The Algebraic Approach to the Phase Problem

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1 Completion of the algebraic approach for x-ray scattering

It has already been anticipated that, in the case of x-ray scattering, difficulties **a-c)** reported at the end of §2 were fully removed in papers I and II. In reviewing these results we shall reformulate some of them so as to make their generalization to the neutron case possible. Besides, it should also be stressed that some aspects of this reformulation are original. In this respect we first observe that x-ray and neutron scattering can be presented in a unified way by using some notions of elementary Quantum Mechanics. In fact, in appendix A we show that the subtracted intensities, defined by (I-16), and the scattering density of the infinitely resolved Patterson map, defined by (I-17), are two different representations of a single hermitian operator, denoted by $\mathcal{Q}$, within an $\bar{\mathcal{N}}$-dimensional Hilbert space $\mathcal{H}(\bar{\mathcal{N}})$. More definitely, one has

$$\mathcal{I}_{\mathbf{h}-\mathbf{k}} = \langle \mathbf{k}|\mathcal{Q}|\mathbf{h}\rangle, \quad \mathbf{h},\mathbf{k} \in \mathcal{Z}^3, \tag{1}$$

$$\nu_i \delta_{i,j} = \langle \vec{\delta}_i|\mathcal{Q}|\vec{\delta}_j\rangle, \quad i,j = 1,\ldots,\bar{\mathcal{N}}. \tag{2}$$

Here $|\mathbf{h}\rangle$ and $|\mathbf{k}\rangle$ are two vectors of the Goedkoop lattice $\mathcal{G}(\bar{\mathcal{N}})$ that is now defined as consisting of the vectors

$$|\mathbf{h}\rangle \equiv \sum_{j=1}^{\bar{\mathcal{N}}} e^{-i2\pi \mathbf{h}\cdot\vec{\delta}_j} |\vec{\delta}_j\rangle, \qquad \mathbf{h} \in \mathcal{Z}^3. \tag{3}$$

where the vectors $|\vec{\delta}_j\rangle$, with $j = 1,\ldots,\bar{\mathcal{N}}$, form a complete orthonormal basis of $\mathcal{H}(\bar{\mathcal{N}})$. Moreover they are the eigenvectors of the position operator $\vec{\mathcal{R}}$ with eigenvalues equal to the positions of the $\bar{\mathcal{N}}$ "charges" present in (I-17), since they obey to

$$\vec{\mathcal{R}}|\vec{\delta}_j\rangle = \vec{\delta}_j|\vec{\delta}_j\rangle, \qquad j = 1,\ldots,\bar{\mathcal{N}}. \tag{4}$$

Eq (3) shows that the vectors of $\mathcal{G}(\bar{\mathcal{N}})$ only depend on the positions of the charges and are independent on the latter values. It is stressed that this property holds true both for x-ray and for neutron scattering. The vector lattice $\mathcal{G}(\bar{\mathcal{N}})$ contains $\bar{\mathcal{N}}$ linearly independent vectors due to the property shown in appendix A of I. Our first task is to single out in $\mathcal{G}(\bar{\mathcal{N}})$ a set of $\bar{\mathcal{N}}$ linearly independent vectors. If the $\vec{\delta}_j$s were known, the task would be very simple. In fact, considering the components of $\vec{\delta}_j$, one has $\vec{\delta}_j = (x_j, y_j, z_j)$. We denote the distinct x_j values as $\bar{x}_{\hat{\imath}}$ with $\hat{\imath} = 1,\ldots,M$. The distinct y_j values of the $\vec{\delta}_j$s that have x_j equal to a particular $\bar{x}_{\hat{\imath}}$ are denoted by $\bar{y}_{\hat{\imath},\hat{\jmath}}$ and the different z_j values of the $\vec{\delta}_j$s having their first two components equal to a given pair $(\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}})$ by $\bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}$. For a fixed $\hat{\imath}$, index $\hat{\jmath}$ in $\bar{y}_{\hat{\imath},\hat{\jmath}}$ will run between 1 and $\mu_{\hat{\imath}}$, $\mu_{\hat{\imath}}$ being a integer greater than zero and, similarly, for a fixed pair $(\hat{\imath},\hat{\jmath})$ with $1 \le \hat{\jmath} \le \mu_{\hat{\imath}}$, index $\hat{\ell}$ in $\bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}$ will run between 1 and $\mu_{\hat{\imath},\hat{\jmath}}$ with $\mu_{\hat{\imath},\hat{\jmath}}$ integer and such that $\mu_{\hat{\imath},\hat{\jmath}} \ge 1$. In this way, we have the bijective mapping

$$\{\vec{\delta}_j | j = 1, \ldots, \bar{\mathcal{N}}\} \leftrightarrow \{(\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}) \;\;|\;\; \hat{\imath} = 1, \ldots, M,\; \hat{\jmath} = 1, \ldots, \mu_{\hat{\imath}}, \\ \hat{\ell} = 1, \ldots, \mu_{\hat{\imath},\hat{\jmath}}\} \tag{5}$$

that can also be seen as a bijective mapping of the integer set $\{1, \ldots, \bar{\mathcal{N}}\}$ onto the subset $\mathcal{I}$ of $\mathcal{Z}^3$ defined as

$$\mathcal{I} \equiv \{(\hat{\imath}, \hat{\jmath}, \hat{\ell}) | \hat{\imath} = 1, \ldots, M,\; \hat{\jmath} = 1, \ldots, \mu_{\hat{\imath}},\; \hat{\ell} = 1, \ldots, \mu_{\hat{\imath},\hat{\jmath}}\} \tag{6}$$

so that the $\mu_{\hat{\imath},\hat{\jmath}}$s obey to

$$\sum_{\hat{\imath}=1}^{M} \sum_{\hat{\jmath}=1}^{\mu_i} \mu_{\hat{\imath},\hat{\jmath}} = \bar{\mathcal{N}}. \tag{7}$$

$\mathcal{I}$ can also be identified as a subset of the reciprocal lattice. In particular, if we translate $\mathcal{I}$ by $(-1, -1, -1)$, we obtain the set of reflections

$$\mathcal{B}_{\mathbf{c}^*\mathbf{b}^*\mathbf{a}^*} \equiv \{(h_1, h_2, h_3) \;\Big|\; h_1 = 0, \ldots, (M-1), h_2 = 0, \ldots, (\mu_{h_1+1} - 1), \\ h_3 = 0, \ldots, (\mu_{h_1+1, h_2+1} - 1)\} \tag{8}$$

where subscript $\mathbf{c}^*\mathbf{b}^*\mathbf{a}^*$ on the lhs is a reminder of the fact that we considered first the different components of the $\vec{\delta}_j$ along $\mathbf{a}$, then those along $\mathbf{b}$ and lastly along $\mathbf{c}$. The vectors of $\mathcal{G}(\bar{\mathcal{N}})$ associated to these reflections are linearly independent. This important property is proven in Appendix B. It implies that any vector $|\mathbf{h}\rangle$ of $\mathcal{G}(\bar{\mathcal{N}})$ can be written as

$$|\mathbf{h}\rangle = \sum_{\mathbf{h}_l \in \mathcal{B}_{\mathbf{c}^*\mathbf{b}^*\mathbf{a}^*}} \alpha_{\mathbf{h},\mathbf{h}_l} |\mathbf{h}_l\rangle, \tag{9}$$

and, by Eq(1), that

$$\mathcal{I}_{\mathbf{h}} = \langle \mathbf{0} | \mathcal{Q} | \mathbf{h} \rangle = \sum_{\mathbf{h}_l \in \mathcal{B}(\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*)} \alpha_{\mathbf{h},\mathbf{h}_l} \langle \mathbf{0} | \mathcal{Q} | \mathbf{h}_l \rangle = \sum_{\mathbf{h}_l \in \mathcal{B}(\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*)} \alpha_{\mathbf{h},\mathbf{h}_l} \mathcal{I}_{\mathbf{h}_l}. \tag{10}$$

