\,(m+1)\,(m+2)}-\ldots\right\}. \tag{I.7}$$

Finally, Weber's first exponential integral (Watson, 1958, p. 393),

$$\int_0^\infty \exp\,(-pt^2)J_0(at)tdt=\frac{1}{2p}\exp\left(-\frac{a^2}{4p}\right), \tag{I.8}$$

also finds important application in the sequel.

APPENDIX II
The derivation of g_λ

Suppressing the index λ of the vector $\mathbf{r}$ in (2.4) and combining by means of (I.1)–(I.3), the four terms in the exponent of (2.4) which involve $\mathbf{l}$, one finds

$$\begin{aligned}\frac{i}{N^{1/2}}\{&\varrho_3\cos\,(2\pi\mathbf{l}\,.\,\mathbf{r}-\theta_3)+\varrho_4\cos\,[2\pi(\mathbf{h}+\mathbf{k}+\mathbf{l})\,.\,\mathbf{r}+\theta_4]\\&+\varrho_{23}\cos\,[2\pi(\mathbf{k}+\mathbf{l})\,.\,\mathbf{r}-\theta_{23}]\\&+\varrho_{31}[\cos\,2\pi(\mathbf{l}+\mathbf{h})\,.\,\mathbf{r}-\theta_{31}]\}\\&=\frac{i}{N^{1/2}}X\cos\,(2\pi\mathbf{l}\,.\,\mathbf{r}+\xi)\end{aligned} \tag{II.1}$$

where

$$\begin{aligned}X=\{&\varrho_3^2+\varrho_4^2+\varrho_{23}^2+\varrho_{31}^2+2\varrho_3\varrho_4\\&\times\cos\,[2\pi(\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}+\theta_3+\theta_4]\\&+2\varrho_3\varrho_{23}\cos\,(2\pi\mathbf{k}\,.\,\mathbf{r}+\theta_3-\theta_{23})\\&+2\varrho_3\varrho_{31}\cos\,(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3-\theta_{31})\\&+2\varrho_4\varrho_{23}\cos\,(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_4+\theta_{23})\\&+2\varrho_4\varrho_{31}\cos\,(2\pi\mathbf{k}\,.\,\mathbf{r}+\theta_4+\theta_{31})\\&+2\varrho_{23}\varrho_{31}\cos\,[2\pi(\mathbf{h}-\mathbf{k})\,.\,\mathbf{r}+\theta_{23}-\theta_{31}]\}^{1/2},\end{aligned} \tag{II.2}$$

$$\begin{aligned}X\exp\,(i\xi)=&\varrho_3\exp\,(-i\theta_3)+\varrho_4\exp\,i[2\pi(\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}+\theta_4]\\&+\varrho_{23}\exp\,i(2\pi\mathbf{k}\,.\,\mathbf{r}-\theta_{23})\\&+\varrho_{31}\exp\,i(2\pi\mathbf{h}\,.\,\mathbf{r}-\theta_{31})\end{aligned} \tag{II.3}$$

so that X and ξ are independent of $\mathbf{l}$ but not of $\mathbf{h}$ or $\mathbf{k}$. Then (2.4) becomes

$$\begin{aligned}g_\lambda=\Big\langle\exp\Big\{&\frac{i}{N^{1/2}}[\varrho_1\cos\,(2\pi\mathbf{h}\,.\,\mathbf{r}-\theta_1)\\&+\varrho_2\cos\,(2\pi\mathbf{k}\,.\,\mathbf{r}-\theta_2)+\varrho_{12}\cos\,[2\pi(\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}-\theta_{12})\\&+X\cos\,(2\pi\mathbf{l}\,.\,\mathbf{r}+\xi)]\Big\}\Big\rangle_{\mathbf{h},\mathbf{k},\mathbf{l}}\,.\end{aligned} \tag{II.4}$$

Assume that the three components of $\mathbf{r}$ are linearly independent, *i.e.* that no linear combination of these components with integer coefficients not all zero is equal to an integer. Since $\mathbf{l}$ is assumed to be uniformly distributed throughout reciprocal space, it follows that the fractional part of $\mathbf{l}\,.\,\mathbf{r}$ is uniformly distributed in the interval (0, 1) [see *e.g.* Hauptman & Karle (1953), Appendix]. Since X and ξ are independent of $\mathbf{l}$, the average over $\mathbf{l}$ in (II.4) is readily carried out by means of (I.4):

$$\begin{aligned}g_\lambda=\Big\langle\exp\Big\{&\frac{i}{N^{1/2}}[\varrho_1\cos\,(2\pi\mathbf{h}\,.\,\mathbf{r}-\theta_1)\\&+\varrho_2\cos\,(2\pi\mathbf{k}\,.\,\mathbf{r}-\theta_2)+\varrho_{12}\\&\times\cos\,(2\pi(\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}-\theta_{12})]\Big\}J_0\left(\frac{X}{N^{1/2}}\right)\Big\rangle_{\mathbf{h},\mathbf{k}}.\end{aligned} \tag{II.5}$$

