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FINITE FRAMES AND FINITE FRAME QUANTIZATIONS*

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Abstract. A finite-dimensional Hilbert space is usually described in terms of an orthonormal basis, but in certain applications a description in terms of a finite overcomplete system of vectors, called a finite frame, may offer some advantages. The use of a finite frame may lead to a simpler description of the symmetry transformations, to a simpler and more symmetric form of invariants or the possibility to define new mathematical objects with physical meaning. We present some general results concerning the notion of finite frame, several examples and suggest some possible applications.

Key words: finite frames, overcomplete basis, Klauder-Berezin-Toeplitz quantization.

1. INTRODUCTION

Although, at first glance, a system described by a finite-dimensional Hilbert space looks much simpler than one described by an infinite dimensional space, there is much more knowledge about the latter than the former. Our aim is to present some results concerning the finite frames [1, 3, 5] and their applications in physics. Particularly, we try to prove that some mathematical methods used in modeling crystalline or quasicrystalline structures are in fact based on certain finite frames. The descriptions of a physical system in terms of a finite frame allows us to associate a linear operator to a classical observable. The procedure, not necessarily a path to a quantum approach, can be regarded as an extended version of the Klauder-Berezin-Toeplitz quantization and represents a change of point of view in considering the physical system [4].

2. FINITE FRAMES

Let **K** be the field **R** or **C**, and let ***H*** be a n-dimensional Hilbert space over **K** with $\{|1\rangle,\ |2\rangle,\ \ldots,|n\rangle\}$ a fixed orthonormal basis. A system of vectors $|u_1\rangle, |u_2\rangle, \ldots, |u_m\rangle$ from ***H*** will be called a (finite) *frame* if

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$$\langle u_i \mid u_i \rangle = 1 \text{ for any } i \in \{1,2,...,m\} \tag{1}$$

and there exist some positive constants $k_1, k_2, \ldots, k_m$ such that

$$\sum_{i=1}^{m} k_i |u_i\rangle\langle u_i| = \mathrm{I}_H \tag{2}$$

that is,

$$\sum_{i=1}^{m} k_i |u_i\rangle\langle u_i \mid v\rangle = |v\rangle \quad \text{for any } |v\rangle \in \boldsymbol{H}. \tag{3}$$

In this case we have

$$\langle v \mid w\rangle = \sum_{i=1}^{m} k_i \langle v \mid u_i\rangle\langle u_i \mid w\rangle,\ \|\mathrm{v}\|^2 = \sum_{i=1}^{m} k_i\, |\langle u_i \mid v\rangle|^2, \tag{4}$$

for any $|v\rangle$, $|w\rangle \in \boldsymbol{H}$ and one can remark that

$$n = \sum_{j=1}^{n} \langle j \mid j\rangle = \sum_{j=1}^{n}\sum_{i=1}^{m} k_i\, |\langle u_i \mid j\rangle|^2 = \sum_{i=1}^{m} k_i \sum_{j=1}^{n} |\langle u_i \mid j\rangle|^2 = \sum_{i=1}^{m} k_i. \tag{5}$$

Particularly, if $k_1 = k_2 = ... = k_m$ the the relations (2) and (4) become

$$\frac{n}{m}\sum_{i=1}^{m} |u_i\rangle\langle u_i| = I_H \tag{6}$$

and

$$\langle v \mid w\rangle = \frac{n}{m}\sum_{i=1}^{m} \langle v \mid u_i\rangle\langle u_i \mid w\rangle, \quad \|\mathrm{v}\|^2 = \sum_{i=1}^{m} |\langle u_i \mid v\rangle|^2. \tag{7}$$

3. FINITE FRAMES DEFINED BY USING GROUP REPRESENTATIONS

Some useful frames can be defined in a natural way by using the group representations. Let $\{g : \boldsymbol{H} \to \boldsymbol{H} \mid g \in \boldsymbol{G}\}$ be an orthogonal (resp. unitary) irreductible representation of a finite group G in the real (resp. complex) n-dimensional Hilbert space $\boldsymbol{H}$, and let $|u\rangle \in \boldsymbol{H}$ be a fixed unit vector. The elements $g \in \boldsymbol{G}$ with the property

$$g|u\rangle = \alpha|u\rangle, \tag{8}$$

where α is a scalar depending on g, form the stationary group $\boldsymbol{G}_u$ of $|u\rangle$.

