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# The determinants of some multilevel Vandermonde and Toeplitz matrices 

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#### Abstract

The closed algebraic expressions of the determinants of some multivariate (multilevel) Vandermonde matrices and the associated Toeplitz/KarleHauptman matrices are worked out. The formula can usefully be applied to evaluate the determinant of the Karle-Hauptman matrix generated by a principal basic set of reflections, the knowledge of which determines the full diffraction pattern of an ideal crystal.


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## 1. Introduction

The explicit expression of the Vandermonde determinant has long been known. Recently, there has been interest in evaluating different generalizations of the Vandermonde determinant, including the multivariate (multilevel) case [1, 2], since these matrices and their determinants are useful in many fields, such as crystallography [3-10] or signal theory [2,11,12]. The reason why these fields are interested in Vandermonde matrices depends on the fact that the relevant basic problem can be formulated in the one-dimensional (1D) case as follows: to determine the quantities $v_{j} \mathrm{~s}$ and $x_{j} \mathrm{~s}$ (with $0 \leqslant x_{j}<1$ ) defining the distribution $\rho(x) \equiv \sum_{j=1}^{N} v_{j} \delta\left(x-x_{j}\right)$, knowing the latter's Fourier transform $F_{h}=\sum_{j=1}^{N} v_{j} \xi_{j}{ }^{h}$ (with $\xi_{j} \equiv \mathrm{e}^{\mathrm{i} 2 \pi x_{j}}$ ) at an appropriate set of integers $h$. It is evident that with $h=0,1, \ldots, N-1$ we have a system of $N$ linear equations characterized by a Vandermonde matrix. When the problem is generalized to the more realistic case of a higher dimensional space, i.e. $D \geqslant 2$, the involved matrices become multilevel Vandermonde matrices denoted by $(\mathcal{V})$ in the following.
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Associated with these matrices there are Toeplitz matrices [13, 1], known as KarleHauptman matrices in crystallography [3, 4] and having the following structure $(\mathcal{D})=$ $(\mathcal{V})^{\dagger}(\Delta)(\mathcal{V})$ (see section 3 for precise definition) with $(\Delta)$ a diagonal matrix.

The study of these matrices of the kind found in x-ray or neutron scattering from an ideal crystal has helped us to find that their determinants have a simple closed algebraic expression that will be reported here.

## 2. Generalized multilevel Vandermonde matrix

In this section, we define a generalized $D$-level Vandermonde matrix in the context of Fourier transforms of weighted discrete sets of points in a $D$-dimensional space. In the first part of this section we evaluate its determinant in the case $D=2$; and in the second part, we treat the cases $D>2$ (section 2.2) that only involve more bookkeeping.

Take a set $\mathcal{S}_{D}$ of $N$ distinct points in $[0,1)^{D}$. In general, some points may have some but not all of their coordinates equal. Then we enumerate the points in $\mathcal{S}_{D}$ by the different values of the first (leading) coordinate, then by the different values of the second (trailing) coordinate and so on, employing $D$ indices.

### 2.1. Case $D=2$

For $D=2$, we have

$$
\begin{equation*}
\mathcal{S}_{2} \equiv\left\{\mathbf{r}_{r, s} \equiv\left(x_{r}, y_{r, s}\right) \mid r=1, \ldots, M, s=1, \ldots, m_{r}\right\} \tag{1}
\end{equation*}
$$

Here, $m_{r}$ counts the points which share the same $r$ th value of the first (leading) coordinate. Clearly, $1 \leqslant m_{r} \leqslant N$ whatever $r$, and $\sum_{r=1}^{M} m_{r}=N$. Further, in labelling the different $x_{r} \mathrm{~s}$, we choose label $r$ in such a way that

$$
\begin{equation*}
m_{1} \geqslant m_{2} \geqslant \cdots \geqslant m_{M} \tag{2}
\end{equation*}
$$

It is observed that set $\mathcal{S}_{2}$ can bijectively be mapped onto subset $\mathcal{I}_{2}$

$$
\begin{equation*}
\mathcal{I}_{2} \equiv\left\{\mathbf{k} \equiv(h, k) \mid h=0, \ldots, M-1, k=0, \ldots, m_{h+1}-1\right\} \tag{3}
\end{equation*}
$$

of the $\mathbb{Z}^{2}$ lattice by putting $h=r-1$ and $k=s-1$. We remark that the labelling used in (1) depends on the order in which the coordinates are considered. Therefore there are $D$ ! possible different realizations but, in the following, we shall confine ourselves to the one defined above.