In order to carry out the average over $\mathbf{k}$ it is necessary first to analyze X since, as reference to (II.2) shows, X depends on $\mathbf{k}$. Using (I.1)–(I.3), combine the four terms involving $\mathbf{k}$ under the radical of X as follows:

$$\begin{aligned}2\varrho_3\varrho_4&\cos\,[2\pi(\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}+\theta_3+\theta_4]\\&+2\varrho_3\varrho_{23}\cos\,(2\pi\mathbf{k}\,.\,\mathbf{r}+\theta_3-\theta_{23})\\&+2\varrho_4\varrho_{31}\cos\,(2\pi\mathbf{k}\,.\,\mathbf{r}+\theta_4+\theta_{31})\\&+2\varrho_{23}\varrho_{31}\cos\,[2\pi(-\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}-\theta_{23}+\theta_{31}]\\&=2Y\cos\,(2\pi\mathbf{k}\,.\,\mathbf{r}+\eta)\end{aligned} \tag{II.6}$$

where

$$\begin{aligned}Y=[&\varrho_3^2\varrho_4^2+\varrho_3^2\varrho_{23}^2+\varrho_4^2\varrho_{31}^2+\varrho_{23}^2\varrho_{31}^2\\&+2\varrho_3^2\varrho_4\varrho_{23}\cos\,(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_4+\theta_{23})\\&+2\varrho_3\varrho_4^2\varrho_{31}\cos\,(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3-\theta_{31})\\&+2\varrho_3\varrho_4\varrho_{23}\varrho_{31}\cos\,(4\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3+\theta_4+\theta_{23}-\theta_{31})\\&+2\varrho_3\varrho_4\varrho_{23}\varrho_{31}\cos\,(\theta_3-\theta_4-\theta_{23}-\theta_{31})\\&+2\varrho_3\varrho_{23}^2\varrho_{31}\cos\,(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3-\theta_{31})\\&+2\varrho_4\varrho_{23}\varrho_{31}^2\cos\,(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_4+\theta_{23})]^{1/2},\end{aligned} \tag{II.7}$$

$$\begin{aligned}Y\exp\,(i\eta)=&\varrho_3\varrho_4\exp\,[i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3+\theta_4)]\\&+\varrho_3\varrho_{23}\exp\,[i(\theta_3-\theta_{23})]\\&+\varrho_4\varrho_{31}\exp\,[i(\theta_4+\theta_{31})]\\&+\varrho_{23}\varrho_{31}\exp\,[-i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_{23}-\theta_{31})].\end{aligned} \tag{II.8}$$

If x_1 and x_2 are defined by

$$x_1=[\varrho_3^2+\varrho_{31}^2+2\varrho_3\varrho_{31}\cos\,(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3-\theta_{31})]^{1/2} \tag{II.9}$$

$$x_2=[\varrho_4^2+\varrho_{23}^2+2\varrho_4\varrho_{23}\cos\,(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_4+\theta_{23})]^{1/2}, \tag{II.10}$$

then the six terms not involving $\mathbf{k}$ under the radical of X in (II.2) may be written

$$x_1^2+x_2^2 \tag{II.11}$$

and, as reference to (II.7) shows,

$$x_1x_2 = Y. \tag{II.12}$$

Hence, in view of (II.2) and (II.6), X may be written

$$X = [x_1^2 + x_2^2 + 2x_1x_2 \cos(2\pi\mathbf{k}\,.\,\mathbf{r}+\eta)]^{1/2}. \tag{II.13}$$

Then, from (I.6) with $\nu = 0$,

$$J_0\left(\frac{X}{N^{1/2}}\right) = \sum_{\mu=-\infty}^{\infty} (-1)^\mu J_\mu\left(\frac{x_1}{N^{1/2}}\right) J_\mu\left(\frac{x_2}{N^{1/2}}\right) \times \exp[i\mu(2\pi\mathbf{k}\,.\,\mathbf{r}+\eta)], \tag{II.14}$$

and (II.5) becomes

$$g_\lambda = \sum_{\mu=-\infty}^{\infty} (-1)^\mu \left\langle \exp\left\{\frac{i}{N^{1/2}}[\varrho_1\cos(2\pi\mathbf{h}\,.\,\mathbf{r}-\theta_1) + \varrho_2\cos(2\pi\mathbf{k}\,.\,\mathbf{r}-\theta_2) + \varrho_{12}\cos(2\pi(\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}-\theta_{12})]\right\} \times J_\mu\left(\frac{x_1}{N^{1/2}}\right) J_\mu\left(\frac{x_2}{N^{1/2}}\right)\exp[i\mu(2\pi\mathbf{k}\,.\,\mathbf{r}+\eta)]\right\rangle_{\mathbf{h},\mathbf{k}}, \tag{II.15}$$

where x_1, x_2, and η are given by (II.9), (II.10) and (II.7), (II.8) respectively and are seen to be independent of **k**.

The two cosine terms involving **k** in the exponent of (II.15) may be combined by (I.1)–(I.3) as follows:

$$\frac{i}{N^{1/2}}\{\varrho_2\cos(2\pi\mathbf{k}\,.\,\mathbf{r}-\theta_2)+\varrho_{12}\cos[2\pi(\mathbf{h}+\mathbf{k})\,.\,\mathbf{r}-\theta_{12}]\} = \frac{i}{N^{1/2}} Z\cos(2\pi\mathbf{k}\,.\,\mathbf{r}+\zeta) \tag{II.16}$$

where

$$Z = [\varrho_2^2+\varrho_{12}^2+2\varrho_2\varrho_{12}\cos(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_2-\theta_{12})]^{1/2}, \tag{II.17}$$

$$Z\exp(i\zeta) = \varrho_2\exp(-i\theta_2)+\varrho_{12}\exp[i(2\pi\mathbf{h}\,.\,\mathbf{r}-\theta_{12})]. \tag{II.18}$$

