Joint probability distribution of the invariants comprising
determinantal inequalities: Heuristic derivation

(crystal structure/phase determination/phase refinement/conditional probability)

JEROME KARLE

Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, D.C. 20375

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ABSTRACT

Joint probability distributions are derived that are expressed in terms of the determinants that form the
determinantal inequalities associated with the non-negative Fourier series that represent crystal structures. The derivation
involves heuristic considerations. It is therefore appropriate to test the distributions extensively by making comparisons with
results obtained by other theoretical means and evaluations of the implications of the distributions. Those performed thus far
on the low-order determinants (third and fourth orders) have provided satisfactory results. The determinantal probability
distributions imply a general maximum determinant rule, contain a wealth of information, and provide numerous paths
that may be followed for future development.

There are several reasons for developing probability distributions associated with the determinantal inequalities (1, 2), the
relations among the crystal structure factors that arise from the fact that the electron density in a crystal is a non-negative
function. For example, applications of higher order determinants to the determination of the phases of the structure factors
could be considerably facilitated by appropriate probability distributions. As has been often noted (2-4), the main formula
for phase determination that provides the basis for the direct method of phase determination derives from the third-order
determinantal inequality (1) and its probabilistic implications (2). It is therefore reasonable to consider the possibility of using
fourth and higher order determinants in phase determination. Procedures based on such determinants would involve the use
of accompanying joint probability distributions.

In another type of application, investigations have been performed to develop techniques for phase refinement and extension, particularly for crystals of macromolecules (5-8). The applications made so far are based on special properties of the
high-order determinants and require, for their probabilistic support, special probability functions—namely, conditional probability functions (2, 9) in which the values of a large number of the structure factors are known, at least approximately. It is readily conceivable that the availability of more
general joint probability distributions could facilitate progress in phase refinement and extension.

Conditional joint probability distributions for determinants of any order, with structure factors as elements, have been
derived by Tsoucaris (9). These give the joint probability distribution of the elements in the last row of a determinant, subject to knowledge of the values of all the elements in the determinant except those in the last row and column. Here I shall derive joint probability distributions of the elements of the determinants which resemble closely the distributions of Tsoucaris (9) but for which there are no conditions on any elements—i.e., no requirements that the values of any of the elements be known. When the same conditions as those of Tsoucaris are applied to the general distributions, the results are quite
similar, affording evidence for the validity of the new distributions. The difference concerns a factor that enhances the
probabilities and depends, in part, upon how great the magnitudes of appropriate structure factors are.

The general joint probability distributions to be presented here have a number of features:

1. Determinantal joint distributions are readily composed.
2. Special cases of the joint distributions can be derived from the determinantal distributions. The manipulations involved
in achieving this concern rules of formation that generate determinantal distributions having closely related elements,
rules of combination that facilitate the combining of the latter distributions, adjustments that account for the presence of heavy
atoms, and mathematical operations that can eliminate phases or magnitudes (or both) to specialize the resulting probability
distributions.
3. The determinants have a general validity for all 230 space groups. Space group equivalents and their relationships can be
readily introduced directly into the determinants. In addition, a formalism for taking space group symmetry into consideration
has been developed by Goedkoop (10).
4. The determinants facilitate the identification of the closely related structure factors—i.e., those structure factors that form
the most strongly interrelated joint probability distributions.
5. The joint probability distributions imply a general maximum determinant rule that has potential for practical application.
The rule is that the most probable set of values of the variates in a determinant composed of structure factors is the one that makes the value of the determinant a maximum. The maximum determinant rule derived by Tsoucaris (9) for the conditional probability distributions is a special case of the
general rule.
6. The determinantal distributions are in the desirable exponential form in contrast to the series form that generally has
convergence difficulties.
7. The determinantal form affords a very compact representation of the probabilistic information.

One step in the derivation of the joint distributions is heuristic. Evaluations of the validity of these distributions can be
obtained from comparisons with probability distributions known in special cases from derivations involving the more
rigorous application of the techniques of probability theory, from calculations of statistical properties that are subject to
numerical tests, and from general applications of the new theory in procedures designed to facilitate phase determination.

JOINT PROBABILITY DISTRIBUTION

In an earlier paper (2), high-order determinantal inequalities
were used to obtain a generalization of the tangent formula (11)
for phase determination. Accompanying probability measures associated with the determination of the value of a phase angle were derived by making use of expected values and estimates of the variance, obtainable from the determinantal inequalities, as required for application of the central limit theorem (12).