Take now a set of $N$ orthonormal vectors $\left|\mathbf{r}_{r, s}\right\rangle \equiv\left|x_{r}, y_{r, s}\right\rangle\left(\mathbf{r}_{r, s} \in \mathcal{S}_{2}\right)$ forming an orthonormal complete basis of the $N$-dimensional Hilbert space $\mathcal{H}$. We consider the vectors $|\mathbf{k}\rangle \equiv|(h, k)\rangle$, with $\mathbf{k} \in \mathbb{Z}^{2}$, defined as

$$
\begin{equation*}
|\mathbf{k}\rangle \equiv \sum_{r=1}^{M} \sum_{s=1}^{m_{r}} \mathrm{e}^{-\mathrm{i} 2 \pi \mathbf{k} \cdot \mathbf{r}_{r, s}}\left|\mathbf{r}_{r, s}\right\rangle \equiv \sum_{r=1}^{M} \sum_{s=1}^{m_{r}} \mathrm{e}^{-\mathrm{i} 2 \pi h x_{r}} \mathrm{e}^{-\mathrm{i} 2 \pi k y_{r, s}}\left|x_{r}, y_{r, s}\right\rangle . \tag{4}
\end{equation*}
$$

Equivalently, setting

$$
\begin{equation*}
\xi_{r} \equiv \mathrm{e}^{-\mathrm{i} 2 \pi x_{r}} \quad \text { and } \quad \eta_{r, s} \equiv \mathrm{e}^{-\mathrm{i} 2 \pi y_{r, s}} \tag{5}
\end{equation*}
$$

we have

$$
\begin{equation*}
|\mathbf{k}\rangle=\sum_{r=1}^{M} \sum_{s=1}^{m_{r}} \xi_{r}^{h} \eta_{r, s}^{k}\left|x_{r}, y_{r, s}\right\rangle \tag{6}
\end{equation*}
$$

These vectors form a lattice of vectors belonging to $\mathcal{H}$. We restrict now ourselves to the set of the $N$ vectors $|\mathbf{k}\rangle=|(h, k)\rangle$ with $\mathbf{k} \in \mathcal{I}_{2}$. Then (6) describes a linear transformation
between two sets of $N$ vectors of $\mathcal{H}$ that is represented by matrix $(\mathcal{V})$ with elements $\mathcal{V}_{(r, s),(h, k)} \equiv\left\langle\mathbf{r}_{r, s} \mid \mathbf{k}\right\rangle=\xi_{r}^{h} \eta_{r, s}^{k}$. The considered $N$ vectors $|\mathbf{k}\rangle$ are linearly independent iff $(\mathcal{V})$ is non-singular. We write $(\mathcal{V})$ in the factored-block form

$$
(\mathcal{V})=\left|\begin{array}{llll}
\xi_{1}^{0}\left(B_{1,1}\right) & \xi_{1}^{1}\left(B_{1,2}\right) & \ldots & \xi_{1}^{M-1}\left(B_{1, M}\right)  \tag{7}\\
\xi_{2}^{0}\left(B_{2,1}\right) & \xi_{2}^{1}\left(B_{2,2}\right) & \ldots & \xi_{2}^{M-1}\left(B_{2, M}\right) \\
& & \ldots & \\
\xi_{M}^{0}\left(B_{M, 1}\right) & \xi_{M}^{1}\left(B_{M, 2}\right) & \ldots & \xi_{M}^{M-1}\left(B_{M, M}\right)
\end{array}\right|
$$

where the generic ( $B_{r, r^{\prime}}$ ) element is the $m_{r} \times m_{r^{\prime}}$ matrix defined as

$$
\left(B_{r, r^{\prime}}\right) \equiv\left|\begin{array}{cccc}
\eta_{r, 1}^{0} & \eta_{r, 1}^{1} & \ldots & \eta_{r, 1}^{m_{r^{\prime}}-1}  \tag{8}\\
\eta_{r, 2}^{0} & \eta_{r, 2}^{1} & \ldots & \eta_{r, 2}^{m_{r, 2}-1} \\
& & \ldots & \\
\eta_{r, m_{r}}^{0} & \eta_{r, m_{r}}^{1} & \ldots & \eta_{r, m_{r}}^{m_{r}-1}
\end{array}\right|
$$

and $\xi_{r}^{r^{\prime}-1}\left(B_{r, r^{\prime}}\right)$ denotes the $m_{r} \times m_{r^{\prime}}$ matrix obtained by entrywise (element by element) multiplication of matrix $\left(B_{r, r^{\prime}}\right)$ by scalar $\xi_{r}^{r^{\prime}-1}$. This identifies $(\mathcal{V})$ as a two-level Vandermonde matrix. Clearly, for dimension $D>2$, we shall have a $D$-level block structure. Diagonal blocks ( $B_{r, r}$ ) are square Vandermonde matrices and

$$
\begin{equation*}
\operatorname{det}\left(B_{r, r}\right)=\prod_{1 \leqslant s^{\prime}<s \leqslant m_{r}}\left(\eta_{r, s}-\eta_{r, s^{\prime}}\right) \tag{9}
\end{equation*}
$$

To facilitate the reader in understanding the way to form matrix $(\mathcal{V})$, we have included a small example in the appendix.

