Arbitrary unitary rotation of three-dimensional pixellated images

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Abstract

Using the coefficients introduced by Bargmann and Moshinsky for the reduction of the \( su(3) \) algebra of Cartesian three-dimensional oscillator multiplet states into \( so(3) \) angular momentum submultiplets, we implement unitary rotations of three-dimensional Cartesian arrays that form finite pixellated “volume images.” Transforming between the Cartesian and spherical bases, the subgroup of rotations in the latter is converted into rotations of the former, allowing for proper concatenation and inversion of these unitary transformations, which entail no loss of information.

1 Introduction

Unitary rotations of three-dimensional (3D) pixellated ‘images’ in a cube of \( N^3 \) volumetric data, will be imported from the rotations of the 3D quantum harmonic oscillator wavefunctions between Cartesian and spherical coordinates onto the 3D discrete oscillator model \[1\]. The importation process will follow closely the process which was applied in the 2D case of \( N^2 \) pixellated arrays or screens \[2, 3\]. This work relies heavily on the understanding of group theory, and although it is not a requirement, we do not rely on conventional notation in signal analysis; nevertheless, the reader can follow, without problem, the development of the presented methods.

We start with the well-known \( D \)-dimensional Heisenberg-Weyl algebra of position and momentum operators \( \overline{Q}_i, \overline{P}_i, 1 \in \hbar \omega_i \), with their standard commutation relation \( [\overline{Q}_i, \overline{P}_j] = i\delta_{ij}\lambda \). These serve to construct the raising and lowering operators, \( \overline{Q}_i \pm i\overline{P}_i \), out of which oscillator Hamiltonians for each axis are built as the products \( \overline{H}_i := \frac{1}{2}(\overline{P}_i^2 + \overline{Q}_i^2) \), also defining the number operators \( \overline{N}_i := \overline{H}_i - \frac{1}{2}I \) with integer eigenvalues \( n_i \in \{0, 1, 2, \ldots\} \), as well as the quadratic product operators that shift quanta between the axes, which form the symmetry Lie algebra \( su(D) \) of the \( D \)-dim oscillator system. These operators conserve the total energy \( E_n = \hbar \omega(n + \frac{1}{2}D) \), given by the principal quantum number \( n = n_1 + n_2 + \cdots + n_D \). This \( su(D) \) Lie algebra contains \( D \)-dimensional orthogonal subalgebras \( so(D) \) of rotations.

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The harmonic oscillator wavefunctions are separable in Cartesian coordinates and also in polar or, generally, spherical coordinates. In the former, the quantum numbers \( n_i \) are provided by the \( D \) commuting number operators \( \overline{N}_i \), while the latter use quantum numbers from the rotation subalgebra chain. For \( D = 2 \) dimensions, denoted \( x, y \), the oscillator states are classified by

\[
\overline{N}_x \oplus \overline{N}_y \subset \mathfrak{su}(2) = \mathfrak{so}(3) \supset \mathfrak{so}(2)
\]

\[
n_x \quad n_y \quad n := n_x + n_y = : 2\ell \quad m
\]

\[
n_i \in \{0, 1, \ldots\}, \ i \in \{x, y\} \quad m \in \{-\ell, -\ell + 1, \ldots, \ell - 1, \ell\}.
\]

and form an inverted infinite triangle with apex at the ground state. At level \( n = 2\ell \) there are \( n + 1 = 2\ell + 1 \) states degenerate in energy \( E_n = n + \frac{1}{2} \), that form an angular momentum multiplet of states classified by \( m. \[3] \). Correspondingly, for \( D = 3 \) dimensions, we have the subalgebra chains and quantum numbers given by

\[
\overline{N}_x \oplus \overline{N}_y \oplus \overline{N}_z \subset \mathfrak{su}(3) \supset \mathfrak{so}(3) \supset \mathfrak{so}(2)
\]

\[
n_x \quad n_y \quad n_z \quad n := n_x + n_y + n_z \quad \ell \quad m
\]

\[
n_i \in \{0, 1, \ldots\}, \ i \in \{x, y, z\} \quad \ell \in L(n) := \{n, n - 2, \ldots, 0 \text{ or } 1\} \quad m \in M(\ell) := \{-\ell, -\ell + 1, \ldots, \ell - 1, \ell\}.
\]

In this case, each energy level \( n \) contains states that can be arranged in an inverted infinite triangular prism with apex at the ground state. The multiplet of states with energy \( E_n = n + 1 \) forms triangular numbers \( \tau_n := \sum_{i=0}^{n} (2\ell + 1) = \frac{1}{2} (n + 1)(n + 2), \) which for \( n \geq 2 \) contain more than one angular momentum submultiplet of states. The linear combination coefficients that relate the Cartesian states \( |n_i, n_y, n_z\rangle \) and the spherical 3D quantum oscillator states \( |n, \ell, m\rangle \) were given by Bargmann and Moshinsky in \[3] for the nuclear shell model, and further investigated in \[5, 6\]. We use a round ket because \( \ell \) is NOT the eigenvalue of any one operator in the set, but \( \ell(\ell + 1), \ell \geq 0, \) is the eigenvalue of squared total angular momentum.