By combining probability distributions for the individual elements derived in this fashion, the joint probability distribution of the elements comprising a determinantal inequality is obtained. The details will now be described.

The quasi-normalized structure factor is defined,

\[ \mathcal{E}_h = \left( \sum_{j=1}^{N} f_j \right)^{-1/2} \sum_{j=1}^{N} f_j \exp(2\pi i h \cdot r_j) \]  

or

\[ \mathcal{E}_h \sim \sigma_0^{-1/2} \sum_{j=1}^{N} Z_j \exp(2\pi i h \cdot r_j) \]

in which

\[ \sigma_0 = \sum_{j=1}^{N} Z_j. \]

The quantity \( f_j \) is the atomic scattering factor for the \( j \)th atom in a unit cell containing \( N \) atoms, \( Z_j \) is its atomic number, and the components of \( h \) are the Miller indices for a particular reflection intensity.

A typical determinantal inequality representing the infinite set appropriate to point atoms may be written in the form (1)

\[
D_m,p = \begin{vmatrix}
0 & \mathcal{E}_{-k_1} & \mathcal{E}_{-k_2} & \ldots & \mathcal{E}_{-k_{m-1}} \\
\mathcal{E}_{k_1} & 0 & \mathcal{E}_{k_2} & \ldots & \mathcal{E}_{k_{m-1}} \\
\mathcal{E}_{k_{m-2}} & \mathcal{E}_{k_{m-2}-k_1} & 0 & \ldots & \mathcal{E}_{k_{m-1}-k_{m-2}} \\
\mathcal{E}_{k_{m-1}} & \mathcal{E}_{k_{m-1}-k_{m-2}} & \ldots & \ldots & 0 \\
\end{vmatrix} \geq 0 \quad [4]
\]

\((\text{rank } N)\)

The determinant \( D_{m,p} \) of order \( m \) is formed by composing the first column with \( \mathcal{E}_0 \) as the first element followed by \( m - 1 \) selected structure factors. Note that \( \mathcal{E}_0 = \mathcal{E}_{000} \) or \( \mathcal{E}_h \) with \( h = (0,0,0) \). Here \( D_{m,p} \) differs slightly from \( D_{m,p}(h) \), defined in an earlier paper (2), in that the vector \( k_{m-1} \) replaces \( h \). The subscript \( p \) labels a particular set of \( m - 1 \) vectors \( k_1, \ldots, k_{m-1} \) such that \( D_{m,p} = D_{m,k_1, \ldots, k_{m-1}} \). Once the first column is specified, the remainder of the determinant is readily constructed by first forming the first row with the complex conjugates of the elements in the first column in the same sequence. Each element in the body of the determinant is a structure factor whose subscript is the sum of the subscripts of the elements in the first row and first column corresponding to the row and column of the element of interest.

Any off-diagonal element in inequality 4 can be bounded by use of the determinantal inequality. If we are concerned with a noncentrosymmetric reflection, the element is bounded by a circle in the complex plane. The center and radius of the circle can be defined in terms of determinants derivable from \( D_{m,p} \).

This type of bound has been exhibited (1, 2) for the case in which the element of interest is the lowest one of the first column of \( D_{m,p} \). The result is quite general, however, because any element in the determinant can be placed in this position, with the form of the determinant preserved, by appropriate interchanges of rows and interchanges of columns. It is convenient here to define the bound without changing the position of occurrence of the element of interest. This is accomplished by use of the following definitions with respect to the arbitrary element \( \mathcal{E}_{k_0} \):

\[ \Delta_{m,p} \] is formed from \( D_{m,p} \) by omitting the row and column that contain \( \mathcal{E}_{-k_0} \), replacing the element \( \mathcal{E}_{k_0} \) by zero, and multiplying by \((-1)^{r+s}\) where \( r \) is the row and \( s \) is the column in which \( \mathcal{E}_{k_0} \) occurs. In the notation of inequality 4, \( k_0 = k_{r-1} - k_{s-1} \), where \( k_0 = (0,0,0) \).

\[ \Delta_{m,p} \] is formed from \( D_{m,p} \) by omitting the rows and columns in which \( \mathcal{E}_{k_0} \) and \( \mathcal{E}_{-k_0} \) occur.

\[ \Delta_{1,m,p} \] is formed from \( D_{m,p} \) by omitting the row in which \( \mathcal{E}_{k_0} \) occurs and the column in which \( \mathcal{E}_{-k_0} \) occurs.

\[ \Delta_{2,m,p} \] is formed from \( D_{m,p} \) by omitting the column in which \( \mathcal{E}_{-k_0} \) occurs and the row in which \( \mathcal{E}_{k_0} \) occurs.