THEOREM. *If g_1, g_2,...,g_m is a system of representatives of the left cosets of **G** on $\boldsymbol{G}_u$ then*

$$|u_1\rangle = g_1|u\rangle,\ |u_2\rangle = g_2|u\rangle,\ldots,\ |u_m\rangle = g_{2m}|u\rangle \tag{9}$$

*is a frame in **H**, namely*

$$\frac{n}{m}\sum_{i=1}^{m}|u_i\rangle\langle u_i| = I_H\ . \tag{10}$$

Proof. The operator $\Lambda : \boldsymbol{H}\to\boldsymbol{H},\ \Lambda\,|v\rangle=\sum_{i=1}^{m}|u_i\rangle\langle u_i\mid v\rangle$ is self-adjoint

$$\langle w\,|\,(\Lambda\,|\,v\rangle\,)=\sum_{i=1}^{m}\langle w\,|\,u_i\rangle\langle u_i\mid v\rangle=(\langle w\,|\,\Lambda)\,|\,v\rangle$$

and therefore, it has a real eigenvalue λ. Since the eigenspace $\{|v\rangle;\ \Lambda\,|v\rangle = \lambda|v\rangle\}$ corresponding to λ is **G**-invariant

$$\Lambda\,(\mathrm{g}|v\rangle\,)=\sum_{i=1}^{m}|u_i\rangle\langle u_i\mid(g\mid v\rangle = \sum_{i=1}^{m}g|u_i\rangle\langle u_i\mid v\rangle = g(\langle\Lambda\mid v\rangle)$$

and the representation is irreductible we must have
$\Lambda|v\rangle = \lambda|v\rangle$ for any $|v\rangle\in\boldsymbol{H}$. By using an orthogonal basis $\{|1\rangle,\ |2\rangle,\ \ldots,|n\rangle\}$ of **H** we get $n\lambda=\sum_{j=1}^{n}\langle j\,|\,\Lambda\,|\,j\rangle=\sum_{j=1}^{n}\sum_{i=1}^{m}\langle j\,|\,u_i\rangle\langle u_i\,|\,j\rangle=\sum_{i=1}^{m}\sum_{j=1}^{n}|\langle j\,|\,u_i\rangle|^2=m.$

4. HONEYCOMB LATTICE IN TERMS OF A FINITE FRAME

The unit vectors $|u_1\rangle=(1,0),\ |u_2\rangle=\left(-\frac{1}{2},\frac{\sqrt{3}}{2}\right),\ |u_3\rangle=\left(-\frac{1}{2},-\frac{\sqrt{3}}{2}\right)$ (11)

from a frame in $\mathbf{R}^2$, namely, $\frac{2}{3}\sum_{i=1}^{3}|u_i\rangle\langle u_i\,|\,v\rangle=|v\rangle$ for any $|v\rangle\in\mathbf{R}^2$. (12)

The symmetry properties of certain discrete sets can be simpler described by using a frame instead of a basis. Honeycomb lattice is a discrete subset £ of the plane such that each point P ∈ £ has three nearest neighbours forming an equilateral triangle with the center at P. It can be described in a natural way by using the frame (11) as the set [6]

$$£ = \{ n_1 \left| u_1 \right\rangle + n_2 \left| u_2 \right\rangle + n_3 \left| u_3 \right\rangle \quad | \ (n_1, n_2, n_3) \in \mathbf{L} \} \tag{13}$$