Since the vectors of the present Goedkoop lattice do not depend on the charges, the same property applies to the coefficients present in linear combinations (9) and (10) and, more generally, in any linear relation originated by a set of linearly dependent vectors. Unfortunately the $\vec{\delta}_j$s are the unknowns of our problem. Thus set (9) and any other set of linearly dependent reflections must be singled from the knowledge of a convenient set of $\mathcal{I}_{\mathbf{h}}$

values. In § 2.2 above Eq(I-20) we already mentioned a procedure able to ascertain whether a set of vectors is linearly independent or not. This procedure is a particular case of a more general mathematical property: consider a set $\mathcal{B}_M$ of M vectors of a Hilbert space and the matrix elements $\langle \mathbf{h}_m|A|\mathbf{h}_n\rangle$ of a Hermitian positive-definite operator A between any pair of two vectors of $\mathcal{B}_M$, then the vectors of $\mathcal{B}_M$ are linearly independent or dependent depending on whether $\det(A) > 0$ or $\det(A) = 0$, respectively. [Note that the positiveness of A implies that the inequality $\det(A) < 0$ never occurs.] In the case of x-ray scattering, according to (2) the operator $\mathcal{Q}$ is a positive-definite operator and, according to (1), the matrix elements of $\mathcal{Q}$ are the subtracted intensities. In this way, Eqs (I-20)-(I-28) are also valid in the present case provided $|\mathbf{h}\rangle$ is interpreted as a vector defined according to (3) and the $F_{\mathbf{h}}$s are substituted with the $\mathcal{I}_{\mathbf{h}}$s. In order to isolate the set $\mathcal{B}_{\mathbf{c}^*\mathbf{b}^*\mathbf{a}^*}$ we proceed as follows. We start with the reflection set containing the only reflection $\mathbf{h}_1 = \mathbf{0}$, *i.e.* $\mathcal{B}_1 \equiv \{\mathbf{h}_1\}$. Then we enlarge $\mathcal{B}_1$ to the set $\mathcal{B}_2 \equiv \{\mathbf{h}_1, \mathbf{h}_2\}$ obtained by "adding" to $\mathcal{B}_1$ the next reflection $\mathbf{h}_2 = (1, 0, 0)$ lying on the positive half-axis $\mathbf{a}^*$. The matrix elements of $\mathcal{Q}$ between the vectors determined by $\mathcal{B}_2$ is the (2×2) KH matrix $(\mathcal{D}_2)$ having its (i, j)th element equal $\langle \mathbf{h}_i|\mathcal{Q}|\mathbf{h}_j\rangle = \mathcal{I}_{\mathbf{h}_j-\mathbf{h}_i}$ with $i, j = 1, 2$. If $\det(\mathcal{D}_2) > 0$, we go on with the described enlargement procedure. The dimension of $\mathcal{G}(\bar{\mathcal{N}})$ is finite and therefore after, say, $(m+1)$ steps we must find a KH matrix $(\mathcal{D}_{m+1})$ such that $\det(\mathcal{D}_{m+1}) = 0$. At this point we shall say to have found a KH *zero* since we have found a KH matrix with determinant equal to zero. We conclude that the vector $|\mathbf{h}_{m+1}\rangle$ associated to last added reflection $\mathbf{h}_{m+1} = (m, 0, 0)$ is linearly dependent on $|\mathbf{h}_1\rangle, \ldots, |\mathbf{h}_m\rangle$. Besides, from (3.7) we also obtain that $M = m$ and in this way M is determined. Furthermore, the $\bar{\xi}_{\hat{\imath}}$ [see Eq (36)] are the roots of the polynomial equation obtained adapting (I-28) and (I-22) to the present case, namely

$$x^M - \sum_{i=0}^{M-1} \alpha_{M-1-i} x^i = 0 \tag{11}$$

with

$$\alpha_i = \sum_{j=1}^{M} \mathcal{D}^{-1}_{M;i+1,j} \mathcal{I}_{(M+1-j,0,0)}, \quad i = 0, \ldots, M-1. \tag{12}$$

The roots of (11) determine the $\bar{\xi}_{\hat{\imath}}$s that in turn determine the $\bar{x}_{\hat{\imath}}$s by (36). The vectors $|\bar{x}_{\hat{\imath}}, h_2, h_3\rangle$ are given from Eq (41) and one finds

$$\begin{aligned}\langle \bar{x}_{\hat{\imath}}, h'_2, h'_3|\mathcal{Q}|\bar{x}_{\hat{\imath}}, h_2, h_3\rangle &= \sum_{h_1, h'_1=0}^{M-1} \overline{\mathcal{V}^{-1}_{M;\hat{\imath},h'_1}(\bar{\xi})} \mathcal{V}^{-1}_{M;\hat{\imath},h_1}(\bar{\xi}) \langle h'_1, h'_2, h'_3|\mathcal{Q}|h_1, h_2, h_3\rangle \\ &= \sum_{h_1, h'_1=0}^{M-1} \overline{\mathcal{V}^{-1}_{M;\hat{\imath},h'_1}(\bar{\xi})} \mathcal{V}^{-1}_{M;\hat{\imath},h_1}(\bar{\xi}) \mathcal{I}_{(h_1-h'_1, h_2-h'_2, h_3-h'_3)}. \end{aligned} \tag{13}$$

It is stressed that the rhs is known in terms of quantities that are either experimentally known [the $\mathcal{I}_{(h_1-h'_1,h_2-h'_2,h_3-h'_3)}$s] or determined at the previous step [$\mathcal{V}^{-1}_{M;\hat{\imath},h_1}(\bar{\xi})$ being the $(\hat{\imath},h_1)$th element of the inverse of matrix (40)]. In the previous equation we set $h_3 = h'_3 = 0$ and we put

$$
\begin{aligned}
(\mathcal{D}_{\hat{\imath},m})_{h'_2,h_2} &\equiv \langle \bar{x}_{\hat{\imath}}, h'_2, 0|\mathcal{Q}|\bar{x}_{\hat{\imath}}, h_2, 0\rangle \\
&= \sum_{h_1,h'_1=0}^{M-1} \overline{\mathcal{V}^{-1}_{M;\hat{\imath},h'_1}(\bar{\xi})}\mathcal{V}^{-1}_{M;\hat{\imath},h_1}(\bar{\xi})\mathcal{I}_{(h_1-h'_1,h_2-h'_2,0)},
\end{aligned}
\tag{14}
$$