We now show that the analytical expression of the determinant of $(\mathcal{V})$ is also remarkably simple. To this aim, consider the following four points:
(i) The determinant of $(\mathcal{V})$ is a homogeneous polynomial in variables $\{\xi\}$ and $\{\eta\}$. In fact, $\operatorname{det}(\mathcal{V})$ is a sum of terms all having the degrees $Q$ and $P$ in the variables $\{\eta\}$ and $\{\xi\}$, respectively, where

$$
\begin{align*}
Q & =\sum_{h=0}^{M-1} \sum_{k=0}^{m_{h+1}-1} k=\frac{1}{2}\left(-N+\sum_{h=0}^{M-1} m_{h+1}^{2}\right)  \tag{10}\\
P & =\sum_{h=0}^{M-1} h m_{h+1} . \tag{11}
\end{align*}
$$

If, whatever $r, \eta_{r, s}=\eta_{r, s^{\prime}}$ with $s \neq s^{\prime}$, two rows of $(\mathcal{V})$ are equal and the determinant must have a zero. This happens for any ( $s, s^{\prime}$ ) pair and for any $r$. Hence, using (9), it must result

$$
\begin{equation*}
\operatorname{det}(\mathcal{V})=\mathcal{R}(\{\xi\}) \prod_{r=1}^{M} \operatorname{det}\left(B_{r, r}\right) \tag{12}
\end{equation*}
$$

It is noted that the factor $\mathcal{R}$ cannot depend on variables $\{\eta\}$ because the total degree of the expression inside the square brackets is $Q$. Thus, $\mathcal{R}(\{\xi\})$ is a polynomial of degree $P$ in the $\{\xi\}$ variables.
(ii) Recall now the Laplace expansion of determinants [14, 15]. Evaluate $\operatorname{det}(\mathcal{V})$ by considering the ( $m_{1} \times m_{1}$ ) minors contained in the first $m_{1}$ rows of $(\mathcal{V})$ corresponding to the first row of the matrix reported on the right-hand side of (7). Each of these minors, after factorizing the appropriate powers of $\xi$ common to each column, is a Vandermonde-like matrix having the same exponent sequence in all its rows, the $s$ th of these consisting only powers of $\eta_{1, s}$. The determinants of the minors that do not contain the full set of exponents $0,1, \ldots, m_{1}-1$ will be 0 . Consider now the only minors with nonzero determinant. Recalling the ordering (2), we can say that only minors containing the leftmost $m_{2}+1, \ldots, m_{1}$ th columns of $(\mathcal{V})$ and, thus, of ( $B_{1,1}$ ) will contain exponents $m_{2}, \ldots, m_{1}-1$ and could therefore be non-singular. Thus, the relevant $\left(N-m_{1}\right) \times\left(N-m_{1}\right)$ complementary minors will never contain the $\left(m_{2}+1\right)$ th, $\ldots, m_{1}$ th column of $(\mathcal{V})$.
(iii) Choose now $r$ such that $1<r \leqslant M$. Assume that $\xi_{1}=\xi_{r}$. We have $m_{1} \geqslant m_{r}$. We can evaluate $\operatorname{det}(\mathcal{V})$ by considering all the minors contained in a rectangular submatrix built by taking the first $m_{1}$ rows-all and only those having a power of $\xi_{1}$ as factor-and all the $m_{r}$ rows which have a power of $\xi_{r}$ as factor. These correspond to the two block rows $B_{1,1}, \ldots, B_{1, M}$ and $B_{r, 1}, \ldots, B_{r, M}$ superimposed. Having assumed that $\xi_{1}=\xi_{r}$, each column of one of these minors factorizes $\xi_{1}^{h}$ with $h$ in $0, \ldots, M-1$ depending on the considered column. Thus, we are left with an $\left(m_{1}+m_{r}\right) \times\left(m_{1}+m_{r}\right)$ Vandermonde matrix whose elements are $\eta_{1, s^{\prime}}^{k^{\prime}}$ or $\eta_{r, s}^{k}$ with $1 \leqslant s^{\prime} \leqslant m_{1}$ and $1 \leqslant s \leqslant m_{r}$, while $k^{\prime}$ and $k$ belong to $0, \ldots, m_{1}-1$. The rank of this matrix can be at most $m_{1}$ and, therefore, its determinant will have a zero of order at least equal to $m_{r}=\min \left(m_{1}, m_{r}\right)$. Hence, $\operatorname{det}(\mathcal{V})$ evaluated by this procedure will have a zero of order at least equal to $m_{r}$ owing to the hypothesis $\xi_{1}=\xi_{r}$.
(iv) Assume now that $\xi_{2}=\xi_{r^{\prime}}$ for a particular $r^{\prime}$ such that $2<r^{\prime} \leqslant M$. Before repeating the reasoning made in the case $\xi_{1}=\xi_{r}$, we imagine of having $\operatorname{developed} \operatorname{det}(\mathcal{V})$ with respect to the minors contained in the first $m_{1}$ rows. As noted above, there is no need to consider complementary minors containing the columns with exponents $m_{2}, \ldots, m_{1}-1$. Each of these complementary minors can be developed by considering its $\left(m_{2}+m_{r^{\prime}}\right) \times\left(m_{2}+m_{r^{\prime}}\right)$ minors contained in the two blocks rows $B_{2,1}, \ldots, B_{2, M}$ and $B_{r^{\prime}, 1}, \ldots, B_{r^{\prime}, M}$, presenting the factors $\xi_{2}$ and $\xi_{r^{\prime}}$, respectively. By the same reasoning made above for the case $\xi_{1}=\xi_{r}$, one concludes that each $\left(m_{2}+m_{r^{\prime}}\right) \times\left(m_{2}+m_{r^{\prime}}\right)$ minor has a rank at most equal to $m_{2}$ and that $\operatorname{det}(\mathcal{V})$ has a zero at least of order $m_{r^{\prime}}=\min \left(m_{2}, m_{r^{\prime}}\right)$ when $\xi_{2}=\xi_{r^{\prime}}$. Thus, the zero of $\operatorname{det}(\mathcal{V})$ is at least of the order $\min \left(m_{r}, m_{r^{\prime}}\right)$ when $\xi_{r}=\xi_{r^{\prime}}$. Due to the ordering (2), whenever $r>r^{\prime}$ we have that $\min \left(m_{r}, m_{r^{\prime}}\right)=m_{r}=\operatorname{size}\left(B_{r, r}\right)$. Thereafter, one can write that