where the subset

$$\mathbf{L} = \{ n = (n_1, n_2, n_3) \in \mathbf{Z}^3 \} | \ n_1 + n_2 + n_3 \in \{0, 1\} \} \tag{14}$$

of $\mathbf{Z}^3$ can be regarded as a mathematical model. The nearest neighbours of $n \in \mathbf{L}$ are

$$\begin{aligned} n^1 &= (n_1 + v(n), n_2, n_3) \\ n^2 &= (n_1, n_2 + v(n), n_3) \\ n^3 &= (n_1, n_2, n_3 + v(n)), \end{aligned} \tag{15}$$

where $v(n) = (-1)^{n_1 + n_2 + n_3}$

The six points $n^{ij} = (n^i)^j$ corresponding to $i \neq j$ are the next-to-nearest neighbours, and one can remark that $n^{ii} = n$, $n^{ijl} = n^{lji}$, for any $i, j, l \in \{1, 2, 3\}$. The mapping

$$d{:}\mathbf{L} \times \mathbf{L} \to \mathbf{Z} \quad d(n, n') = |n_1 - n'_1| + |n_2 - n'_2| + |n_3 - n'_3| \tag{16}$$

is a distance of **L**, and a point n' is a neighbour of order l of n if $d(n, n') = l$.
The symmetry group **G** of the honeycomb lattice is isomorphic with the group of all the isometries space (**L**, d), group generated by the transformations

$$\begin{aligned} \mathbf{L} \to \mathbf{L}&: (n_1, n_2, n_3) \mapsto (n_2, n_3, n_1) \\ \mathbf{L} \to \mathbf{L}&: (n_1, n_2, n_3) \mapsto (n_1, n_3, n_2) \\ \mathbf{L} \to \mathbf{L}&: (n_1, n_2, n_3) \mapsto (-n_1 + 1, -n_2, -n_3). \end{aligned} \tag{17}$$

Honeycomb lattice is a mathematical model for a grapheme sheet and the use of the indicated frame leads to a simpler and more symmetric form for G-invariant mathematical objects occurring in the description of certain physical properties [2].

5. FINITE FRAME QUANTIZATION

Let $\chi = \{a_1, a_2, \ldots.. a_n\}$ be a set of data concerning a physical system. The space of all the functions $\varphi : \chi \to \mathbf{K}$ is a Hilbert space with the scalar product

$$\langle \varphi | \psi \rangle = \sum_{x \in \chi} \overline{\varphi(x)} \psi(x) \tag{18}$$

and the isometry

$$l^2(\chi) \to K^m : \varphi \mapsto (\varphi(1), \varphi((2), ..., \varphi(m)), \tag{19}$$

allows us to identify the space $l^2(\chi)$ with the usual m-dimensional Hilbert space $\mathbf{K}^m$. The system of functions $\{\delta_1, \delta_2, ..., \delta_m\}$, where

$$\delta_i : \chi \to \mathbf{K}, \qquad \delta_i(x) = \begin{cases} 1 & \text{if} \quad x = a_i \\ 0 & \text{if} \quad x \neq a_i \end{cases} \tag{20}$$

in an orthonormal basis in $l^2(\chi)$

$$\varphi = \sum_{i=1}^{m} \langle \delta_i | \varphi \rangle \delta_i = \sum_{i=1}^{m} \varphi(a_{i1}) \delta_{i.} \tag{21}$$

Let us select among the elements of $l^2(M)$ an orthonormal set

$$\{\phi_{1,} \phi_2, ..., \phi_n\} \text{ such that } \quad k_i = \sum_{j=1}^{n} |\phi_j(a_i)|^2 \neq 0, \quad \text{for all } i \in \{1, 2, ..., m\} \tag{22}$$

and let $\boldsymbol{H}$ = span$\{\phi_1, \phi_2, ..., \phi_n\}$. In view of theorem, the elements

$$|u_i\rangle = \frac{1}{\sqrt{k_i}} \sum_{j=1}^{n} \langle \phi_j | \delta_i \rangle \phi_j = \frac{1}{\sqrt{k_i}} \sum_{j=1}^{n} \overline{\phi_j(a_i)} \phi_j, \quad i \in \{1, 2, ..., m\} \tag{23}$$

form a frame in **H**, namely, $$\sum_{i=1}^{m} k_1 |u_i\rangle \langle u_i| = I_H \tag{24}$$