since we let h_2 and h'_2 vary over $(0,\ldots,m-1)$ so as the matrix elements of $\mathcal{Q}$ in the first row are the matrix elements of an $(m\times m)$ matrix denoted as $(\mathcal{D}_{\hat{\imath},m})$ where subscript $\hat{\imath}$ is a reminder of the first argument $\bar{x}_{\hat{\imath}}$ of the involved vectors. The operator $\mathcal{Q}$ being positive definite, the determinant of $(\mathcal{D}_{\hat{\imath},m})$ will be positive unless the considered vectors $|\bar{x}_{\hat{\imath}}, h_2, 0\rangle$ with $h_2 = 0,\ldots,(m-1)$ are linearly dependent. Similarly to the case just described, one start with $m = 1$ and, as far as $\det(\mathcal{D}_{\hat{\imath},m}) > 0$, one increases m step by step by one till finding $\det(\mathcal{D}_{\hat{\imath},m}) = 0$ that will still be called KH zero referred to matrices $(\mathcal{D}_{\hat{\imath},\cdot})$. In this way one determines the value of $\mu_{\hat{\imath}}$ that will be equal to m and $|\bar{x}_{\hat{\imath}}, m, 0\rangle$ can be written as

$$
|\bar{x}_{\hat{\imath}}, \mu_{\hat{\imath}}, 0\rangle = \sum_{h_2=0}^{\mu_{\hat{\imath}}-1} \alpha_{\hat{\imath},h_2}|\bar{x}_{\hat{\imath}}, h_2, 0\rangle, \quad \hat{\imath} = 1,\ldots,M. \tag{15}
$$

From this equation follows that

$$
\begin{aligned}
\langle \bar{x}_{\hat{\imath}}, h'_2, 0|\mathcal{Q}|\bar{x}_{\hat{\imath}}, \mu_{\hat{\imath}}, 0\rangle &= \sum_{h_2=0}^{\mu_{\hat{\imath}}-1} \alpha_{\hat{\imath},h_2}\langle \bar{x}_{\hat{\imath}}, h'_2, 0|\mathcal{Q}|\bar{x}_{\hat{\imath}}, h_2, 0\rangle, \\
&\qquad \hat{\imath} = 1,\ldots,M, \quad h'_2 = 0,\ldots,\mu_{\hat{\imath}}-1,
\end{aligned}
$$

that, by (14), becomes

$$
\begin{aligned}
(\mathcal{D}_{\hat{\imath},\mu_{\hat{\imath}}+1})_{h'_2,\mu_{\hat{\imath}}} &= \sum_{h_2=0}^{\mu_{\hat{\imath}}-1} (\mathcal{D}_{\hat{\imath},\mu_{\hat{\imath}}})_{h'_2,h_2}\alpha_{\hat{\imath},h_2}, \\
&\qquad \hat{\imath} = 1,\ldots,M, \quad h'_2 = 0,\ldots,\mu_{\hat{\imath}}-1.
\end{aligned}
$$

The solution of this system reads

$$
\begin{aligned}
\alpha_{\hat{\imath},h_2} &= \sum_{h'_2=0}^{\mu_{\hat{\imath}}-1} (\mathcal{D}^{-1}_{\hat{\imath},\mu_{\hat{\imath}}})_{h_2,h'_2}(\mathcal{D}_{\hat{\imath},\mu_{\hat{\imath}}+1})_{h'_2,\mu_{\hat{\imath}}}, \\
&\qquad \hat{\imath} = 1,\ldots,M, \quad h_2 = 0,\ldots,\mu_{\hat{\imath}}-1,
\end{aligned}
\tag{16}
$$

and the coefficients determining the linear combination (15) are now known. In order to get the polynomial equation whose roots determine $\bar{\eta}_{\hat{\imath},\hat{\jmath}}$s we first observe that the matrix element $\langle \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},1} | \bar{x}_{\hat{\imath}}, \mu_{\hat{\imath}}, 0\rangle$ by (15) becomes

$$\langle \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},1} | \bar{x}_{\hat{\imath}}, \mu_{\hat{\imath}}, 0\rangle = \sum_{h_2=0}^{\mu_{\hat{\imath}}-1} \alpha_{\hat{\imath},h_2} \langle \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},1} | \bar{x}_{\hat{\imath}}, h_2, 0\rangle.$$

The scalar products here present are immediately evaluated by (37) and one finds

$$\bar{\eta}_{\hat{\imath},\hat{\jmath}}^{\mu_{\hat{\imath}}} = \sum_{h_2=0}^{\mu_{\hat{\imath}}-1} \alpha_{\hat{\imath},h_2} \bar{\eta}_{\hat{\imath},\hat{\jmath}}^{h_2}, \qquad \hat{\imath} = 1, \ldots, M, \quad \hat{\jmath} = 1, \ldots, \mu_{\hat{\imath},\hat{\jmath}}. \tag{17}$$

Thus, fixed $\hat{\imath}$, the $\bar{\eta}_{\hat{\imath},\hat{\jmath}}$s, for $\hat{\jmath} = 1, \ldots, \mu_{\hat{\imath}}$, are the roots of the same polynomial equation of degree $\mu_{\hat{\imath}}$. The polynomial coefficients are given by Eq (16). Hence, for each $\hat{\imath}$ value, the solutions of the polynomial Eq (17) determine the $\bar{\eta}_{\hat{\imath},hj}$s and, consequently, the $\bar{y}_{\hat{\imath},hj}$s associated to the $\bar{x}_{\hat{\imath}}$s, already determined by solving Eq (11).
The determination of the $\mu_{\hat{\imath},\hat{\jmath}}$s and the $\bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}$s proceeds similarly starting from the vectors $|\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h_3\rangle$s that are given by Eq (46), where the involved matrix elements are know since the $\bar{\eta}_{\hat{\imath},\hat{\jmath}}$s have been determined. The matrix elements of the positive-definite operator $\mathcal{Q}$ between two of these vectors with $\hat{\imath}$ and $\hat{\jmath}$ fixed are

$$\langle \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h'_3 | \mathcal{Q} | \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h_3\rangle = \sum_{h'_2,h_2=0}^{\mu_{\hat{\imath}}-1} \overline{\Big(\mathcal{V}_{\mu_{\hat{\imath}}}{}^{-1}(\bar{\eta})\Big)_{\hat{\jmath},h'_2}} \Big(\mathcal{V}_{\mu_{\hat{\imath}}}{}^{-1}(\bar{\eta})\Big)_{\hat{\jmath},h_2} \times \langle \bar{x}_{\hat{\imath}}, h_2, h_3 | \mathcal{Q} | \bar{x}_{\hat{\imath}}, h_2, h_3\rangle.$$

By Eq (13) this becomes

$$\langle \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h'_3 | \mathcal{Q} | \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h_3\rangle = \sum_{h'_2,h_2=0}^{\mu_{\hat{\imath}}-1} \overline{\Big(\mathcal{V}_{\mu_{\hat{\imath}}}{}^{-1}(\bar{\eta})\Big)_{\hat{\jmath},h'_2}} \Big(\mathcal{V}_{\mu_{\hat{\imath}}}{}^{-1}(\bar{\eta})\Big)_{\hat{\jmath},h_2} \times \sum_{h_1,h'_1=0}^{M-1} \overline{\Big(\mathcal{V}_M^{-1}(\bar{\xi})\Big)_{\hat{\imath},h'_1}} \Big(\mathcal{V}_M^{-1}(\bar{\xi})\Big)_{\hat{\imath},h_1} \mathcal{I}_{(h_1-h'_1,h_2-h'_2,h_3-h'_3)} \tag{18}$$

that shows that the involved matrix elements of $\mathcal{Q}$ are now known. Similarly to (14) we shall now put