Hence, substituting from (II.16) into (II.15), (II.15) finally becomes

$$g_\lambda = \sum_{\mu=-\infty}^{\infty} (-1)^\mu \left\langle \exp\left\{\frac{i}{N^{1/2}}\varrho_1\cos(2\pi\mathbf{h}\,.\,\mathbf{r}-\theta_1)\right\} \times J_\mu\left(\frac{x_1}{N^{1/2}}\right) J_\mu\left(\frac{x_2}{N^{1/2}}\right)\exp\left\{\frac{iZ}{N^{1/2}}\cos(2\pi\mathbf{k}\,.\,\mathbf{r}+\zeta)+i\mu(2\pi\mathbf{k}\,.\,\mathbf{r}+\zeta)\right\}\exp[i\mu(\eta-\zeta)]\right\rangle_{\mathbf{h},\mathbf{k}}, \tag{II.19}$$

where x_1, x_2, Z, ζ and η are independent of **k** as reference to (II.9), (II.10), (II.17), (II.18), (II.7) and (II.8) shows. Hence, employing (I.4) and (I.5) the average of (II.19) over **k** is readily carried out:

$$g_\lambda = \sum_{\mu=-\infty}^{\infty} (-i)^\mu \left\langle \exp\left\{\frac{i}{N^{1/2}}\varrho_1\cos(2\pi\mathbf{h}\,.\,\mathbf{r}-\theta_1)+i\mu(\eta-\zeta)\right\} J_\mu\left(\frac{x_1}{N^{1/2}}\right) J_\mu\left(\frac{x_2}{N^{1/2}}\right) \times J_\mu\left(\frac{Z}{N^{1/2}}\right)\right\rangle_{\mathbf{h}}, \tag{II.20}$$

in which η, ζ, x_1, x_2 and Z all depend on **h**. It remains to carry out the final average over **h**.

In view of (II.9), (II.10) and (II.17), (I.6) implies

$$J_\mu\left(\frac{x_1}{N^{1/2}}\right) = \left\{\frac{\varrho_3+\varrho_{31}\exp[i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3-\theta_{31})]}{\varrho_3+\varrho_{31}\exp[-i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3-\theta_{31})]}\right\}^{1/2\mu} \times \sum_{\mu_1=-\infty}^{\infty}(-1)^{\mu_1}J_{\mu+\mu_1}\left(\frac{\varrho_3}{N^{1/2}}\right) \times J_{\mu_1}\left(\frac{\varrho_{31}}{N^{1/2}}\right)\exp[i\mu_1(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3-\theta_{31})], \tag{II.21}$$

$$J_\mu\left(\frac{x_2}{N^{1/2}}\right) = \left\{\frac{\varrho_4+\varrho_{23}\exp[i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_4+\theta_{23})]}{\varrho_4+\varrho_{23}\exp[-i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_4+\theta_{23})]}\right\}^{1/2\mu} \times \sum_{\mu_2=-\infty}^{\infty}(-1)^{\mu_2}J_{\mu+\mu_2}\left(\frac{\varrho_4}{N^{1/2}}\right) \times J_{\mu_2}\left(\frac{\varrho_{23}}{N^{1/2}}\right)\exp[i\mu_2(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_4+\theta_{23})], \tag{II.22}$$

$$J_\mu(Z) = \left\{\frac{\varrho_2+\varrho_{12}\exp[i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_2-\theta_{12})]}{\varrho_2+\varrho_{12}\exp[-i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_2-\theta_{12})]}\right\}^{1/2\mu} \times \sum_{\nu=-\infty}^{\infty}(-1)^{\nu}J_{\mu+\nu}\left(\frac{\varrho_2}{N^{1/2}}\right)J_\nu\left(\frac{\varrho_{12}}{N^{1/2}}\right) \times \exp[i\nu(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_2-\theta_{12})]. \tag{II.23}$$

Multiplying (II.8) by the complex conjugate of (II.18) and raising both sides to the μth power, it is readily verified that

$$\begin{aligned}\exp[i\mu(\eta-\zeta)] &= \exp[i\mu(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_2+\theta_3+\theta_4)]/(YZ)^\mu \\ &\times\{\varrho_3+\varrho_{31}\exp[-i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3-\theta_{31})]\}^\mu \\ &\times\{\varrho_4+\varrho_{23}\exp[-i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_4+\theta_{23})]\}^\mu \\ &\times\{\varrho_2+\varrho_{12}\exp[-i(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_2-\theta_{12})]\}^\mu.\end{aligned} \tag{II.24}$$