If $\varphi : \chi \to \mathbf{K}$ is such that $\|\varphi\| = \sqrt{\langle \varphi, \varphi \rangle} = 1$ then

$$\sum_{i=1}^{m} \left| \sqrt{k_i} \langle \varphi | u_i \rangle \right|^2 = \sum_{i=1}^{m} k_i \left| \langle \varphi | u_i \rangle \right|^2 = \|\varphi\|^2 = 1 \tag{25}$$

and hence, $\left| \sqrt{k_i} \langle \varphi | u_i \rangle \right|^2$ can be regarded as the probability to find φ in the state $|u_i\rangle$.

To each function $f : \chi \to \mathbf{R}$ which we can regard as a *classical* observable we associate the linear operator

$$\mathrm{A}_f : \boldsymbol{H} \to \boldsymbol{H}, \qquad A_f = \sum_{i-1}^{m} k_i f(a_i) \left| u_i \right\rangle \left\langle u_i \right|. \tag{26}$$

This can be regarded as a Berezin-Klauder type quantization of f , the notion of quantization being considered here a large sense [4]. The function f is called upper (or contravariant) symbol of A_f , and the function

$$\chi \to \mathbf{R}: a_i \mapsto \left\langle u_i \mid A_f \mid u_i \right\rangle \tag{27}$$

is called lower (or covariant) symbol of A_f . To a certain existent, a quantization scheme consists in adopting a certain point of view in dealing with χ. The presented frame quantization $f \mapsto A_f$ depends on the subspace $\boldsymbol{H} \subset l^2(\chi)$ we choose. The validity of the frame quantization corresponding to a certain subspace $\boldsymbol{H}$ is asserted by comparing spectral characteristics of A_f with data provided by specific protocol in the observation of the considered physical system.

6. AN APPLICATION OF THE FRAME QUANTIZATION TO CRYSTALS

The set $\mathbf{Z}\times\mathbf{Z}$ can be regarded as a mathematical model for two-dimensional crystal. By imposing the cyclic boundary condition, the space $\varepsilon = l^2(\mathbf{Z}_N \times \mathbf{Z}_N)$ and the operator

$$\mathrm{H}: \varepsilon \to \varepsilon,$$

$$(\mathrm{H}\psi)(n_1, n_2) = \psi(n_1 + 1, n_2) + \psi(n_1 - 1, n_2) + \psi(n_1, n_2 + 1) + \psi(n_1, n_2 - 1). \tag{28}$$

Allow one to describe the electron evolution inside the crystal in the tight bonding approximation. For any $k=(k_1,k_2) \in \mathbf{Z}_N \times \mathbf{Z}_N$, the function

$$\psi_k : \mathbf{Z}_N \times \mathbf{Z}_N \to \mathbf{C}, \quad \psi_k(n_1, n_2) = \mathrm{e}^{\frac{2\pi i}{N}(k_1 n_1 + k_2 n_2)} \tag{29}$$

is an eigenfunction of H corresponding to the eigenvalue

$$E_k = \mathrm{e}^{\frac{2\pi i}{N}k_1} + e^{-\frac{2\pi i}{N}k_1} + e^{\frac{2\pi i}{N}k_2} + e^{-\frac{2\pi i}{N}k_2} = 2\cos\frac{2\pi}{N}k_1 + 2\cos\frac{2\pi}{N}k_2. \tag{30}$$

That is

$$\mathrm{H}\psi = E_k \psi_k. \tag{31}$$

One can remark that

$$E_k = \sum_{(n_1, n_2 \in C)} \psi_k(n_1, n_2) \tag{32}$$

where C is the cluster

$$C=\{(1,0), (-1,0), (0,1), (0,-1)\} \subset \mathrm{Z}_N \times \mathrm{Z}_N . \tag{33}$$