$$(\mathcal{D}_{\hat{\imath},\hat{\jmath},m})_{h'_3,h_3} \equiv \langle \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h'_3 | \mathcal{Q} | \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h_3\rangle, \qquad \hat{\imath} = 1, \ldots, M, \quad \hat{\jmath} = 1, \ldots, \mu_{\hat{\jmath}}, \tag{19}$$

where h_3 and h'_3 are assumed to run from 0 to $m-1$. Again, fixed $\hat{\imath}$ and $\hat{\jmath}$, we start with $m=1$, we evaluate $\det(\mathcal{D}_{\hat{\imath},\hat{\jmath},m})$ and if the determinant is different from zero we increase m by 1. At a particular step, say m , of this procedure we find a determinant equal to zero that is the KH zero relevant to matrices $(\mathcal{D}_{\hat{\imath},\hat{\jmath},.})$. Then we conclude that $\mu_{\hat{\imath},\hat{\jmath}}=m$ and we can write

$$|\bar{x}_{\hat{\imath}},\bar{y}_{\hat{\imath},\hat{\jmath}},\mu_{\hat{\imath},\hat{\jmath}}\rangle = \sum_{h_3=0}^{\mu_{\hat{\imath},\hat{\jmath}}-1}\alpha_{\hat{\imath},\hat{\jmath},h_3}|\bar{x}_{\hat{\imath}},\bar{y}_{\hat{\imath},\hat{\jmath}},h_3\rangle \tag{20}$$
$$\hat{\imath}=1,\ldots,M,\quad \hat{\jmath}=1,\ldots,\mu_{\hat{\imath}}.$$

The coefficients $\alpha_{\hat{\imath},\hat{\jmath},h_3}$ here present are obtained by solving the system of linear equations obtained considering the matrix elements of $\mathcal{Q}$ between the vectors $|\bar{x}_{\hat{\imath}},\bar{y}_{\hat{\imath},\hat{\jmath}},h_3\rangle$, with $h_3=0,\ldots,\mu_{\hat{\imath},\hat{\jmath}}-1$, and $|\bar{x}_{\hat{\imath}},\bar{y}_{\hat{\imath},\hat{\jmath}},\mu_{\hat{\imath},\hat{\jmath}}\rangle$. In this way, using (20) and definition (19), one finds

$$\alpha_{\hat{\imath},\hat{\jmath},h_3} = \sum_{h'_3=0}^{\mu_{\hat{\imath},\hat{\jmath}}-1}(\mathcal{D}^{-1}_{\hat{\imath},\hat{\jmath},\mu_{\hat{\imath},\hat{\jmath}}})_{h_3,h'_3}(\mathcal{D}_{\hat{\imath},\hat{\jmath},\mu_{\hat{\imath},\hat{\jmath}}+1})_{h'_3,\mu_{\hat{\imath},\hat{\jmath}}}$$
$$\hat{\imath}=1,\ldots,M,\quad \hat{\jmath}=1,\ldots,\mu_{\hat{\imath}}. \tag{21}$$

Finally the scalar product of (20) with $|\bar{x}_{\hat{\imath}},\bar{y}_{\hat{\imath},\hat{\jmath}},\bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}\rangle$ yields

$$\langle\bar{x}_{\hat{\imath}},\bar{y}_{\hat{\imath},\hat{\jmath}},\bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}|\bar{x}_{\hat{\imath}},\bar{y}_{\hat{\imath},\hat{\jmath}},\mu_{\hat{\imath},\hat{\jmath}}\rangle = \sum_{h_3=0}^{\mu_{\hat{\imath},\hat{\jmath}}-1}\alpha_{\hat{\imath},\hat{\jmath},h_3}\langle\bar{x}_{\hat{\imath}},\bar{y}_{\hat{\imath},\hat{\jmath}},\bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}|\bar{x}_{\hat{\imath}},\bar{y}_{\hat{\imath},\hat{\jmath}},h_3\rangle$$

that, using (42) and (34), becomes

$$\bar{\zeta}^{\mu_{\hat{\imath},\hat{\jmath}}}_{\hat{\jmath},\hat{\jmath},\hat{\ell}} = \sum_{h_3=0}^{\mu_{\hat{\imath},\hat{\jmath}}-1}\alpha_{\hat{\imath},\hat{\jmath},h_3}\bar{\zeta}^{h_3}_{\hat{\jmath},\hat{\jmath},\hat{\ell}}, \tag{22}$$
$$\hat{\imath}=1,\ldots,M,\quad \hat{\jmath}=1,\ldots,\mu_{\hat{\imath}},\quad \hat{\ell}=1,\ldots,\mu_{\hat{\imath},\hat{\jmath}}.$$

For fixed $\hat{\imath}$ and $\hat{\jmath}$ values, these equations show that the $\bar{\zeta}_{\hat{\jmath},\hat{\jmath},\hat{\ell}}$ with $\hat{\ell}=1,\ldots,\mu_{\hat{\imath},\hat{\jmath}}$ are the roots of a polynomial equation of the $\mu_{\hat{\imath},\hat{\jmath}}$th degree that is fully known since its coefficients are given by (21). At this point, the determination of the unknowns: M, $\mu_{\hat{\imath}}$, $\mu_{\hat{\imath},\hat{\jmath}}$, $\bar{x}_{\hat{\imath}}$, $\bar{y}_{\hat{\imath},\hat{\jmath}}$ and $\bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}$ is fully accomplished. Hence, from (7) and (5) we conclude that the number of the scattering centres and their spatial location have been determined. The determination of the charges ν_j is now straightforward. To this aim it is sufficient to solve the linear system of equations obtained considering Eq (I-16) for all the $\mathbf{h}$s of the set $\mathcal{B}_{\mathbf{c}^*\mathbf{b}^*\mathbf{a}^*}$ defined by (8).

Once we have also determined the ν_js all the quantities entering in the definition (I-16) of subtracted intensities are known. It follows that $\mathcal{I}_{\mathbf{h}}$ can be

evaluated for any $\mathbf{h}$ and this implies that the full diffraction pattern can be reconstructed from the knowledge of the subtracted intensities required to single out the basic set of reflection $\mathcal{B}_{\mathbf{c}^*\mathbf{b}^*\mathbf{a}^*}$. The reported procedure, able to single out this set, is based on the search of the first singular matrices $(\mathcal{D}_M)$, $(\mathcal{D}_{\hat{\imath},\mu_{\hat{\imath}}+1})$ [see Eq (14)] and $(\mathcal{D}_{\hat{\imath},\hat{\jmath},\mu_{\hat{\imath},\hat{\jmath}}+1})$ [see Eq (19) and (18)]. The expressions of these matrices show that it is necessary to know all the subtracted intensities relevant to the reflections that are difference of any two reflections that belong to set obtained obtained by "adding" to $\mathcal{B}_{\mathbf{c}^*\mathbf{b}^*\mathbf{a}^*}$ all the reflections that are nearest neighbour of its border and contained in the first octant of reciprocal space.
In concluding this section we remark that the most important part of the results first reported in § 2 of I have been obtained again by a different procedure that directly applies to the 3D case and explicitly reports the polynomial equations in a single variable that must be solved in order to determine the positions of the "charges". On the contrary, we must refer to I for the discussion of the iterative procedure that allows us to reconstruct the full diffraction pattern from a complete set of reflections. It is also noted that the basic set $\mathcal{B}_{\mathbf{c}^*\mathbf{b}^*\mathbf{a}^*}$ is different from those worked out in paper II. In particular, it is not one of the basic sets with the smallest size and therefore one should refer to II for the procedure that determines these sets.