Substituting from (II.21)–(II.24) into (II.20), one finds

$$g_\lambda = \sum_{\mu,\mu_1,\mu_2,\nu=-\infty}^{\infty} (-i)^\mu \left\langle \frac{\exp\left\{\frac{i}{N^{1/2}}\varrho_1 \cos(2\pi\mathbf{h}\,.\,\mathbf{r}-\theta_1)+i\mu(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_2+\theta_3+\theta_4)\right\}}{(YZ)^\mu}\right.$$
$$\times\{\varrho_3^2+\varrho_{31}^2+2\varrho_3\varrho_{31}\cos(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3-\theta_{31})\}^{\mu/2}$$
$$\times\{\varrho_4^2+\varrho_{23}^2+2\varrho_4\varrho_{23}\cos(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_4+\theta_{23})\}^{\mu/2}$$
$$\times\{\varrho_2^2+\varrho_{12}^2+2\varrho_2\varrho_{12}\cos(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_2-\theta_{12})\}^{\mu/2}$$
$$\times\ (-1)^{\mu_1+\mu_2+\nu} J_{\mu+\mu_1}\left(\frac{\varrho_3}{N^{1/2}}\right) J_{\mu_1}\left(\frac{\varrho_{31}}{N^{1/2}}\right) J_{\mu+\mu_2}\left(\frac{\varrho_4}{N^{1/2}}\right) J_{\mu_2}\left(\frac{\varrho_{23}}{N^{1/2}}\right)$$
$$\times J_{\mu+\nu}\left(\frac{\varrho_2}{N^{1/2}}\right) J_\nu\left(\frac{\varrho_{12}}{N^{1/2}}\right)\exp\{2\pi i(\mu_1+\mu_2+\nu)\mathbf{h}\,.\,\mathbf{r}+i\mu_1(\theta_3-\theta_{31})+i\mu_2(\theta_4+\theta_{23})$$
$$\left.+i\nu(\theta_2-\theta_{12})\}\right\rangle_{\mathbf{h}}\,. \qquad \text{(II.25)}$$

However it is readily verified from (II.7) and (II.17) that

$$(YZ)^\mu=\{\varrho_3^2+\varrho_{31}^2+2\varrho_3\varrho_{31}\cos(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_3-\theta_{31})\}^{\mu/2}$$
$$\times\{\varrho_4^2+\varrho_{23}^2+2\varrho_4\varrho_{23}\cos(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_4+\theta_{23})\}^{\mu/2}$$
$$\times\{\varrho_2^2+\varrho_{12}^2+2\varrho_2\varrho_{12}\cos(2\pi\mathbf{h}\,.\,\mathbf{r}+\theta_2-\theta_{12})\}^{\mu/2}. \qquad \text{(II.26)}$$

Hence, substituting from (II.26) into (II.25),

$$g_\lambda=\sum_{\mu,\mu_1,\mu_2,\nu=-\infty}^{\infty}(-i)^\mu(-1)^{\mu_1+\mu_2+\nu}J_{\mu+\mu_1}\left(\frac{\varrho_3}{N^{1/2}}\right)$$
$$\times J_{\mu_1}\left(\frac{\varrho_{31}}{N^{1/2}}\right) J_{\mu+\mu_2}\left(\frac{\varrho_4}{N^{1/2}}\right) J_{\mu_2}\left(\frac{\varrho_{23}}{N^{1/2}}\right)$$
$$\times J_{\mu+\nu}\left(\frac{\varrho_2}{N^{1/2}}\right) J_\nu\left(\frac{\varrho_{12}}{N^{1/2}}\right)\left\langle\exp\left\{\frac{i}{N^{1/2}}\varrho_1\right.\right.$$
$$\times\cos(2\pi\mathbf{h}\,.\,\mathbf{r}-\theta_1)+i(\mu+\mu_1+\mu_2+\nu)$$
$$\left.\times(2\pi\mathbf{h}\,.\,\mathbf{r}-\theta_1)\right\}\exp\{i\mu(\theta_1+\theta_2+\theta_3+\theta_4)$$
$$+i\mu_1(\theta_1+\theta_3-\theta_{31})+i\mu_2(\theta_1+\theta_4+\theta_{23})$$
$$\left.+\ i\nu(\theta_1+\theta_2-\theta_{12})\}\right\rangle_{\mathbf{h}}\,. \qquad \text{(II.27)}$$

Replace μ_1 by ϱ, μ_2 by σ and employ (I.4) and (I.5) to evaluate the average over $\mathbf{h}$ in (II.27):

$$g_\lambda=\sum_{\mu,\nu,\varrho,\sigma=-\infty}^{\infty}(-i)^{\nu+\varrho+\sigma}J_{\mu+\nu+\varrho+\sigma}\left(\frac{\varrho_1}{N^{1/2}}\right)$$
$$\times J_{\mu+\nu}\left(\frac{\varrho_2}{N^{1/2}}\right) J_{\mu+\varrho}\left(\frac{\varrho_3}{N^{1/2}}\right) J_{\mu+\sigma}\left(\frac{\varrho_4}{N^{1/2}}\right)$$
$$\times J_\nu\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_\sigma\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_\varrho\left(\frac{\varrho_{31}}{N^{1/2}}\right)$$
$$\times\exp\{i\mu(\theta_1+\theta_2+\theta_3+\theta_4)+i\nu(\theta_1+\theta_2-\theta_{12})$$
$$+i\sigma(\theta_1+\theta_4+\theta_{23})+i\varrho(\theta_1+\theta_3-\theta_{31})\}\,, \qquad \text{(II.28)}$$

which is seen to be independent of λ. Finally, retaining terms up to and including terms of order $1/N^2$, it is readily verified that μ, ν, ϱ, σ take on the 27 sets of values shown in Table 1.