The Hilbert space $l^2(C)$ can be identified with the subspace

$$\boldsymbol{H}:=\{ \varphi : \mathbf{Z}_N \times \mathbf{Z}_N \to \mathbf{C} \mid \varphi(n_1, n_2) = 0 \ \text{ for } (\mathrm{n}_1, n_2) \notin C\}. \tag{34}$$

The N^2 functions $\{ \left| \delta_{(n_1,n_2)} \right\rangle = \delta_{(n_1,n_2)} : \mathbf{Z}_N \times \mathbf{Z}_N \to \mathbf{C}\}_{n_1,n_2 \in Z_N}$

$$\delta_{(n_1,n_2)}(n_1', n_2') = \begin{cases} 1 & \text{if} \quad (n_1', n_2') = (n_1, n_2) \\ 0 & \text{if} \quad (n_1', n_2') \neq (n_1, n_2) \end{cases} \tag{35}$$

and the N^2 functions $\{ \left| \psi_{(k_1,k_2)} \right\rangle = \psi_{(k_1,k_2)} : \mathbf{Z}_N \times \mathbf{Z}_N \to \mathbf{C}\}_{k_1,k_2 \in Z_N}$

$$\psi_{(k_1,k_2)}(n_1, n_2) = \frac{1}{N} \ \mathrm{e}^{\frac{2\pi i}{N}(k_1 n_1 + k_2 n_2)} \tag{36}$$

from two orthonormal bases of ε related through the discrete Fourier transform.

The orthogonal projector corresponding to

$$\boldsymbol{H} \text{ is } \pi = \sum_{(n_1, n_2 \in C)} \left| \delta_{(n_1,n_2)} \right\rangle \left\langle \delta_{(n_1,n_2)} \right| \tag{37}$$

and in the view of theorem, the N^2 functions $\{ \left| k_1, k_2 \right\rangle : \mathbf{Z}_N \times \mathbf{Z}_N \to \mathbf{C}\}_{k_1,k_2 \in Z_N}$

$$\left| k_1, k_2 \right\rangle = \frac{1}{2} \sum_{(n_1,n_2) \in C} \mathrm{e}^{\frac{2\pi \mathrm{i}}{\mathrm{N}}(k_1 n_1 + k_2 n_2)} \left| \delta_{(n_1,n_2)} \right\rangle \tag{38}$$

from a frame in H

$$\frac{4}{N^2} \sum_{k_1,k_2=0}^{N-1} \left| k_1, k_2 \right\rangle \left\langle k_1, k_2 \right| = I_H . \tag{39}$$

They satisfy the relation

$$\left\langle k_1,k_2 \mid k_1^{'},k_2^{'}\right\rangle = \frac{1}{4}\sum_{(n_1,n_2)\in C} \mathrm{e}^{\frac{2\pi \mathrm{i}}{\mathrm{N}}\{(k_1^{'}-k_1)n_1+(k_2^{'}-k_2)n_2\}} =$$

$$= \frac{1}{2}\left[\cos\frac{2\pi}{N}(k_1^{'}-k_1)+\cos\frac{2\pi}{N}(k_2^{'}-k_2)\right]. \tag{40}$$

To a *classical* observation defined by *f*: $\mathbf{Z}_N \times \mathbf{Z}_N \to \mathbf{R}$ we associate the linear operator

$$A_f : \boldsymbol{H}\to \boldsymbol{H},\quad A_f = \frac{4}{N^2}\sum_{k_1,k_2=0}^{N-1} f(k_1,k_2)\left|k_1,k_2\right\rangle\left\langle k_1,k_2\right|, \tag{41}$$

with the lower symbol

$$\left\langle k_1,k_2 \mid A_f \mid k_1,k_2\right\rangle = \sum_{k_1^{'},k_2^{'}=0}^{N-1} f(k_1^{'},k_2^{'})\left[\cos\frac{2\pi}{N}(k_1^{'}-k_1)+\cos\frac{2\pi}{N}(k_2^{'}-k_2)\right]^2 . \tag{42}$$

In the case of the frame quantization we analyze a classical observable by using a suitable smaller dimensional subspace. We can increase the resolution of our analysis by choosing a larger chuster including second order and third order neighbours of (0,0).