2 The algebraic approach for neutron scattering

In the previous section we stressed that the vectors forming the present Goedkoop lattice are independent from the ν_js and only depend on the positions of the scattering centres. Hence a basic set of reflections preserves the property of being a set containing the largest number of linearly independent reflections whatever the charge values. On the other hand, we also stressed that a procedure able to single out a set of basic reflections must use experimentally known quantities. In the case of x-ray scattering it has been possible to find such a procedure because the observable subtracted intensities are the matrix elements of the charge operator $\mathcal{Q}$ that is positive-definite, so that the vanishing of the determinant of any $(m \times m)$ matrix with its elements equal to those of $\mathcal{Q}$ between any pair of vectors associated to a set of m reflections implies that the considered vectors are linearly dependent. This mathematical property can no longer be used in the case of neutron scattering because the charge operator $\mathcal{Q}$ in general is not positive-definite due to the fact that some ν_js can be smaller than zero. Therefore, in order to extend the search procedure of a basic set to the case of neutron scattering, we must find a positive definite operator whose matrix elements with respect to the $|\mathbf{h}\rangle$s are known in terms of the observed $I_{\mathbf{h}}$s. To this aim, denote by $\mathcal{S}_{obs}$ the set of the observed reflections and denote by $\mathcal{S}_1$ the largest subset of $\mathcal{S}_{obs}$ such that, for any two reflections $\mathbf{h}_r$ and $\mathbf{h}_{r'}$ of $\mathcal{S}_1$, it results that $(\mathbf{h}_r - \mathbf{h}_{r'})$ lies in $\mathcal{S}_{obs}$. We denote by $\bar{\mathcal{N}}_1$ the number of reflections contained in $\mathcal{S}_1$. First let us assume that $\mathcal{S}_1$ be large enough to contain a basic set (and the latter's border) so that $\bar{\mathcal{N}}_1 > \bar{\mathcal{N}}$. Consider now the linear operator[1]

$$\mathcal{Q}_{\mathcal{S}_1} \equiv \mathcal{Q} \sum_{r=1}^{\bar{\mathcal{N}}_1} |\mathbf{h}_r\rangle\langle\mathbf{h}_r|\mathcal{Q}. \tag{23}$$

This operator is hermitian and positive definite. The first property is evident. To show the second, we consider the expectation value of $\mathcal{Q}_{\mathcal{S}_1}$ with respect to an arbitrary vector $|a\rangle \in \mathcal{H}(\bar{\mathcal{N}})$. One finds that

$$\langle a|\mathcal{Q}_{\mathcal{S}_1}|a\rangle = \sum_{r-1}^{\bar{\mathcal{N}}_1} \Big|\langle a|\mathcal{Q}|\mathbf{h}_r\rangle\Big|^2$$

This expectation value can be equal to zero either if $\mathcal{Q}|a\rangle (\neq 0)$ is perpendicular to all the $|\mathbf{h}_r\rangle$s, with $r = 1, \ldots, \bar{\mathcal{N}}_1$, or if $\mathcal{Q}|a\rangle = 0$. The first condition is impossible because $\mathcal{S}_1$ is assumed to contain a basic set of vectors. We are left with the condition $\mathcal{Q}|a\rangle = 0$. This implies that $|a\rangle$ is eigenvector of $\mathcal{Q}$ with eigenvalue 0. But this condition is also impossible because the eigenvalues of $\mathcal{Q}$ are all different from zero as it appears evident from Eq. (2). Hence, $\langle a|\mathcal{Q}_{\mathcal{S}_1}|a\rangle > 0$ whatever $|a\rangle (\neq 0)$ and the positivity of $\mathcal{Q}_{\mathcal{S}_1}$ is proven. From (23) follows that the matrix elements of $\mathcal{Q}_{\mathcal{S}_1}$ with respect to the vectors of the Goedkoop lattice are

$$\langle\mathbf{h}|\mathcal{Q}_{\mathcal{S}_1}|\mathbf{k}\rangle = \sum_{r=1}^{\bar{\mathcal{N}}_1} I_{\mathbf{h}-\mathbf{h}_r} I_{\mathbf{h}_r-\mathbf{k}}.$$

If $\mathbf{h}, \mathbf{k} \in \mathcal{S}_1$, the matrix elements of $\mathcal{Q}_{\mathcal{S}_1}$ are fully known and will be denoted as

$$\mathcal{J}_{\mathbf{h}_l,\mathbf{h}_m} \equiv \langle\mathbf{h}_l|\mathcal{Q}_{\mathcal{S}_1}|\mathbf{h}_m\rangle = \sum_{r=1}^{\bar{\mathcal{N}}_1} I_{\mathbf{h}_l-\mathbf{h}_r} I_{\mathbf{h}_r-\mathbf{h}_m}, \quad l, m = 1, \ldots, \bar{\mathcal{N}}_1. \tag{24}$$

[It is noted that the $\mathcal{J}_{\mathbf{h}_l,\mathbf{h}_m}$'s are symmetric since they obey the relation $\mathcal{J}_{\mathbf{h}_l,\mathbf{h}_m} = \mathcal{J}_{\mathbf{h}_m,\mathbf{h}_l}$ that follows from the Friedel property valid for the subtracted

[1] The introduction of this quantity is suggested by the "tensorial" product used by Silva & Navaza (1981) and Navaza & Navaza (1992).

intensities, *i.e.* $I_{\mathbf{h}} = I_{-\mathbf{h}}$.] At this point, the search of a basic set becomes possible through the search of the KH zeros of the generalized KH matrices having their elements dependent on the $\mathcal{J}_{\mathbf{h}_l,\mathbf{h}_m}$s. It will proceed by one of the enlargement procedures described in the previous section or in § 5 of II. Whatever the adopted procedure, the search of a basic set is complete if and only if the final configuration of the found KH zeros is such to prevent a further enlargement of the set. Should the set $\mathcal{S}_1$ be not large enough to contain a basic set of reflections, this will be signaled by the fact that the resulting set can still be enlarged. It should appear clear that the use of $\mathcal{Q}_{\mathcal{S}_1}$ is only necessary to locate the KH zeros and to determine $\bar{\mathcal{N}}$, while the remaining unknowns $\vec{\delta}_j$ and ν_j are determined as in § 4.

A Quantum mechanical formulation

By using some notions of elementary Quantum Mechanics we show here how it is possible to introduce a finite-dimensional Hilbert space and, within the latter, a lattice of vectors in such a way that the scattering density (I-17) and the "subtracted" intensities (I-16) are two different representations of a single hermitian operator. This property holds true in both cases of x-ray and neutron scattering[2].