Table 1. *The* 27 *sets of values for* μ,ν,ϱ,σ *used in* (II.28) *to insure accuracy to order* $1/N^2$

μ	0	0	0	0	0	0	0	1	−1	1	−1	1	−1	1	−1
ν	0	0	0	0	0	1	−1	0	0	0	0	0	0	−1	1
ϱ	0	0	0	1	−1	0	0	0	0	0	0	−1	1	0	0
σ	0	1	−1	0	0	0	0	0	0	−1	1	0	0	0	0

μ	0	0	0	0	0	0	1	−1	1	−1	1	−1
ν	1	−1	1	−1	0	0	−1	1	−1	1	0	0
ϱ	−1	1	0	0	1	−1	−1	1	0	0	−1	1
σ	0	0	−1	1	−1	1	0	0	−1	1	−1	1

Hence g_λ finally becomes

$$
\begin{aligned}
g_\lambda \approx\; & J_0\left(\frac{\varrho_1}{N^{1/2}}\right) J_0\left(\frac{\varrho_2}{N^{1/2}}\right) J_0\left(\frac{\varrho_3}{N^{1/2}}\right) J_0\left(\frac{\varrho_4}{N^{1/2}}\right) J_0\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{31}}{N^{1/2}}\right) \\
& - 2iJ_1\left(\frac{\varrho_1}{N^{1/2}}\right) J_0\left(\frac{\varrho_2}{N^{1/2}}\right) J_0\left(\frac{\varrho_3}{N^{1/2}}\right) J_1\left(\frac{\varrho_4}{N^{1/2}}\right) J_0\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_1+\theta_4+\theta_{23}) \\
& - 2iJ_1\left(\frac{\varrho_1}{N^{1/2}}\right) J_0\left(\frac{\varrho_2}{N^{1/2}}\right) J_1\left(\frac{\varrho_3}{N^{1/2}}\right) J_0\left(\frac{\varrho_4}{N^{1/2}}\right) J_0\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_1+\theta_3-\theta_{31}) \\
& - 2iJ_1\left(\frac{\varrho_1}{N^{1/2}}\right) J_1\left(\frac{\varrho_2}{N^{1/2}}\right) J_0\left(\frac{\varrho_3}{N^{1/2}}\right) J_0\left(\frac{\varrho_4}{N^{1/2}}\right) J_1\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_1+\theta_2-\theta_{12}) \\
& - 2iJ_0\left(\frac{\varrho_1}{N^{1/2}}\right) J_1\left(\frac{\varrho_2}{N^{1/2}}\right) J_1\left(\frac{\varrho_3}{N^{1/2}}\right) J_0\left(\frac{\varrho_4}{N^{1/2}}\right) J_0\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_2+\theta_3-\theta_{23}) \\
& - 2iJ_0\left(\frac{\varrho_1}{N^{1/2}}\right) J_1\left(\frac{\varrho_2}{N^{1/2}}\right) J_0\left(\frac{\varrho_3}{N^{1/2}}\right) J_1\left(\frac{\varrho_4}{N^{1/2}}\right) J_0\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_2+\theta_4+\theta_{31}) \\
& - 2iJ_0\left(\frac{\varrho_1}{N^{1/2}}\right) J_0\left(\frac{\varrho_2}{N^{1/2}}\right) J_1\left(\frac{\varrho_3}{N^{1/2}}\right) J_1\left(\frac{\varrho_4}{N^{1/2}}\right) J_1\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_3+\theta_4+\theta_{12}) \\
& + 2J_1\left(\frac{\varrho_1}{N^{1/2}}\right) J_1\left(\frac{\varrho_2}{N^{1/2}}\right) J_1\left(\frac{\varrho_3}{N^{1/2}}\right) J_1\left(\frac{\varrho_4}{N^{1/2}}\right) J_0\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_1+\theta_2+\theta_3+\theta_4) \\
& + 2J_0\left(\frac{\varrho_1}{N^{1/2}}\right) J_1\left(\frac{\varrho_2}{N^{1/2}}\right) J_1\left(\frac{\varrho_3}{N^{1/2}}\right) J_0\left(\frac{\varrho_4}{N^{1/2}}\right) J_1\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_2-\theta_3+\theta_{31}-\theta_{12}) \\
& + 2J_0\left(\frac{\varrho_1}{N^{1/2}}\right) J_1\left(\frac{\varrho_2}{N^{1/2}}\right) J_0\left(\frac{\varrho_3}{N^{1/2}}\right) J_1\left(\frac{\varrho_4}{N^{1/2}}\right) J_1\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_2-\theta_4-\theta_{12}-\theta_{23}) \\
& + 2J_0\left(\frac{\varrho_1}{N^{1/2}}\right) J_0\left(\frac{\varrho_2}{N^{1/2}}\right) J_1\left(\frac{\varrho_3}{N^{1/2}}\right) J_1\left(\frac{\varrho_4}{N^{1/2}}\right) J_0\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_3-\theta_4-\theta_{23}-\theta_{31}) \\
& + 2J_1\left(\frac{\varrho_1}{N^{1/2}}\right) J_0\left(\frac{\varrho_2}{N^{1/2}}\right) J_0\left(\frac{\varrho_3}{N^{1/2}}\right) J_1\left(\frac{\varrho_4}{N^{1/2}}\right) J_1\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_1-\theta_4-\theta_{31}-\theta_{12}) \\
& + 2J_1\left(\frac{\varrho_1}{N^{1/2}}\right) J_0\left(\frac{\varrho_2}{N^{1/2}}\right) J_1\left(\frac{\varrho_3}{N^{1/2}}\right) J_0\left(\frac{\varrho_4}{N^{1/2}}\right) J_1\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_0\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_1-\theta_3-\theta_{12}+\theta_{23}) \\
& + 2J_1\left(\frac{\varrho_1}{N^{1/2}}\right) J_1\left(\frac{\varrho_2}{N^{1/2}}\right) J_0\left(\frac{\varrho_3}{N^{1/2}}\right) J_0\left(\frac{\varrho_4}{N^{1/2}}\right) J_0\left(\frac{\varrho_{12}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{23}}{N^{1/2}}\right) J_1\left(\frac{\varrho_{31}}{N^{1/2}}\right) \cos(\theta_1-\theta_2+\theta_{23}-\theta_{31}).
\end{aligned}
\tag{II.29}
$$