\( d \) is derived from \( D_{m,p} \) by omitting the row and column that contain \( \mathcal{E}_{-k_0} \).

\( d^* \) is derived from \( D_{m,p} \) by omitting the row and column that contain \( \mathcal{E}_{k_0} \). This determinant is the complex conjugate of \( d \).

With the aid of the above definitions for the various types of determinants, the bound for \( \mathcal{E}_{k_0} \) is

\[ |\mathcal{E}_{k_0} - \delta_{m,p}| \leq r_{m,p} \]

in which \( r_{m,p} \) is the radius of the bounding circle in the complex plane centered about \( \delta_{m,p} \).

\[ \delta_{m,p} = \Delta_{m,p}/\Delta_{m,p} \]

and

\[ r_{m,p} = \Delta_{1/2,1,m,p} \Delta_{1/2,2,m,p} / \Delta_{m,p} \]

By use of the central limit theorem, it is possible to obtain the joint probability distribution of the real and imaginary parts of \( \mathcal{E}_{k_0} \) or, alternatively, the magnitude and phase of \( \mathcal{E}_{k_0} \). For the complex variate, \( \mathcal{E} \), the central limit theorem may be written

\[ P(\mathcal{E}) = P(|\mathcal{E}|, \phi) \exp[-|\mathcal{E}|^2/2\sigma^2] \]

in which \( \mathcal{E} \) represents the expected value of \( \mathcal{E} \) and \( \sigma^2 \) is the associated variance. As has been noted previously (2), the expected value of \( \mathcal{E}_{k_0} \) is

\[ \mathcal{E}_{k_0} = \delta_{m,p} \]

and the standard deviation may be defined in terms of \( r_{m,p} \),

\[ \sigma = |\mathcal{E}_{k_0}| r_{m,p} \]

in which \( \epsilon = 1 \) for centrosymmetric reflections and \( \epsilon = 2^{-1/2} \) for noncentrosymmetric ones.

From (8), (9), and (10), it follows for a noncentrosymmetric reflection that

\[ P(|\mathcal{E}_{k_0}|, \phi_{k_0}) \propto \exp \left[ -\frac{|\mathcal{E}_{k_0} \Delta_{m,p} - \Delta_{m,p}'|^2}{\mathcal{E}_{k_0}^2 \Delta_{1,m,p} \Delta_{2,m,p}} \right] \]

\[ \Delta_{1,m,p} \Delta_{2,m,p} = 1 - dd^*/\Delta_{1,m,p} \Delta_{2,m,p} \]

By equation 20 of ref. 1 (on determinantal inequalities),

\[ \Delta_{1,m,p} \Delta_{2,m,p} = 1 - dd^*/\Delta_{1,m,p} \Delta_{2,m,p} \]

We therefore obtain

\[ P(|\mathcal{E}_{k_0}|, \phi_{k_0}) \propto \exp \left[ \frac{D_{m,p} \Delta_{m,p}}{\mathcal{E}_{k_0}^2 \Delta_{1,m,p} \Delta_{2,m,p}} \right] \]

It is of interest that the determinant \( D_{m,p} \) plays a key role in this probability expression. It is the only factor in the exponential expression that contains the element \( \mathcal{E}_{k_0} \).

We now have the problem of combining the probability distributions for the \( \mathcal{E}_{k_0} \), given by expression 14 to form a joint probability distribution for all the elements in the determinant. Clearly, the individual distributions are not independent and a simple multiplication of them could not be expected to be correct. On the other hand, \( D_{m,p} \) contains all the variates in an
appealingly symmetric fashion, and it appears in each individual probability distribution multiplied by an appropriate ratio of $\Delta_{m,p,q}/\Delta_{1,m,p,q}\Delta_{2,m,p,q}$. The subscript $q$ is now added to the labeling of the determinants to emphasize that the determinants involved will vary as the element in question changes with $q$. $D_{m,p}$ does not change.