To this aim we recall that the position and momentum operator, respectively denoted by $\vec{\mathcal{R}}$ and $\vec{\mathcal{P}}$, have eigenvectors $|\mathbf{r}\rangle$ and $|\mathbf{p}\rangle$ whose eigenvalues $\mathbf{r}$ and $\mathbf{p}$ span the full 3D space R^3. Consider now the eigenvalues $\mathbf{p}$ equal to $-2\pi\mathbf{h}$, $\mathbf{h}$ being a triple of integers, and put $|\mathbf{h}) \equiv |-2\pi\mathbf{h}\rangle$. As $\mathbf{h}$ ranges over the 3D lattice $\mathcal{Z}^3$, the set of $|\mathbf{h})$'s defines a lattice of vectors lying within the infinite-dimensional Hilbert space $\mathcal{H}$ spanned by the eigenvectors $|\mathbf{p}\rangle$ or $|\mathbf{r}\rangle$. Introduce now the linear operator

$$\mathcal{Q} \equiv \sum_{\hat{\jmath}=1}^{\bar{\mathcal{N}}} |\vec{\delta}_{\hat{\jmath}}\rangle \nu_{\hat{\jmath}} \langle \vec{\delta}_{\hat{\jmath}}|, \tag{25}$$

where $|\vec{\delta}_{\hat{\jmath}}\rangle$ is the eigenvector of $\vec{\mathcal{R}}$ with eigenvalue $\vec{\delta}_{\hat{\jmath}}$ equal to the position vector of the $\hat{\jmath}$th scattering centre. Due to the property $\langle \mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}')$, the matrix elements of $\mathcal{Q}$ with respect to the eigenvectors of $\vec{\mathcal{R}}$ are

$$\langle \mathbf{r}|\mathcal{Q}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}') \sum_{\hat{\jmath}=1}^{\bar{\mathcal{N}}} \nu_{\hat{\jmath}} \delta(\mathbf{r}-\vec{\delta}_{\hat{\jmath}}) \tag{26}$$

[2] In passing we observe that this approach is not a simple mathematical trick as it is confirmed by the papers of Bethanis *et al.*(2002) and Ciccariello(2005).

At the same time, the matrix elements of $\mathcal{Q}$ with respect to the lattice vectors $|\mathbf{h})$ are

$$(\mathbf{h}|\mathcal{Q}|\mathbf{h}') = (2\pi)^{-3} \sum_{\hat{j}=1}^{\bar{\mathcal{N}}} \nu_{\hat{j}} e^{-i2\pi\vec{\delta}_{\hat{j}}\cdot(\mathbf{h}-\mathbf{h}')}, \tag{27}$$

where we used the property that $\langle \mathbf{p}|\mathbf{r}\rangle = e^{i\mathbf{p}\cdot\mathbf{r}}/(2\pi)^{3/2}$ and units such that $\hbar = 1$ (Messiah, 1959). Comparison of (26) with (I-17) shows that the scattering density (I-17) coincides with the diagonal matrix elements of $\mathcal{Q}$ (leaving aside the divergent factor related to the value $\delta(\mathbf{0})$ of the 1st Dirac function). On the other hand, the comparison of (27) with (I-16) shows that all the subtracted intensities (I-16) are $(2\pi)^3$ times the matrix elements of $\mathcal{Q}$ with respect to the lattice vectors $|\mathbf{h})$. Moreover, Eq.(25) shows that the "charge density" operator $\mathcal{Q}$ is determined only by the $\bar{\mathcal{N}}$ eigenvectors $|\vec{\delta}_1\rangle, \ldots, |\vec{\delta}_{\bar{\mathcal{N}}}\rangle$ of $\vec{\mathcal{R}}$ with eigenvalues equal to the positions of the $\bar{\mathcal{N}}$ scattering centres, and by the $\bar{\mathcal{N}}$ real numbers $\nu_1, \ldots, \nu_{\bar{\mathcal{N}}}$ equal to the weights of the scattering centres. Hence, we can restrict ourselves to the finite-dimensional Hilbert space $\mathcal{H}(\bar{\mathcal{N}})$ spanned by the vectors $|\vec{\delta}_1\rangle, \ldots, |\vec{\delta}_{\bar{\mathcal{N}}}\rangle$ and defined as

$$\mathcal{H}(\bar{\mathcal{N}}) \equiv \Big\{ |v\rangle = \sum_{j=1}^{\bar{\mathcal{N}}} \alpha_j |\vec{\delta}_j\rangle \Big| \;\; \alpha_1, \ldots, \alpha_{\bar{\mathcal{N}}} \in C \Big\}.$$

Vectors $|\vec{\delta}_1\rangle, \ldots, |\vec{\delta}_{\bar{\mathcal{N}}}\rangle$ obey the orthonormality condition[3]

$$\langle \vec{\delta}_{j'}|\vec{\delta}_j\rangle = \delta_{j',j}, \quad j, j' = 1, \ldots, \bar{\mathcal{N}} \tag{28}$$

as well as the completeness relation

$$\sum_{j=1}^{\bar{\mathcal{N}}} |\vec{\delta}_j\rangle\langle\vec{\delta}_j| = 1. \tag{29}$$

In order to preserve the validity of (27), we still need to assume that $\mathcal{H}(\bar{\mathcal{N}})$ contains a lattice of vectors $|\mathbf{h}\rangle$ [not to be confused with $|\mathbf{h})$ or with the eigenvectors of $\vec{\mathcal{P}}$, see the following Eq. (32)] defined by Eq (3). After taking the scalar product of $|\mathbf{h}\rangle$ with with $|\vec{\delta}_{j'}\rangle$ one gets

$$\langle \vec{\delta}_{j'}|\mathbf{h}\rangle = e^{-i2\pi\mathbf{h}\cdot\vec{\delta}_{j'}}, \quad \forall \mathbf{h} \in \mathcal{Z}^3, \; j' = 1, 2, \ldots, \bar{\mathcal{N}}. \tag{30}$$

From the above two relations it follows that vectors $|\mathbf{h}\rangle$ are no longer orthogonal since from (3) and (28) one gets

$$\langle \mathbf{h}|\mathbf{h}'\rangle = \sum_{j=1}^{\bar{\mathcal{N}}} e^{i2\pi\vec{\delta}_j\cdot(\mathbf{h}-\mathbf{h}')} = \langle \mathbf{h}+\mathbf{m}|\mathbf{h}'+\mathbf{m}\rangle, \quad \forall\; \mathbf{h}, \mathbf{h}', \mathbf{m} \in \mathcal{Z}^3, \tag{31}$$

[3] By so doing, the previous normalization $\langle \vec{\delta}_{j'}|\vec{\delta}_j\rangle = \delta(\vec{\delta}_{j'} - \vec{\delta}_j)$ has been scaled to $\langle \vec{\delta}_{j'}|\vec{\delta}_j\rangle = \delta_{j',j}$.

with $\langle \mathbf{h}|\mathbf{h}\rangle = \bar{\mathcal{N}}$. This property is not surprising if one observes that $|\mathbf{h}\rangle$ and $|\mathbf{h})$ are related as follows

$$|\mathbf{h}\rangle = (2\pi)^{3/2} \sum_{j=1}^{\bar{\mathcal{N}}} |\vec{\delta}_j\rangle\langle\vec{\delta}_j|\mathbf{h}) \tag{32}$$

so that $|\mathbf{h}\rangle$ is the projection of $|\mathbf{h})(\in \mathcal{H})$ into $\mathcal{H}(\bar{\mathcal{N}})$ and, therefore, it is no longer an eigenvector of $\vec{\mathcal{P}}$. It is straightforward to show by (3) and (28) that

$$\langle \mathbf{h}'|\mathcal{Q}|\mathbf{h}\rangle = \sum_{j=1}^{\bar{\mathcal{N}}} \nu_j e^{-i2\pi\vec{\delta}_j\cdot(\mathbf{h}'-\mathbf{h})} = I_{\mathbf{h}'-\mathbf{h}},$$