APPENDIX III

The derivation of $\prod_{\lambda=1}^{N} g_\lambda$

Employing (I.7), (II.29) becomes

$$
\begin{aligned}
g_\lambda = 1 & - \frac{1}{4N}(\varrho_1^2+\varrho_2^2+\varrho_3^2+\varrho_4^2+\varrho_{12}^2+\varrho_{23}^2+\varrho_{31}^2) \\
& - \frac{i}{4N^{3/2}}[\varrho_1\varrho_4\varrho_{23}\cos(\theta_1+\theta_4+\theta_{23}) \\
& + \text{five similar terms}] \\
& + \frac{1}{8N^2}[\varrho_1\varrho_2\varrho_3\varrho_4\cos(\theta_1+\theta_2+\theta_3+\theta_4) \\
& + \varrho_2\varrho_3\varrho_{31}\varrho_{12}\cos(\theta_2-\theta_3+\theta_{31}-\theta_{12}) \\
& + \text{five similar terms}] + \mathrm{O}\left(\frac{1}{N^2}\right),
\end{aligned}
\tag{III.1}
$$

where $\mathrm{O}(1/N^2)$ represents terms of order $1/N^2$ or higher in which the terms of order $1/N^2$ are independent of the θ's. Then

$$
\begin{aligned}
N\log g_\lambda = & -\tfrac{1}{4}(\varrho_1^2+\ldots) \\
& - \frac{i}{4N^{1/2}}[\varrho_1\varrho_4\varrho_{23}\cos(\theta_1+\theta_4+\theta_{23})+\ldots] \\
& + \frac{1}{8N}[\varrho_1\varrho_2\varrho_3\varrho_4\cos(\theta_1+\theta_2+\theta_3+\theta_4)+\ldots] \\
& + \mathrm{O}\left(\frac{1}{N}\right)
\end{aligned}
\tag{III.2}
$$

and

$$\prod_{\lambda=1}^{N} g_\lambda = g_\lambda^N = \exp(N \log g_\lambda)$$
$$= \exp\Big\{-\tfrac{1}{4}(\varrho_1^2+\varrho_2^2+\varrho_3^3+\varrho_4^2+\varrho_{12}^2+\varrho_{23}^2+\varrho_{31}^2)$$
$$-\frac{i}{4N^{1/2}}[\varrho_1\varrho_4\varrho_{23}\cos(\theta_1+\theta_4+\theta_{23})$$
$$+\varrho_1\varrho_3\varrho_{31}\cos(\theta_1+\theta_3-\theta_{31})$$
$$+\varrho_1\varrho_2\varrho_{12}\cos(\theta_1+\theta_2-\theta_{12})$$
$$+\varrho_2\varrho_3\varrho_{23}\cos(\theta_2+\theta_3-\theta_{23})$$
$$+\varrho_2\varrho_4\varrho_{31}\cos(\theta_2+\theta_4+\theta_{31})$$
$$+\varrho_3\varrho_4\varrho_{12}\cos(\theta_3+\theta_4+\theta_{12})]$$
$$+\frac{1}{8N}[\varrho_1\varrho_2\varrho_3\varrho_4\cos(\theta_1+\theta_2+\theta_3+\theta_4)$$
$$+\varrho_2\varrho_3\varrho_{31}\varrho_{12}\cos(\theta_2-\theta_3+\theta_{31}-\theta_{12})$$
$$+\varrho_2\varrho_4\varrho_{12}\varrho_{23}\cos(\theta_2-\theta_4-\theta_{12}-\theta_{23})$$
$$+\varrho_3\varrho_4\varrho_{23}\varrho_{31}\cos(\theta_3-\theta_4-\theta_{23}-\theta_{31})$$
$$+\varrho_1\varrho_4\varrho_{31}\varrho_{12}\cos(\theta_1-\theta_4-\theta_{31}-\theta_{12})$$
$$+\varrho_1\varrho_3\varrho_{12}\varrho_{23}\cos(\theta_1-\theta_3-\theta_{12}+\theta_{23})$$
$$+\varrho_1\varrho_2\varrho_{23}\varrho_{31}\cos(\theta_1-\theta_2+\theta_{23}-\theta_{31})]\Big\}$$
$$\times\left\{1+O\left(\frac{1}{N}\right)\right\} \qquad \text{(III.3)}$$

where $O(1/N)$ represents the terms of order $1/N$ or higher in which the terms of order $1/N$ are independent of the θ's.