$$
\begin{equation*}
\operatorname{det}(\mathcal{V})=\mathcal{R}_{1}(\{\eta\}) \prod_{1 \leqslant r^{\prime}<r \leqslant M}\left(\xi_{r}-\xi_{r^{\prime}}\right)^{\operatorname{size}\left(B_{r, r}\right)} \tag{13}
\end{equation*}
$$

The degree in the variables $\{\xi\}$ in the above product is equal to $P$, so that $\mathcal{R}_{1}$ is a polynomial of the variables $\{\eta\}$ only. Thus, combining equation (12) with (13), one finds that

$$
\begin{equation*}
\mathcal{R}_{1}(\{\eta\})=\mathcal{R}_{0} \prod_{r=1}^{M} \operatorname{det}\left(B_{r, r}\right) \tag{14}
\end{equation*}
$$

where $\mathcal{R}_{0}$ is a simple constant. Comparing the 'diagonal' term $\prod_{r=1}^{M}\left(\xi_{r}{ }^{(r-1) m_{r}} \prod_{s=1}^{m_{r}} \eta_{r, s}^{s-1}\right)$ resulting from the calculation of $\operatorname{det}(\mathcal{V})$, starting from the explicit expression of $(\mathcal{V})$, with the corresponding term obtained developing the products present in (13) combined with (14), one
finds that $\mathcal{R}_{0}=1$. Hence, the remarkably simple expression of the determinant of matrix $(\mathcal{V})$ reads

$$
\begin{equation*}
\operatorname{det}(\mathcal{V})=\left(\prod_{1 \leqslant r^{\prime}<r \leqslant M}\left(\xi_{r}-\xi_{r^{\prime}}\right)^{\operatorname{size}\left(B_{r, r}\right)}\right)\left(\prod_{r=1}^{M} \operatorname{det}\left(B_{r, r}\right)\right) \tag{15}
\end{equation*}
$$