7. DISCRETE VERSION OF THE SPHERE AND ITS QUANTIZATION

The subset *C*= $\{u_1,u_2,...,u_{12}\}$of the unit sphere $S^2=\{x\in\mathbf{R}^3;\ \|x\|=1\}$ formed by the twelve vertices of a regular icosahedron

$$\begin{aligned} &u_1=-u_7=\frac{1}{\sqrt{\tau+2}}(1,\tau,0), && u_2=-u_8=\frac{1}{\sqrt{\tau+2}}(-1,\tau,0),\\ &u_3=-u_9=\frac{1}{\sqrt{\tau+2}}(-\tau,0,1) && u_4=-u_{10}=\frac{1}{\sqrt{\tau+2}}(0,-1,\tau),\\ &u_5=-u_{11}=\frac{1}{\sqrt{\tau+2}}(\tau,0,1), && u_6=-u_{12}=\frac{1}{\sqrt{\tau+2}}(0,1,\tau), \end{aligned} \tag{43}$$

where $\tau=(1+\sqrt{5})/2$ can be regarded as a discrete version of S^2. The group I of all the rotations of $\mathbf{R}^3$ leaving the set C invariant is called *icosahedral group* and is generated by the rotations

$$r(\alpha,\beta,\gamma)=\left(\frac{\tau-1}{2}\alpha-\frac{\tau}{2}\beta+\frac{1}{2}\lambda,\frac{\tau}{2}\alpha+\frac{1}{2}\beta+\frac{\tau-1}{2}\gamma,-\frac{1}{2}\alpha+\frac{\tau-1}{2}\beta+\frac{\tau}{2}\gamma\right),$$

$$s(\alpha,\beta,\gamma)=(-\alpha,-\beta,\gamma) \tag{44}$$

satisfy the relation $r^5=s^2=(rs)^3=I_{R^3}$. The stationary group $\Im_{u_1}$ of u_1 is formed by the rotations $g\in\Im$ with $gu_1\in\{u_1,-u_1\}$, and we can choose the representatives $g_1,g_2,...,g_6$ of the cosets of $\Im$ on $\Im_{u_1}$ such that

$$g_1u_1=u_1,\quad g_2u_1=u_2,\quad g_3u_1=u_3,\quad g_4u_1=u_4,\quad g_5u_1=u_5,\quad g_6u_1=u_6.$$

In view of theorem, the vectors $|u_1\rangle$, $|u_2\rangle,...,$ $|u_6\rangle$ from a frame in $\mathbf{R}^3$

$$\frac{3}{6}\sum_{i=1}^{6}|u_i\rangle\langle u_i|=\mathrm{I}_{R^3}. \tag{45}$$

From (43) it follows that

$$\frac{3}{12}\sum_{i=1}^{12}|u_i\rangle\langle u_i|=\mathrm{I}_{R^3} \tag{46}$$

that is, the whole orbit C is also a frame in $\mathbf{R}^3$.