which coincides with (1). Thus, on the one hand, all the matrix elements of $\mathcal{Q}$ with respect to the lattice of vectors $|\mathbf{h}\rangle$ reproduce the full diffraction pattern. On the other hand, the diagonal matrix elements of $\mathcal{Q}$ with respect to the basis vectors $|\vec{\delta}_j\rangle$ are the weights of the scattering density (I-17). In this way, it has been shown that: both for X-ray and for neutron scattering it can be introduced a finite-dimensional Hilbert space $\mathcal{H}(\bar{\mathcal{N}})$ spanned by the $\bar{\mathcal{N}}$ eigenvectors of $\vec{\mathcal{R}}$ associated to the position vectors of the $\bar{\mathcal{N}}$ scattering centres; within $\mathcal{H}(\bar{\mathcal{N}})$ it exists a $\mathcal{G}(\bar{\mathcal{N}})$ vector lattice formed by the vectors $|\mathbf{h}\rangle$ defined by Eq. (3); it exists a hermitian linear operator $\mathcal{Q}$ whose matrix elements with respect to the basis vectors $|\vec{\delta}_j\rangle$ and to the vectors of $\mathcal{G}(\bar{\mathcal{N}})$ yield all the weights of the scattering density and all the subtracted intensities $I_{\mathbf{h}}$, respectively.

B Linear independence of the reflection set (8)

We prove now that the reflection of the set defined by Eq (8) are linearly independent. To this aim, we start by observing that Eq (5) allows us to write $\vec{\delta}_j$ as

$$|\vec{\delta}_j\rangle = |\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}\rangle \tag{33}$$

and Eq (28) implies that

$$\langle \bar{x}_{\hat{\imath}'}, \bar{y}_{\hat{\imath}',\hat{\jmath}'}, \bar{z}_{\hat{\imath}',\hat{\jmath}',\hat{\ell}'}|\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}\rangle = \delta_{\hat{\imath}',\hat{\imath}}\delta_{\hat{\jmath}',\hat{\jmath}}\delta_{\hat{\ell}',\hat{\ell}} \tag{34}$$

Then, the generic vector $|\mathbf{h}\rangle$ of $\mathcal{G}(\bar{\mathcal{N}})$ can be written as

$$|h_1, h_2, h_3\rangle = \sum_{\hat{\imath}=1}^{M} \sum_{\hat{\jmath}=1}^{\mu_{\hat{\imath}}} \sum_{\hat{\ell}=1}^{\mu_{\hat{\imath},\hat{\jmath}}} \bar{\xi}_{\hat{\imath}}^{h_1} \bar{\eta}_{\hat{\imath},\hat{\jmath}}^{h_2} \bar{\zeta}_{\hat{\imath},\hat{\jmath},\hat{\ell}}^{h_3} |\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}\rangle \tag{35}$$

where the rhs follows from (3), (34), (35) and the following definitions

$$\bar{\xi}_{\hat\imath} \equiv e^{-i2\pi\bar{x}_{\hat\imath}},\ \bar{\eta}_{\hat\imath,\hat\jmath} \equiv e^{-i2\pi\bar{y}_{\hat\imath,\hat\jmath}},\ \bar{\zeta}_{\hat\imath,\hat\jmath,\hat\ell} \equiv e^{-i2\pi\bar{z}_{\hat\imath,\hat\jmath,\hat\ell}} \tag{36}$$

similar to (I-26). Putting

$$|\bar{x}_{\hat\imath}, h_2, h_3\rangle \equiv \sum_{\hat\jmath=1}^{\mu_{\hat\imath}} \sum_{\hat\ell=1}^{\mu_{\hat\imath,\hat\jmath}} \bar{\eta}_{\hat\imath,\hat\jmath}^{h_2} \bar{\zeta}_{\hat\imath,\hat\jmath,\hat\ell}^{h_3} |\bar{x}_{\hat\imath}, \bar{y}_{\hat\imath,\hat\jmath}, \bar{z}_{\hat\imath,\hat\jmath,\hat\ell}\rangle \tag{37}$$

Eq (35) becomes

$$|h_1, h_2, h_3\rangle = \sum_{\hat\imath=1}^{M} \bar{\xi}_{\hat\imath}^{h_1} |\bar{x}_{\hat\imath}, h_2, h_2\rangle \tag{38}$$

The vectors $|\bar{x}_{\hat\imath}, h_2, h_3\rangle$ with h_2 and h_3 fixed and $\hat\imath = 1, \ldots, M$ are linearly independent because they are each other orthogonal since

$$\begin{aligned}\langle \bar{x}_{\hat\imath'}, h_2, h_3 | \bar{x}_{\hat\imath}, h_2, h_3\rangle \ &= \sum_{\hat\jmath'=1}^{\mu_{\hat\imath'}} \sum_{\hat\ell'=1}^{\mu_{\hat\imath',\hat\jmath'}} \sum_{\hat\jmath=1}^{\mu_{\hat\imath}} \sum_{\hat\ell=1}^{\mu_{\hat\imath,\hat\jmath}} \bar{\eta}_{\hat\imath',\hat\jmath'}^{-h_2} \bar{\zeta}_{\hat\imath',\hat\jmath',\hat\ell'}^{-h_3} \bar{\eta}_{\hat\imath,\hat\jmath}^{h_2} \bar{\zeta}_{\hat\imath,\hat\jmath,\hat\ell}^{h_3} \times \\ &\quad \langle \bar{x}_{\hat\imath'}, \bar{y}_{\hat\imath',\hat\jmath'}, \bar{z}_{\hat\imath',\hat\jmath',\hat\ell'} | \bar{x}_{\hat\imath}, \bar{y}_{\hat\imath,\hat\jmath}, \bar{z}_{\hat\imath,\hat\jmath,\hat\ell}\rangle = \delta_{\hat\imath',\hat\imath} \sum_{\hat\jmath=1}^{\mu_{\hat\imath}} \mu_{\hat\imath,\hat\jmath},\end{aligned} \tag{39}$$

where the last equality follows from (34). It follows that, fixed h_2 and h_3, the M vectors $|h_1, h_2, h_3\rangle$, with $h_1 = 0, 1, \ldots, (M-1)$, are linearly independent because, on the basis of (38), they are related to the $|\bar{x}_{\hat\imath}, h_2, h_3\rangle$ by a non-singular $(M \times M)$ Vandermonde matrix $\Big(\mathcal{V}_M(\bar\xi)\Big)$ having its $(h_1, \hat\imath)$th element equal to

$$\Big(\mathcal{V}_M(\bar\xi)\Big)_{h_1,\hat\imath} \equiv \bar{\xi}_{\hat\imath}^{h_1} = e^{-2i\pi\bar{x}_{\hat\imath}h_1}. \tag{40}$$

[The non singularity of this matrix is ensured by the property that $\bar\xi_1 \neq \bar\xi_2 \ldots \neq \bar\xi_M$ due to the facts that $\bar{x}_1 \neq \ldots \neq \bar{x}_M$ and $0 \le \bar{x}_{\hat\imath} < 1$ for $\hat\imath = 1, \ldots, M$.] Hence, by inverting (38), one can write

$$|\bar{x}_{\hat\imath}, h_2, h_3\rangle = \sum_{h_1=0}^{M-1} \Big({\mathcal{V}^{-1}}_M(\bar\xi)\Big)_{\hat\imath,h_1} |h_1, h_2, h_3\rangle. \tag{41}$$