APPENDIX IV

Evaluating the fourteenfold integral (2.3)

IV.1. *The θ_1 integration*

Substitute for $\prod_{\lambda=1}^{N} g_\lambda$ from (III.3) into (2.3) and combine the eight terms involving θ_1 in the exponent of the integrand as follows:

$$-i\varrho_1\Big\{R_1\cos(\theta_1-\Phi_1)$$
$$+\frac{1}{4N^{1/2}}[\varrho_4\varrho_{23}\cos(\theta_1+\theta_4+\theta_{23})$$
$$+\varrho_3\varrho_{31}\cos(\theta_1+\theta_3-\theta_{31})+\varrho_2\varrho_{12}\cos(\theta_1+\theta_2-\theta_{12})]$$
$$+\frac{i}{8N}[\varrho_2\varrho_3\varrho_4\cos(\theta_1+\theta_2+\theta_3+\theta_4)$$
$$+\varrho_4\varrho_{31}\varrho_{12}\cos(\theta_1-\theta_4-\theta_{31}-\theta_{12})$$
$$+\varrho_3\varrho_{12}\varrho_{23}\cos(\theta_1-\theta_3-\theta_{12}+\theta_{23})$$
$$+\varrho_2\varrho_{23}\varrho_{31}\cos(\theta_1-\theta_2+\theta_{23}-\theta_{31})]\Big\}$$
$$=-i\varrho_1X_1\cos(\theta_1+\xi_1), \qquad \text{(IV.1)}$$

where, in view of (I.1)–(I.3),

$$X_1=\Big\{R_1^2+\frac{R_1}{2N^{1/2}}[\varrho_4\varrho_{23}\cos(\Phi_1+\theta_4+\theta_{23})$$
$$+\varrho_3\varrho_{31}\cos(\Phi_1+\theta_3-\theta_{31})+\varrho_2\varrho_{12}\cos(\Phi_1+\theta_2-\theta_{12})]$$
$$+\frac{iR_1}{4N}[\varrho_2\varrho_3\varrho_4\cos(\Phi_1+\theta_2+\theta_3+\theta_4)$$
$$+\varrho_4\varrho_{31}\varrho_{12}\cos(\Phi_1-\theta_4-\theta_{31}-\theta_{12})$$
$$+\varrho_3\varrho_{12}\varrho_{23}\cos(\Phi_1-\theta_3-\theta_{12}+\theta_{23})$$
$$+\varrho_2\varrho_{23}\varrho_{31}\cos(\Phi_1-\theta_2+\theta_{23}-\theta_{31})]$$
$$+\frac{1}{8N}[\varrho_3\varrho_4\varrho_{23}\varrho_{31}\cos(\theta_3-\theta_4-\theta_{23}-\theta_{31})$$
$$+\varrho_2\varrho_4\varrho_{12}\varrho_{23}\cos(\theta_2-\theta_4-\theta_{12}-\theta_{23})$$
$$+\varrho_2\varrho_3\varrho_{31}\varrho_{12}\cos(\theta_2-\theta_3+\theta_{31}-\theta_{12})]$$
$$+O\left(\frac{1}{N}\right)\Big\}^{1/2} \qquad \text{(IV.2)}$$

$$X_1\exp(i\xi_1)=R_1\exp(-i\Phi_1)+\ldots \qquad \text{(IV.3)}$$

so that X_1 and ξ_1 are independent of ϱ_1 and θ_1 and $O(1/N)$ consists of all terms of order $1/N$ or higher in which the terms of order $1/N$ are independent of the θ's and the Φ's. Hence, in view of (I.4) and (IV.1), the integration of (2.3) with respect to θ_1 is readily carried out:

$$P=\frac{1}{(2\pi)^{13}}R_1R_2R_3R_4R_{12}R_{23}R_{31}$$
$$\times\int_{\varrho_1,\ldots,\varrho_{31}=0}^{\infty}\int_{\theta_2,\ldots,\theta_{31}=0}^{2\pi}\varrho_1\varrho_2\varrho_3\varrho_4\varrho_{12}\varrho_{23}\varrho_{31}$$
$$\times\exp\Big\{-\tfrac{1}{4}(\varrho_1^2+\varrho_2^2+\varrho_3^2+\varrho_4^2+\varrho_{12}^2+\varrho_{23}^2+\varrho_{31}^2)$$
$$-i[R_2\varrho_2\cos(\theta_2-\Phi_2)+R_3\varrho_3\cos(\theta_3-\Phi_3)$$
$$+R_4\varrho_4\cos(\theta_4-\Phi_4)+R_{12}\varrho_{12}\cos(\theta_{12}-\Phi_{12})$$
$$+R_{23}\varrho_{23}\cos(\theta_{23}-\Phi_{23})+R_{31}\varrho_{31}\cos(\theta_{31}-\Phi_{31})]$$
$$-\frac{i}{4N^{1/2}}[\varrho_2\varrho_3\varrho_{23}\cos(\theta_2+\theta_3-\theta_{23})$$
$$\times\varrho_2\varrho_4\varrho_{31}\cos(\theta_2+\theta_4+\theta_{31})$$
$$+\varrho_3\varrho_4\varrho_{12}\cos(\theta_3+\theta_4+\theta_{12})]$$
$$+\frac{1}{8N}[\varrho_2\varrho_3\varrho_{31}\varrho_{12}\cos(\theta_2-\theta_3+\theta_{31}-\theta_{12})$$
$$+\varrho_2\varrho_4\varrho_{12}\varrho_{23}\cos(\theta_2-\theta_4-\theta_{12}-\theta_{23})$$
$$+\varrho_3\varrho_4\varrho_{23}\varrho_{31}\cos(\theta_3-\theta_4-\theta_{23}-\theta_{31})]\Big\}J_0(\varrho_1X_1)$$
$$\times\left\{1+O\left(\frac{1}{N}\right)\right\}d\varrho_1\ldots d\varrho_{31}d\theta_2\ldots d\theta_{31} \qquad \text{(IV.4)}$$

where $O(1/N)$ consists of all terms of order $1/N$ or higher in which the terms of order $1/N$ are independent of the θ's and the Φ's.