The heuristic conjecture is now made that, for the probability distributions given by expression 14 for the various elements in $D_{m,p}$, the effect of multiplying the individual distributions is to achieve the proper form for the joint distribution of the variates but also to exaggerate the probability measures. The acceptance of this conjecture would permit the joint distribution to be obtained by multiplication of the individual distributions, with appropriate scaling included to adjust the probability measures. This path will be followed here.

The proposed joint probability distribution $P_{\epsilon}$ of all the variates in $D_{m,p}$ is then,

$$P_{\epsilon}(\mathcal{E}_{k_1}, \ldots, \mathcal{E}_{k_n}, \varphi_{k_1}, \ldots, \varphi_{k_n}) = \exp \left[ \frac{\Delta_{m,p,q}}{\Delta_{1,m,p,q}\Delta_{2,m,p,q}} \right] \ , \ [15]$$

in which the subscript $\epsilon$ refers to noncentrosymmetric structure factors, $n = m(m-1)/2$, $1 \leq q \leq m(m-1)/2$, and the scaling adjustment is effected by replacing the sum of terms involving the ratio of determinants of the type $\Delta_{1}/\Delta_{2}$ by the average value of such terms, where it is understood that this average term is computed for those values of the variates that make $D_{m,p}$ a maximum. If this is not feasible because of limited information, various approximations may be considered such as the use of individual expected values for the phase invariants. The $\mathcal{E}_{k_j}$ are generally known from experiment. Phase values may also be available from various sources. Such information is immediately usable in expression 15 to effect the realization of conditional probability distributions.

**Independent Triplet Invariants.** The main feature of expression 15 is the determinant $D_{m,p}$. The factor formed by the average term is a fixed number computed from a particular set of values for the variates. If the determinants are written out, they are found to be expressible in terms of polynomials of structure factor magnitudes and sums of cosine functions of phase invariants that have structure factor magnitudes as coefficients. The phase invariants are linear combinations of phases whose subscripts sum to zero. The concept of invariant in this case derives from the fact that the values of the linear combinations of phases are independent of the choice of origin in a crystal. The values of the magnitudes of the structure factors are also invariant in this respect. It is apparent therefore that the determinants $D_{m,p}$ are also invariants, being composed of linear combinations of invariants.

The structure factor magnitudes $|\mathcal{E}|$ are generally known from experiment. We assume this to be the case and direct our attention to the phase invariants. Starting with third-order determinants ($m = 3$), the $D_{m,p}$ contain phase invariants composed of three phases (triplets), four phases (quartets), five phase (quintets), and so forth up to $m$ phases. All the phase invariants are expressible in terms of the values of an independent set of $(m-1)(m-2)/2$ triplets. These are formed by adding a phase from an element in the first column, a phase from an element in the first row, and a phase from a subset which subscript cancels the other two. Formally, we have for $D_{m,p}$

$$\tau_{ij} = \phi_{k_i} + \phi_{k_j} + \phi_{k_{i+j}}(1 \leq i \leq m - 2; \ i < j \leq m - 1) \ . \ [16]$$

It is easy to show that the $(m - 1)(m - 2)/2$ triplets are independent and that all the phase invariants occurring in the expression of $D_{m,p}$ can be defined in terms of these triplets. In view of this and the fact that we expect the magnitudes $|\mathcal{E}|$ to be known from experiment, we can now reinterpret the probability expression 15 as

$$P_{\epsilon}(\tau_{1,1}, \tau_{1,2}, \ldots, \tau_{m-2,m-1}; |\mathcal{E}_{k_1}|, \ldots, |\mathcal{E}_{k_n}|) = N_{\epsilon} \exp \left[ \frac{\Delta_{m,p,q}}{\Delta_{1,m,p,q}\Delta_{2,m,p,q}} \right] \ . \ [17]$$

in which $P_{\epsilon}$ is the joint probability distribution of the independent triplets, conditioned by the fact that the magnitudes of the structure factors are known, and $N_{\epsilon}$ is a normalizing constant.