The frame quantization of a *classical* observable f: $C\rightarrow\mathbf{R}$ consists in associating to f the operator

$$\mathrm{A}_f:\mathbf{R}^3\rightarrow\mathbf{R}^3,\qquad A_f=\frac{3}{12}\sum_{i=1}^{12}f(u_i)|u_i\rangle\langle u_i|. \tag{47}$$

We can increase the resolution of our discrete description of S^2 by using longer orbits of $\Im$. For example, we can use the orbit $C'=\{u'_1,u'_2,...,u'_{20}\}$ formed by vertices of a regular dodecahedron

$$\begin{aligned}
&u_1^{'} = -u_{11}^{'} = \frac{1}{\sqrt{3}}(1,1,1), && u_2^{'} = -u_{12}^{'} = \frac{1}{\sqrt{3}}(0,\tau,\tau-1),\\
&u_3^{'} = -u_{13}^{'} = \frac{1}{\sqrt{3}}(-1,1,1) && u_4^{'} = -u_{14}^{'} = \frac{1}{\sqrt{3}}(1,-\tau,0,-\tau),\\
&u_5^{'} = -u_{15}^{'} = \frac{1}{\sqrt{3}}(\tau-1,0,\tau), && u_6^{'} = -u_{16}^{'} = \frac{1}{\sqrt{3}}(1,-1,1),\\
&u_7^{'} = -u_{17}^{'} = \frac{1}{\sqrt{3}}(\tau,\tau-1,0), && u_8^{'} = -u_{18}^{'} = \frac{1}{\sqrt{3}}(0,\tau,1-\tau),\\
&u_9^{'} = -u_{19}^{'} = \frac{1}{\sqrt{3}}(-\tau,\tau-1,0), && u_{10}^{'} = -u_{120}^{'} = \frac{1}{\sqrt{3}}(-1,-1,1),
\end{aligned} \tag{48}$$

satisfying the relation

$$\frac{3}{20}\sum_{i=1}^{20}\left|u_i^{'}\right\rangle\left\langle u_i^{'}\right| = \mathrm{I}_{R^3}\,, \tag{49}$$

we can increase further the resolution by using a union of orbits. If we add the relations (46) and (49) multiplied respectively by $\frac{12}{32}$ and $\frac{20}{32}$ then we get the relation

$$\frac{3}{32}\left(\sum_{i=1}^{12}\left|u_i\right\rangle\left\langle u_i\right| + \sum_{i=1}^{20}\left|u_i^{'}\right\rangle\left\langle u_i^{'}\right|\right) = \mathrm{I}_{R^3}\,, \tag{50}$$

which shows that $C \cup C^{'}$ is a frame. Some of these frame quantizations may be useful in the study of fullerenes.

8. QUASIPERIODIC PATTERNS OBTAINED BY PROJECTION

The embedding into a superspace defined by a frame offers the mathematical possibility to obtain some remarkable quasiperiodic sets. The frame (see (45))

$$\begin{aligned}
&\left|u_1\right\rangle = \frac{1}{\sqrt{\tau+2}}(1,\tau,0), && \left|u_2\right\rangle = \frac{1}{\sqrt{\tau+2}}(-1,\tau,0),\\
&\left|u_3\right\rangle = \frac{1}{\sqrt{\tau+2}}(-\tau,0,1) && \left|u_4\right\rangle = \frac{1}{\sqrt{\tau+2}}(0,-1,\tau),\\
&\left|u_5\right\rangle = \frac{1}{\sqrt{\tau+2}}(\tau,0,1), && \left|u_6\right\rangle = \frac{1}{\sqrt{\tau+2}}(0,1,\tau)
\end{aligned} \tag{50}$$

allows us to identify the space ***H***= $\mathbf{R}^3$, with the subspace

$$\tilde{H}=\{\alpha_1\left|\phi_1\right\rangle+\alpha_2\left|\phi_2\right\rangle+\alpha_3\left|\phi_3\right\rangle \mid \alpha_1,\alpha_2,\alpha_3\in\mathbf{R}\}$$

of the superspace $\mathbf{R}^6$, by using the isometry

$$\mathbf{R}^3\to\tilde{H}:\left|v\right\rangle=(\alpha_1,\alpha_2,\alpha_3)\mapsto\left|\tilde{v}\right\rangle=\alpha_1\left|\phi_1\right\rangle+\alpha_2\left|\phi_2\right\rangle+\alpha_3\left|\phi_3\right\rangle, \tag{52}$$

where

$$\begin{aligned}\left|\phi_1\right\rangle&=\frac{1}{\sqrt{5+\sqrt{5}}}(1,-1,-\tau,0,\tau,0),\\ \left|\phi_2\right\rangle&=\frac{1}{\sqrt{5+\sqrt{5}}}(\tau,\tau,0,-1,0,1)\\ \left|\phi_3\right\rangle&=\frac{1}{\sqrt{5+\sqrt{5}}}(0,0,1,\tau,1,\tau).\end{aligned} \tag{53}$$