IV.2. *The* ϱ_1 *integration*

Since X_1 is independent of ϱ_1, one employs (I.8) with $p=\frac{1}{4}$, $a=X_1$, using (IV.2), to carry out the ϱ_1 integration:

$$\begin{aligned} P = & \frac{1}{2^{12}\pi^{13}} R_1R_2R_3R_4R_{12}R_{23}R_{31} \exp(-R_1^2) \\ & \times \int_{\varrho_2,\ldots,\varrho_{31}=0}^{\infty} \int_{\theta_2,\ldots,\theta_{31}=0}^{2\pi} \varrho_2\varrho_3\varrho_4\varrho_{12}\varrho_{23}\varrho_{31} \\ & \times \exp\Big\{-\tfrac{1}{4}(\varrho_2^2+\varrho_3^2+\varrho_4^2+\varrho_{12}^2+\varrho_{23}^2+\varrho_{31}^2) \\ & -i[R_2\varrho_2\cos(\theta_2-\Phi_2)+R_3\varrho_3\cos(\theta_3-\Phi_3) \\ & +R_4\varrho_4\cos(\theta_4-\Phi_4)+R_{12}\varrho_{12}\cos(\theta_{12}-\Phi_{12}) \\ & +R_{23}\varrho_{23}\cos(\theta_{23}-\Phi_{23})+R_{31}\varrho_{31}\cos(\theta_{31}-\Phi_{31})] \\ & -\frac{i}{4N^{1/2}}[\varrho_2\varrho_3\varrho_{23}\cos(\theta_2+\theta_3-\theta_{23}) \\ & +\varrho_2\varrho_4\varrho_{31}\cos(\theta_2+\theta_4+\theta_{31}) \\ & +\varrho_3\varrho_4\varrho_{12}\cos(\theta_3+\theta_4+\theta_{12})] \\ & -\frac{R_1}{2N^{1/2}}[\varrho_4\varrho_{23}\cos(\Phi_1+\theta_4+\theta_{23}) \\ & +\varrho_3\varrho_{31}\cos(\Phi_1+\theta_3-\theta_{31})+\varrho_2\varrho_{12}\cos(\Phi_1+\theta_2-\theta_{12})] \\ & -\frac{iR_1}{4N}[\varrho_2\varrho_3\varrho_4\cos(\Phi_1+\theta_2+\theta_3+\theta_4) \\ & +\varrho_4\varrho_{31}\varrho_{12}\cos(\Phi_1-\theta_4-\theta_{31}-\theta_{12}) \\ & +\varrho_3\varrho_{12}\varrho_{23}\cos(\Phi_1-\theta_3-\theta_{12}+\theta_{23}) \\ & +\varrho_2\varrho_{23}\varrho_{31}\cos(\Phi_1-\theta_2+\theta_{23}-\theta_{31})]\Big\} \\ & \times\left\{1+O\left(\frac{1}{N}\right)\right\} d\varrho_2 d\varrho_3 d\varrho_4 d\varrho_{12} d\varrho_{23} d\varrho_{31} \\ & \times d\theta_2 d\theta_3 d\theta_4 d\theta_{12} d\theta_{23} d\theta_{31}, \end{aligned} \quad \text{(IV.5)}$$

where again $O(1/N)$ consists of those terms of order $1/N$ or higher in which the terms of order $1/N$ are independent of the θ's and the Φ's.

IV.3. *The remaining* 12 *integrations*

One continues in this way, carrying out the successive integrations $\theta_2, \varrho_2, \theta_3, \varrho_3$, *etc.*, until finally (2.5) is obtained.

APPENDIX V

The question of convergence

It would be desirable to obtain an upper bound for $O(1/N)$, the terms of order $1/N$ or higher, in (2.5). However the rigorous derivation of a sharp upper bound appears to require a subtle analysis and lengthy calculation which is hardly justified here. Instead only a brief argument is given which makes plausible the several approximations used.

For fixed μ it is known that, as z approaches infinity,

$$J_\mu(z) \approx \left(\frac{2}{\pi z}\right)^{1/2} \cos(z-\tfrac{1}{2}\pi\mu-\tfrac{1}{4}\pi) \to 0, \quad \text{(V.1)}$$

(Watson, 1958, p. 195). If, on the other hand, z is fixed and μ approaches infinity, then

$$J_\mu(z) \approx \frac{\mu^{-\mu}e^{\mu}(\frac{1}{2}z)^{\mu}}{\sqrt{2\pi\mu}} \approx \frac{(\frac{1}{2}z)^{\mu}}{\mu!} \to 0, \quad \text{(V.2)}$$

(Watson, 1958, p. 225). Hence (II.28) implies that g_λ tends toward zero as any one of $\varrho_1/N^{1/2}$, $\varrho_2/N^{1/2}$, ..., $\varrho_{31}/N^{1/2}$ approaches infinity. In view of the factor $\prod_{\lambda=1}^{N} g_\lambda$ in the integrand of (2.3) it follows that, for large N, the integrand makes a substantial contribution to the value of the integral only when the ϱ's are in the neighborhood of zero (but are not necessarily small). More precisely, one makes an arbitrarily small error in (2.3) if the infinite limits of the ϱ integrations are replaced by sufficiently large but finite positive numbers, provided also that N is chosen sufficiently large. Hence the expansions (II.29), (III.1)–(III.3) are justified and the error term $O(1/N)$ in (2.5) may be made as small as desired provided that N is sufficiently large.

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