For centrosymmetric crystals, the phases of the structure factors can assume only two values, 0 or $\pi$, for an appropriately chosen origin in the crystal and, in this case, the variates are the structure factors $\mathcal{E}$. The latter assume a positive or negative value depending upon whether the associated phase is 0 or $\pi$, respectively. In the context of the interpretation of expression 5, a centrosymmetric reflection is bounded within a line segment on the real axis whose center is $\delta_{m,p}$ and radius is $r_{m,p}$. In carrying out a derivation leading to a joint distribution comparable to expression 15, it is noted that $\epsilon = 1$ in Eq. 10 giving

$$P_{\epsilon}(\mathcal{E}_{k_1}, \mathcal{E}_{k_2}, \ldots, \mathcal{E}_{k_n}) = N_{\epsilon} \exp \left[ \frac{1}{2} \frac{\Delta_{m,p,q}}{\Delta_{1,m,p,q}\Delta_{2,m,p,q}} \right] \ . \ [18]$$

in which the subscript $\epsilon$ refers to real (centrosymmetric) structure factors, $N_{\epsilon}$ is a normalizing constant, $n = m(m-1)/2$, and $1 \leq q \leq m(m-1)/2$. The factor averaged over $q$ is evaluated with those values of the variates that make $D_{m,p}$ a maximum.

On expanding $D_{m,p}$ for the centrosymmetric case, it is found to be a linear combination of invariants consisting of products of the $\mathcal{E}_k$. Similarly to the noncentrosymmetric case, there is an independent set of $(m - 1)(m - 2)/2$ triplets in $D_{m,p}$ of the type $\mathcal{E}_k\mathcal{E}_{-k}\mathcal{E}_{-k+k}$. In terms of whose signs the signs of other triple products and higher order products can be expressed. Evidently, the sign to be associated with even powers of any $\mathcal{E}_k$ is plus. Given the values of the structure factor magnitudes from expression, expression 18 can be regarded as the joint discontinuous distribution of the signs of the independent triplet products. If we define

$$S_{ij} = \text{sign} \mathcal{E}_{k_i}\mathcal{E}_{-k_i}\mathcal{E}_{-k_i+k_i} \ . \ [19]$$

we may write for expression 18

$$P_{s}(S_{1,2},S_{1,3}, \ldots, S_{(m-2),(m-1)}; |\mathcal{E}_{k_1}|, \ldots, |\mathcal{E}_{k_n}|) = N_{s} \exp \left[ \frac{1}{2} \frac{\Delta_{m,p,q}}{\Delta_{1,m,p,q}\Delta_{2,m,p,q}} \right] \ . \ [20]$$

in which the subscript $s$ implies a joint discontinuous distribution for signs of invariants, $n = m(m-1)/2$, and $1 \leq q \leq m(m-1)/2$. The factor averaged over $q$ is evaluated with those values of the variates that make $D_{m,p}$ a maximum.

Many noncentrosymmetric space groups may have structure factors that are complex and others that may be real or pure imaginary. Those that are real or pure imaginary are associated with joint distributions such as expression 18, which is distinguished from the joint distribution 18 by the presence of the factor of $\frac{1}{2}$ in the exponent. The question arises concerning how joint distributions are to be written when complex, real and/or pure imaginary structure factors occur in $D_{m,p}$. A suggested rule is as follows: Expand the determinant. An invariant composed of only complex structure factors would be left as is, an

*Note: The reference to "Proc. Natl. Acad. Sci. USA 75 (1978) 2547" and "Applied Mathematical and Physical Sciences: Karle" is not relevant to the content of the text and is not included in the natural text representation.*
invariant composed of only real and/or pure imaginary structure factors would be divided by 2, and all others would be divided by a number between 1 and 2 depending on the proportion of each type of structure factor comprising the invariant. Such a rule would generally interfere with use of the determinants in their compact form, a matter that could be of considerable importance in the higher orders. On balance then, it might be best in some applications to select an overall factor and retain the determinantal form.

Unequal Atoms. As has already been noted by Tsoucaris (9), the determinantal form for the probability distribution applies only to structures that do not have atoms with rather disparate atomic numbers. The presence of hydrogen atoms can ordinarily be excepted in this context. The determinantal form is not a suitable form for the probability distributions for structures with atoms having disparate atomic numbers because of the nature of the coefficients that are appropriate for the invariants comprising the expanded determinant. It is possible to adjust the coefficients of an expanded determinant to make the probability distribution more appropriate for structures with unequal atoms.