### 2.2. Case $D>2$

In the case $D=3$, the set $\mathcal{S}_{3}$ of the position vectors will be written as
$\mathcal{S}_{3} \equiv\left\{\mathbf{r}_{r, s, t} \equiv\left(x_{r}, y_{r, s}, z_{r, s, t}\right) \mid r=1, \ldots, M, s=1, \ldots, M_{r}, t=1, \ldots, m_{r, s}\right\}$
where $M_{r}$ counts the different values of the first subleading coordinate of the points sharing the same $r$ th value of the leading coordinate while $m_{r, s}$ counts the number of the points of $\mathcal{S}_{3}$ that have as second coordinate the $s$ th of the possible values when its first coordinate is the $r$ th of the possible values. Clearly, $\sum_{s=1}^{M_{r}} m_{r, s}=m_{r}$ where $m_{r}$, similarly to definition (1), is the number of the points of $\mathcal{S}_{3}$ that share the $r$ th leading coordinate so as to have $m_{r} \geqslant M_{r}$ and, as before, $N=\sum_{r=1}^{M} m_{r}$. Labels $r$ and $s$ are now chosen in such a way that $M_{1} \geqslant M_{2} \geqslant \cdots \geqslant M_{M}$ and $m_{r, 1} \geqslant m_{r, 2} \geqslant \cdots \geqslant m_{r, M_{r}}$. Set $\mathcal{S}_{3}$ can be bijectively mapped onto subset $\mathcal{I}_{3}$
$\mathcal{I}_{3} \equiv\left\{\mathbf{k} \equiv(h, k, l) \mid h=0, \ldots, M-1, k=0, \ldots, M_{h+1}-1, l=0, \ldots, m_{h+1, k+1}-1\right\}$
of the $\mathbb{Z}^{3}$ lattice. The vectors $|\mathbf{k}\rangle$, with $\mathbf{k} \in \mathbb{Z}^{3}$, are now defined as
$|\mathbf{k}\rangle \equiv|(h, k, l)\rangle \equiv \sum_{r=1}^{M} \sum_{s=1}^{M_{r}} \sum_{t=1}^{m_{r, s}} \mathrm{e}^{-\mathrm{i} 2 \pi \mathbf{k} \cdot \mathbf{r}_{r, s, t}}\left|\mathbf{r}_{r, s, t}\right\rangle \equiv \sum_{r=1}^{M} \sum_{s=1}^{M_{r}} \sum_{t=1}^{m_{r, s}} \xi_{r}^{h} \eta_{r, s}^{k} \zeta_{r, s, t}^{l}\left|x_{r}, y_{r, s}, z_{r, s, t}\right\rangle$,
where

$$
\begin{equation*}
\xi_{r} \equiv \mathrm{e}^{-\mathrm{i} 2 \pi x_{r}} ; \quad \eta_{r, s} \equiv \mathrm{e}^{-\mathrm{i} 2 \pi y_{r, s}} ; \quad \zeta_{r, s, t} \equiv \mathrm{e}^{-\mathrm{i} 2 \pi z_{r, s, t}} \tag{19}
\end{equation*}
$$

At the same time, the vectors $\left|\mathbf{r}_{r, s, t}\right\rangle \equiv\left|x_{r}, y_{r, s}, z_{r, s, t}\right\rangle$ form an orthonormal complete basis of the $N$-dimensional Hilbert space $\mathcal{H}$. Take now the $N$ vectors $|\mathbf{k}\rangle=|(h, k, l)\rangle$ with $\mathbf{k} \in \mathcal{I}_{3}$. The generic element of the 3-level Vandermonde matrix $(\mathcal{V})$, obtained from the sets $\mathcal{S}_{3}$ and $\mathcal{I}_{3}$, is $\mathcal{V}_{(r, s, t),(h, k, l)} \equiv\left\langle\mathbf{r}_{r, s, t} \mid \mathbf{k}\right\rangle=\xi_{r}^{h} \eta_{r, S}^{k} \zeta_{r, s, t}^{l}$. From these considerations, it appears clear how sets $\mathcal{S}_{D}$ and $\mathcal{I}_{D}$ are defined if $D>3$.

It is evident that the expression of the determinant of the corresponding Vandermonde matrix, obtained by $\mathcal{S}_{D}$ and the associated $\mathcal{I}_{D}$ for the case $D>2$, is exactly the same as in (15), with the proviso that now all the $\left(B_{r, r}\right)$ blocks there present are $(D-1)$-level Vandermonde matrices with (leading) variables $\eta_{r, s}$ with $s=1, \ldots, \operatorname{size}\left(B_{r, r}\right)$ and sub-blocks $\left(C_{r ; s, p}\right)$ which are again ( $D-2$ )-level Vandermonde matrices in the trailing variables. To be more explicit, in the case $D=3$ one has