We apply now the same procedure to the vectors defined by (37). Putting

$$|\bar{x}_{\hat\imath}, \bar{y}_{\hat\imath,\hat\jmath}, h_3\rangle \equiv \sum_{\hat\ell=1}^{\mu_{\hat\imath,\hat\jmath}} \bar{\zeta}_{\hat\imath,\hat\jmath,\hat\ell}^{h_3} |\bar{x}_{\hat\imath}, \bar{y}_{\hat\imath,\hat\jmath}, \bar{z}_{\hat\imath,\hat\jmath,\hat\ell}\rangle \tag{42}$$

vectors (37) can be written as

$$|\bar{x}_{\hat\imath}, h_2, h_3\rangle \equiv \sum_{\hat\jmath=1}^{\mu_{\hat\imath}} \bar{\eta}_{\hat\imath,\hat\jmath}^{h_2} |\bar{x}_{\hat\imath}, \bar{y}_{\hat\imath,\hat\jmath}, h_3\rangle. \tag{43}$$

Similarly to (39), the scalar products of two vectors (42) with the same h_3 value yield

$$\begin{aligned}\langle \bar{x}_{\hat{\imath}'}, \bar{y}_{\hat{\imath}',\hat{\jmath}'}, h_3 | \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h_3\rangle &= \sum_{\hat{\ell}'=1}^{\mu_{\hat{\imath}',\hat{\jmath}'}} \sum_{\hat{\ell}=1}^{\mu_{\hat{\imath},\hat{\jmath}}} \bar{\zeta}_{\hat{\imath}',\hat{\jmath}',\hat{\ell}'}^{-h_3} \bar{\zeta}_{\hat{\imath},\hat{\jmath},\hat{\ell}}^{h_3} \langle \bar{x}_{\hat{\imath}'}, \bar{y}_{\hat{\imath}',\hat{\jmath}'}, \bar{z}_{\hat{\imath}',\hat{\jmath}',\hat{\ell}'} | \bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}\rangle \\ &= \delta_{\hat{\imath}',\hat{\imath}} \delta_{\hat{\jmath}',\hat{\jmath}} \mu_{\hat{\imath},\hat{\jmath}}. \end{aligned} \tag{44}$$

Thus, at fixed $\hat{\imath}$ and h_3, we have $\mu_{\hat{\imath}}$ linearly independent $|\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h_3\rangle$ vectors. If we let h_2 range from 0 to $(\mu_{\hat{\imath}} - 1)$ in (43), one realizes that the resulting $(\mu_{\hat{\imath}} - 1)$ vectors $|\bar{x}_{\hat{\imath}}, h_2, h_3\rangle$ [with $\hat{\imath}$ and h_3 fixed] are related to the previous vectors by a $(\mu_{\hat{\imath}} \times \mu_{\hat{\imath}})$ Vandermonde matrix with elements

$$\Big(\mathcal{V}_{\mu_{\hat{\imath}}}(\bar{\eta})\Big)_{h_2,\hat{\jmath}} \equiv \bar{\eta}_{\hat{\imath},\hat{\jmath}}^{h_2} = e^{-2i\pi \bar{y}_{\hat{\imath},\hat{\jmath}} h_2}. \tag{45}$$

The involved $\bar{\eta}_{\hat{\imath},\hat{\jmath}}$s being all different among themselves once $\hat{\imath}$ has been fixed, the matrix is non-singular and (43) can be inverted to read

$$|\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h_3\rangle \equiv \sum_{h_2=0}^{\mu_{\hat{\imath}}-1} \Big(\mathcal{V}_{\mu_{\hat{\imath}}}{}^{-1}(\bar{\eta})\Big)_{\hat{\jmath},h_2} |\bar{x}_{\hat{\imath}}, h_2, h_3\rangle. \tag{46}$$

Similar considerations applied to Eq (42) show that the vectors $|\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h_3\rangle$, with $h_3 = 0, \ldots, (\mu_{\hat{\imath},\hat{\jmath}} - 1)$ and fixed $\hat{\imath}$ and $\hat{\jmath}$, are linearly independent because they are related to the $\mu_{\hat{\imath},\hat{\jmath}}$ vectors present on the rhs of (42) by the $(\mu_{\hat{\imath},\hat{\jmath}} \times \mu_{\hat{\imath},\hat{\jmath}})$ Vandermonde matrix, with elements

$$\Big(\mathcal{V}_{\mu_{\hat{\imath},\hat{\jmath}}}(\bar{\zeta})\Big)_{h_3,\hat{\ell}} \equiv \bar{\zeta}_{\hat{\imath},\hat{\jmath},\hat{\ell}}^{h_3} = e^{-2i\pi \bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}} h_3}, \tag{47}$$

which is non-singular because all the $\bar{\zeta}_{\hat{\imath},\hat{\jmath},\hat{\ell}}$ are different among themselves for $\hat{\ell} = 1, \ldots, \mu_{\hat{\imath},\hat{\jmath}}$ and $\hat{\imath}$ and $\hat{\jmath}$ fixed. Thus, (42) can be inverted to read

$$|\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}\rangle = \sum_{h_3=0}^{\mu_{\hat{\imath},\hat{\jmath}}-1} \Big(\mathcal{V}_{\mu_{\hat{\imath},\hat{\jmath}}}^{-1}(\bar{\zeta})\Big)_{\hat{\ell},h_3} |\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, h_3\rangle. \tag{48}$$

We observe now that, if $\mathbf{h}$ belongs to the set defined by (8), $|\mathbf{h}\rangle$ can be written as

$$\begin{aligned}|h_1, h_2, h_3\rangle &= \sum_{\hat{\imath}=1}^{M} \sum_{\hat{\jmath}=1}^{\mu_{\hat{\imath}}} \sum_{\hat{\ell}=1}^{\mu_{\hat{\imath},\hat{\jmath}}} \Big(\mathcal{V}_M(\bar{\xi})\Big)_{h_1,\hat{\imath}} \Big(\mathcal{V}_{\mu_{\hat{\imath}}}(\bar{\eta})\Big)_{h_2,\hat{\jmath}} \times \\ &\quad \Big(\mathcal{V}_{\mu_{\hat{\imath},\hat{\jmath}}}(\bar{\zeta})\Big)_{h_3,\hat{\ell}} |\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}\rangle,\end{aligned} \tag{49}$$

that, due to the non-singularity of the involved matrices, can be inverted as

$$|\bar{x}_{\hat{\imath}}, \bar{y}_{\hat{\imath},\hat{\jmath}}, \bar{z}_{\hat{\imath},\hat{\jmath},\hat{\ell}}\rangle = \sum_{h_1=0}^{M-1} \sum_{h_2=0}^{\mu_{\hat{\imath}}-1} \sum_{h_3=0}^{\mu_{\hat{\imath},\hat{\jmath}}-1} \Big(\mathcal{V}_M^{-1}(\bar{\xi})\Big)_{\hat{\imath},h_1} \times \Big(\mathcal{V}_{\mu_{\hat{\imath}}}^{-1}(\bar{\eta})\Big)_{\hat{\jmath},h_2} \Big(\mathcal{V}_{\mu_{\hat{\imath},\hat{\jmath}}}^{-1}(\bar{\zeta})\Big)_{\hat{\ell},h_3} |h_1, h_2, h_3\rangle. \tag{50}$$

In this way, the linear independence of the reflections of the set (8) is proven. In passing, it is also noted that the determinant of the block-matrix relating the rhs to the lhs of (49) has a simple algebraic expression (Cervellino & Ciccariello, 2005).

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