If we consider the joint distribution 15, for example, we can factor \( \mathbf{\tilde{e}}^{-2} \) from the average term and write this average term in terms of unitary structure factors, \( U_{\mathbf{a}} = e_{\mathbf{a}}/\mathbf{e} \). On expanding the determinant \( D_{m,p} \), there will arise powers of \( e_{\mathbf{a}} \) in the denominators of the coefficients of the invariants. \( \mathbf{e}^{-1} \) appears in the coefficient of the cosine of a triplet invariant, \( \mathbf{e}^{-2} \) appears in the coefficient of the cosine of a quartet invariant, and so forth. For a more accurate representation of the joint distribution when unequal atoms are present in a structure, the negative powers of \( \mathbf{e} \) are replaced by appropriate polynomials in the \( Q_n \), in which

\[ Q_n = \sigma_n/\sigma^2, \quad (n = 3, 4, 5, \ldots) \tag{21} \]

From knowledge acquired from the application of the method of characteristic functions to obtain joint probability distributions and insight derived from the reduction of complex distributions to simpler ones by integration over the variables, the desired polynomials in the \( Q_n \) can be readily obtained in many instances. In the limiting case of all atoms equal, \( \mathbf{e}^{-(n-2)/2} = Q_n = N^{-(n-2)/2} \).

Maximum Determinant Rule. It is immediately apparent that given the joint distributions 15 and 18, for example, the most probable configuration of the variates is that which makes \( D_{m,p} \) a maximum. On the assumption of the validity of these distributions we would have a general maximum determinant rule. With knowledge of the structure factor magnitudes from experiment, the rule would state that the most probable set of values for the phases in \( D_{m,p} \) is that which makes \( D_{m,p} \) a maximum.

CONCLUDING REMARKS

It is possible to construct determinants \( D_{m,p} \) in which the elements are not all distinct. Redundancy in the elements leads to redundancy in the invariants that are formed on expansion. The latter have the wrong coefficients for the formation of accurate probability distributions and should be avoided.

A set of operations has been found that produces a sequence of determinants that contain a minimal number of changes in the elements from one determinant to the other. A matter of interest is how probability information from sequences of determinants is to be combined. Useful criteria for effecting this have been developed. They are based on the requirement that the resulting distribution, with appropriate manipulations, must reproduce the original ones from which it was composed as well as other requirements regarding the form and character of the terms in the distributions.

Several calculations and comparisons with joint distributions obtained in other ways have shown that the joint distributions derived here. Test calculations, for example, have been performed on the statistical properties of large numbers of triplet invariants as given by the probability distributions obtained from third order determinants. Among the many aspects of the probability distributions that such calculations test is the factor \( (\Delta_{m,p,q}/\Delta_{m,p,q}^2)_{2,2,m,p,q} \) in [15]. The experimental distribution of the expected value of \( \cos(\phi_1 + \phi_{-k} + \phi_{-h+k}) \) as a function of \( 2(\sigma^2/\sigma^2) \mathbf{e}^{-2} \mathbf{e}^{-k} \mathbf{e}^{-h+k} \) was reproduced by the theory to within 1% with an average error of about 0.5% for an equal-atom test case and for one that contained a heavy atom.

Distributions for quartets have been obtained from fourth-order determinants that agree well with those obtained by Hauptman (equation 2.5 in ref. 15) by means of other techniques in probability theory. It is also possible, by examination of probability distributions obtained from fourth-order determinants, to select triplet invariants that have a greater reliability of having a value close to zero than can be ascertained from probability distributions obtained from third-order determinants. Such invariants can be especially useful in procedures for phase determination.

After this manuscript was completed, it was learned, at the International School of Crystallography (Erci, Trapani, Italy, Mar. 28 to Apr. 9, 1978) that successful numerical tests of the general maximum determinant rule have been carried out by M. M. Woolfson and P. Main of the University of York in accordance with the plan described by Woolfson (14) to test its validity and utility for evaluating the symbolic definitions of phases used with "magic integers." It was also learned from H. Krabbe-Kamdem and J. J. L. Heinerman, H. Krabbenend and J. Kron of the University of Utrecht have obtained a rigorous proof of the validity of the determinantal probability distributions up to and including \( N^{-1} \) terms (i.e., the quartet terms). One of their results is the proof of the maximum determinant rule up to and including that order.