$$
\left(B_{r, r}\right)=\left|\begin{array}{cccc}
\eta_{r, 1}^{0}\left(C_{r ; 1,1}\right) & \eta_{r, 1}^{1}\left(C_{r ; 1,2}\right) & \ldots & \eta_{r, 1}^{M_{r}-1}\left(C_{r ; 1, M_{r}}\right)  \tag{20}\\
\eta_{r, 2}^{0}\left(C_{r ; 2,1}\right) & \eta_{r, 2}^{1}\left(C_{r ; 2,2}\right) & \ldots & \eta_{r, 2}^{M_{r}-1}\left(C_{r ; 2, M_{r}}\right) \\
& & \ldots & \\
\eta_{r, M_{r}}^{0}\left(C_{r ; M_{r}, 1}\right) & \eta_{r, M_{r}}^{1}\left(C_{r ; M_{r}, 2}\right) & \ldots & \eta_{r, M_{r}}^{M_{r}-1}\left(C_{r ; M_{r}, M_{r}}\right)
\end{array}\right|
$$

where the symbol $\left(C_{r ; s, p}\right)$ represents the $m_{r, s} \times m_{r, p}$ matrix defined as

$$
\left(C_{r ; s, p}\right) \equiv\left|\begin{array}{llll}
\zeta_{r, s, 1}^{0} & \zeta_{r, s, 1}^{1} & \ldots & \zeta_{r, s, p}^{m_{r, p}-1}  \tag{21}\\
\zeta_{r, s, 2}^{0} & \zeta_{r, s, 2}^{1} & \ldots & \zeta_{r, s, 2}^{m_{r, p}-1} \\
& & \ldots & \\
\zeta_{r, s, m_{r, s}}^{0} & \zeta_{r, s, m_{r, s}}^{1} & \ldots & \zeta_{r, s, m_{r, s}}^{m_{r, p}-1}
\end{array}\right|
$$

and the first index $r$ specifies that sub-blocks $\left(C_{r ; s, p}\right)$ refer to matrix ( $B_{r, r}$ ). This implies that the evaluation of the $D$-level determinant $\operatorname{det}(\mathcal{V})$ involves a recursive application of (15) down to level 1 . In fact, to see that (15) holds in general for any level $D>2$ we can proceed by induction assuming that (15) holds at level $D-1$ and showing that it still holds at $D$. For this aim, it is sufficient to trace back steps (i)-(iv).

## 3. Evaluation of Karle-Hauptman determinants

To write down the explicit form of a Karle-Hauptman matrix $(\mathcal{D})$, it is convenient to re-index sets $\mathcal{S}_{D}$ and $\mathcal{I}_{D}$ by unique indices, denoted as $\rho$ and $\sigma$, respectively, both ranging over $1, \ldots, N$ and preserving the hierarchical order. For $D=2$, this means

$$
\begin{equation*}
\rho \equiv \rho(r, s) \equiv s+\sum_{p=1}^{r-1} m_{p} ; \quad \sigma \equiv \sigma(h, k) \equiv k+1+\sum_{p=0}^{h-1} m_{p+1} . \tag{22}
\end{equation*}
$$

If $D>2$, the expressions are quite similar. The $\left(\sigma, \sigma^{\prime}\right)$ element of $(\mathcal{D})$ is defined as
$\mathcal{D}_{\sigma, \sigma^{\prime}} \equiv \sum_{\rho=1}^{N} \mathcal{V}_{\sigma, \rho}^{\dagger} v_{\rho} \mathcal{V}_{\rho, \sigma^{\prime}}=\sum_{\rho=1}^{N} v_{\rho} \exp \left(\mathrm{i} 2 \pi\left(\mathbf{k}_{\sigma^{\prime}}-\mathbf{k}_{\sigma}\right) \cdot \mathbf{r}_{\rho}\right), \quad \sigma, \sigma^{\prime}=1, \ldots, N$
where $v_{\rho}$ are given complex numbers. Putting $(\Delta) \equiv \operatorname{diag}\left\{v_{1}, \nu_{2}, \ldots, v_{N}\right\}$, we can write

$$
\begin{equation*}
(\mathcal{D}) \equiv(\mathcal{V})^{\dagger}(\Delta)(\mathcal{V}) \tag{24}
\end{equation*}
$$

that clearly coincides with the Karle-Hauptman matrices defined in [3, 4, 8]. At the same time, as the $\left(\sigma, \sigma^{\prime}\right)$ th element depends only on the difference $\mathbf{k}_{\sigma^{\prime}}-\mathbf{k}_{\sigma},(\mathcal{D})$ is a generalized Toeplitz matrix (for $D>1$, a multilevel Toeplitz matrix). (Considering the case $D=1$, in fact, (23) is a classical Toeplitz matrix if $\mathbf{k}_{\sigma^{\prime}}=\left(\sigma^{\prime}-1\right)$ and $\mathbf{k}_{\sigma}=(\sigma-1)$.)