The orthogonal projectors corresponding to $\tilde{H}$ and

$$\tilde{H}^{\perp}=\left\{x=(x_1,x_2,...,x_6)\in R^6 \mid \sum_{i=1}^{6}x_i\left|u_i\right\rangle=0\right\} \tag{54}$$

are $\pi=\wp\,(1/2,\sqrt{5}/10)$ and $\pi^{\perp}=\wp\,(1/2\ ,\ -\sqrt{5}/10)$, where

$$\wp(\beta,\gamma)=\begin{pmatrix}\beta&\gamma&-\gamma&-\gamma&\gamma&\gamma\\ \gamma&\beta&\gamma&-\gamma&-\gamma&\gamma\\ -\gamma&\gamma&\beta&\gamma&-\gamma&\gamma\\ -\gamma&-\gamma&\gamma&\beta&\gamma&\gamma\\ \gamma&-\gamma&-\gamma&\gamma&\beta&\gamma\\ \gamma&\gamma&\gamma&\gamma&\gamma&\beta\end{pmatrix} \tag{55}$$

and we have

$$\pi(\sqrt{2},0,0,0,0,0)=\left|\tilde{u}_1\right\rangle\ ,\ \ \pi(0,\sqrt{2},00,0,0,0)=\left|\tilde{u}_2\right\rangle,...,\pi(0,0,0,0,0,\sqrt{2})=\left|\tilde{u}_6\right\rangle.$$

Therefore

$$\pi(\sqrt{2}\,\mathbf{Z}^6)=\left\{\alpha_1\left|\tilde{u}_1\right\rangle+\alpha_2\left|\tilde{u}_2\right\rangle+...+\alpha_6\left|\tilde{u}_6\right\rangle \mid \alpha_1,\alpha_2,...,\alpha_6\in\sqrt{2}\mathrm{Z}\right\}. \tag{56}$$

If we project only the points belonging to the strip

$$\tilde{H} + \left[0, \sqrt{2}\right]^6 = \{x \in \mathbf{R}^6 \mid \pi^\perp x \in \pi^\perp([0, \sqrt{2}]^6)\} \tag{57}$$

obtained by shifting the hypercube $[0, \sqrt{2}]^6$ along $\tilde{H}$, we get the quasiperiodic set

$$\mathrm{Q} = \{ \pi x \mid x \in \sqrt{2}\,\mathbf{Z}^6,\ \pi^\perp x \in \pi^\perp([0, \sqrt{2}]^6)\}. \tag{58}$$

The set Q is a discrete set, and the nearest neighbours of a point $\pi x \in \mathrm{Q}$ belong to the set of all the vertices of a regular icosahedron, namely,

$$\left\{ \pi x + \left| \tilde{u}_1 \right\rangle, \pi x - \left| \tilde{u}_1 \right\rangle, \pi x + \left| \tilde{u}_2 \right\rangle, \pi x - \left| \tilde{u}_2 \right\rangle, \ldots, \pi x + \left| \tilde{u}_6 \right\rangle, \pi x - \left| \tilde{u}_6 \right\rangle \right\}.$$

The diffraction pattern corresponding to Q computed by using the Fourier transform is similar to the experimental diffraction patterns obtained in the case of certain icosahedral quasicrystals [6]. Quasiperiodic sets corresponding to other quasicrystals can be obtained by starting from finite frames, and they help us to better understand the atomic structure of these materials.

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