By the results of the previous section and (24) we find that

$$
\begin{equation*}
\operatorname{det}(\mathcal{D})=|\operatorname{det}(\mathcal{V})|^{2} \prod_{\rho=1}^{N} v_{\rho} \tag{25}
\end{equation*}
$$

where $\operatorname{det}(\mathcal{V})$ is given by (15). This expression is valid for general complex numbers $v_{\rho}$. Therefore, it applies to the phase problem [3, 4, 10] both for x-ray and for neutrons, and also for anomalous scattering. One concludes that $\operatorname{det}(\mathcal{D})$ is certainly different from zero if no $v_{\rho}$ is equal to zero and all $\mathbf{r}_{\rho}$ s are distinct.


Figure 1. Example of an $\mathcal{S}_{2}$ set associated with a set of seven distinct points in a 2 D space.

## 4. Conclusion

We have shown that the algebraic expression of the determinant of the multilevel Vandermonde matrix generated by the sets $\mathcal{S}_{D}$ and $\mathcal{I}_{D}$ is obtained by the recursive application of (15). Similarly, the determinant of the Toeplitz or Karle-Hauptman matrix defined by equations (23) and (24) is given by (25).

## Appendix

Here, we report an example on the construction of a two-level $(D=2)$ Vandermonde matrix. Consider a set $\mathcal{S}_{2}$ of $N=7$ points in the $[0,1) \times[0,1)$ square, as shown in figure 1 . Choosing the horizontal $(x)$ as leading coordinate, we have only $M=4$ distinct $x$ values. We label the seven points according to their respective $x$-degeneracy, ordered as
$\mathcal{S}_{2}=\left\{\left(x_{1}, y_{1,1}\right),\left(x_{1}, y_{1,2}\right),\left(x_{1}, y_{1,3}\right),\left(x_{2}, y_{2,1}\right),\left(x_{2}, y_{2,2}\right),\left(x_{3}, y_{3,1}\right),\left(x_{4}, y_{4,1}\right)\right\}$.
This labelling fulfils the condition in (2), as $m_{1}=3 \geqslant m_{2}=2 \geqslant m_{3}=1 \geqslant m_{4}=1$. Note that only for the last two points, having the same degeneracy, we could have exchanged labels. Note also that if we had chosen $y$ as leading coordinate, evidently there would be no degeneracy $\left(M=N=7 ; m_{r}=1, r=1, \ldots, 7\right)$ and all labels $\left(y_{r}, x_{r, 1}\right), r=1, \ldots, 7$ could have been arbitrarily assigned to the points.

We also assign now the Fourier space ordered point set as in (3),

$$
\begin{equation*}
\mathcal{I}_{2}=\{(0,0),(0,1),(0,2),(1,0),(1,1),(2,0),(3,0)\} . \tag{A.2}
\end{equation*}
$$

Matrix $\mathcal{V}$ now is built taking the exponential of $2 \pi i$ multiplied by the scalar product of the elements of $\mathcal{S}_{2}$ (in row order) times the elements of $\mathcal{I}_{2}$ (in column order). This gives
$(\mathcal{V})=\left|\begin{array}{lllllll}1 & \mathrm{e}^{\mathrm{i} 2 \pi\left(y_{1,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 y_{1,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{1}+y_{1,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 x_{1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(3 x_{1}\right)} \\ 1 & \mathrm{e}^{\mathrm{i} 2 \pi\left(y_{1,2}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 y_{1,2}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{1}+y_{1,2}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 x_{1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(3 x_{1}\right)} \\ 1 & \mathrm{e}^{\mathrm{i} 2 \pi\left(y_{1,3}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 y_{1,3}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{1}+y_{1,3}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 x_{1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(3 x_{1}\right)} \\ 1 & \mathrm{e}^{\mathrm{i} 2 \pi\left(y_{2,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 y_{2,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{2}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{2}+y_{2,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 x_{2}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(3 x_{2}\right)} \\ 1 & \mathrm{e}^{\mathrm{i} 2 \pi\left(y_{2,2}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 y_{2,2}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{2}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{2}+y_{2,2}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 x_{2}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(3 x_{2}\right)} \\ 1 & \mathrm{e}^{\mathrm{i} 2 \pi\left(y_{3,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 y_{3,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{3}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{3}+y_{3,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 x_{3}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(3 x_{3}\right)} \\ 1 & \mathrm{e}^{\mathrm{i} 2 \pi\left(y_{4,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 y_{4,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{4}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(x_{4}+y_{4,1}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(2 x_{4}\right)} & \mathrm{e}^{\mathrm{i} 2 \pi\left(3 x_{4}\right)}\end{array}\right|$.

After passing to variables $\xi, \eta$ as in (5), with

$$
\begin{equation*}
\xi_{1}=\mathrm{e}^{\mathrm{i} 2 \pi x_{1}}, \quad \xi_{2}=\mathrm{e}^{\mathrm{i} 2 \pi x_{2}}, \ldots ; \quad \eta_{1,1}=\mathrm{e}^{\mathrm{i} 2 \pi y_{1,1}}, \quad \eta_{1,2}=\mathrm{e}^{\mathrm{i} 2 \pi y_{1,2}}, \ldots \tag{A.4}
\end{equation*}
$$

we can write

$$
(\mathcal{V})=\left|\begin{array}{llll}
\xi_{1}^{0}\left(\begin{array}{lll}
\eta_{1,1}^{0} & \eta_{1,1}^{1} & \eta_{1,1}^{2} \\
\eta_{1,2}^{0} & \eta_{1,2}^{1} & \eta_{1,2}^{2} \\
\eta_{1,3}^{0} & \eta_{1,3}^{1} & \eta_{1,3}^{2}
\end{array}\right) & \xi_{1}^{1}\left(\begin{array}{ll}
\eta_{1,1}^{0} & \eta_{1,1}^{1} \\
\eta_{1,2}^{0} & \eta_{1,2}^{1} \\
\eta_{1,3}^{0} & \eta_{1,3}^{1}
\end{array}\right) & \xi_{1}^{2}\left(\begin{array}{l}
\eta_{1,1}^{0} \\
\eta_{1,2}^{0} \\
\eta_{1,3}^{0}
\end{array}\right) & \xi_{1}^{3}\left(\begin{array}{l}
\eta_{1,1}^{0} \\
\eta_{1,2}^{0} \\
\eta_{1,3}^{0}
\end{array}\right)  \tag{A.5}\\
\xi_{2}^{0}\left(\begin{array}{lll}
\eta_{2,1}^{0} & \eta_{2,1}^{1} & \eta_{2,1}^{2} \\
\eta_{2,2}^{0} & \eta_{2,2}^{1} & \eta_{2,2}^{2}
\end{array}\right) & \xi_{2}^{1}\left(\begin{array}{ll}
\eta_{2,1}^{0} & \eta_{2,1}^{1} \\
\eta_{2,2}^{0} & \eta_{2,2}^{1}
\end{array}\right) & \xi_{2}^{2}\binom{\eta_{2,1}^{0}}{\eta_{2,2}^{0}} & \xi_{2}^{3}\binom{\eta_{2,1}^{0}}{\eta_{2,2}^{0}} \\
\xi_{3}^{0}\left(\eta_{3,1}^{0}\right. & \eta_{3,1}^{1} & \left.\eta_{3,1}^{2}\right) & \xi_{3}^{1}\left(\eta_{3,1}^{0}\right. \\
\left.\eta_{3,1}^{1}\right) & \xi_{3}^{2}\left(\eta_{3,1}^{0}\right) & \xi_{3}^{3}\left(\eta_{3,1}^{0}\right) \\
\xi_{4}^{0}\left(\eta_{4,1}^{0}\right. & \eta_{4,1}^{1} & \left.\eta_{4,1}^{2}\right) & \xi_{4}^{1}\left(\eta_{4,1}^{0}\right. \\
\left.\eta_{4,1}^{1}\right) & \xi_{4}^{2}\left(\eta_{4,1}^{0}\right) & \xi_{4}^{3}\left(\eta_{4,1}^{0}\right)
\end{array}\right|
$$

where the ( $B_{r, r^{\prime}}$ ) block matrices are evidenced (cf (7)). By (15) immediately follows that

$$
\begin{align*}
\operatorname{det}(\mathcal{V})=\left(\xi_{2}-\right. & \left.\xi_{1}\right)^{2}\left(\xi_{3}-\xi_{1}\right)\left(\xi_{4}-\xi_{1}\right)\left(\xi_{3}-\xi_{2}\right)\left(\xi_{4}-\xi_{2}\right)\left(\xi_{4}-\xi_{3}\right) \\
& \times\left(\eta_{1,2}-\eta_{1,1}\right)\left(\eta_{1,3}-\eta_{1,1}\right)\left(\eta_{1,3}-\eta_{1,2}\right)\left(\eta_{2,2}-\eta_{2,1}\right) \tag{A.6}
\end{align*}
$$

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