The finite model oscillator was proposed in \[17\] to form a system with oscillator dynamics but with a finite number \( N \) of energy states. This was achieved from the Heisenberg-Weyl algebra by substituting \( \overline{Q}_i \) and \( \overline{P}_i \) with the triads of operators \( Q_i, P_i, K_i \in \mathfrak{su}(2) \) with the commutation relations \([Q_i, P_i] = iK_i, \ [K_i, Q_i] = iP_i, \ [K_i, P_i] = -iQ_i\) and, in the irreducible representation \( j \in \{0, \frac{1}{2}, 1, \frac{3}{2}, \ldots\} \) of \( \mathfrak{su}(2) \), the ‘displaced finite oscillator number operators’ \( N_i := K_i + jI \) whose multiplets have \( N := 2j + 1 \) states with ‘number’ and ‘energy’ eigenvalues \( n = E_n^{(N)} - \frac{1}{2} \in \{0, 1, 2, \ldots, N - 1\} \). Finally, the symmetry importation from the continuous to the discrete model is performed by applying the rotation linear combination coefficients of the former, given by the Wigner Big-\( D \) matrices \( D^\ell_{m, m'}(\alpha, \beta, \gamma) \), onto the latter.

In Sect. \[2\] we give a short account of the construction of the transformation coefficients for the continuous system; in Sect. \[3\] we import this symmetry onto the discrete cube of data, give the correct implementation of the explicit expression given by \[5\]. In Sect. \[4\] we present some examples of unitary rotations and their concatenation.
2 Transformation coefficients for the 3D quantum oscillator

To conform with the prevailing notations in the field, instead of the position and momentum operators, \(Q_i, P_i\) we use the creation and annihilation operators*:

\[
\eta_i := \frac{1}{\sqrt{2}}(Q_i + iP_i), \quad \xi_i := \frac{1}{\sqrt{2}}(Q_i - iP_i), \quad [\xi_i, \eta_j] = \delta_{i,j}I, \quad i, j \in \{x, y, z\}
\] (3)

The three Cartesian commuting oscillator boson creation operators \(\vec{\eta} = (\eta_x, \eta_y, \eta_z)\), and their three adjoint (hermitian conjugate) annihilation operators \(\vec{\xi} = (\xi_x, \xi_y, \xi_z)\), \(\xi_i = \eta_i^\dagger\), act on the independent oscillator mode states, indicated by \(|n_i\rangle\) in Dirac ket notation,

\[
\eta_i |n_i\rangle = \sqrt{n_i + 1} |n_i + 1\rangle, \quad \xi_i |n_i\rangle = \sqrt{n_i} |n_i - 1\rangle, \quad \eta \xi_i |n_i\rangle = n_i |n_i\rangle.
\] (4)

They serve to create the Cartesian oscillator states out of the ground state \(|0\rangle\) as

\[
|n_x, n_y, n_z\rangle = \frac{n_x^{n_x} n_y^{n_y} n_z^{n_z}}{\sqrt{n_x! n_y! n_z!}} |0\rangle.
\] (5)

Equivalently it is useful to define their three polar complex linear combinations,

\[
\eta_+ := -\frac{1}{\sqrt{2}}(\eta_x + i\eta_y), \quad \eta_0 := \eta_z, \quad \eta_- := +\frac{1}{\sqrt{2}}(\eta_x - i\eta_y),
\] (6)

\[
\xi_+ := -\frac{1}{\sqrt{2}}(\xi_x - i\xi_y), \quad \xi_0 := \xi_z, \quad \xi_- := +\frac{1}{\sqrt{2}}(\xi_x + i\xi_y),
\]

where \(\xi_r = \eta^\dagger_r\) and \([\xi_r, \eta_s] = \delta_{r,s}I\) and \(r, s \in \{+, 0, -\}\). The inverse transformation is

\[
\eta_x := -\frac{1}{\sqrt{2}}(\eta_+ + \eta_-), \quad \eta_y := +\frac{1}{\sqrt{2}}(\eta_+ - \eta_-), \quad \eta_z := \eta_0,
\] (7)

\[
\xi_x := -\frac{1}{\sqrt{2}}(\xi_+ - \xi_-), \quad \xi_y := -\frac{1}{\sqrt{2}}(\xi_+ + \xi_-), \quad \xi_z := \xi_0,
\]

The polar operators act, as the Cartesian ones in (8), on states \(|n_r\rangle^\circ, r \in \{+, 0, -\}\), through

\[
\eta_r |n_r\rangle^\circ = \sqrt{n_r + 1} |n_r + 1\rangle^\circ, \quad \xi_r |n_r\rangle^\circ = \sqrt{n_r} |n_r - 1\rangle^\circ, \quad \eta \xi_r |n_r\rangle^\circ = n_r |n_r\rangle^\circ.
\] (8)

Thus one defines the polar mode states

\[
|n_+, n_0, n_-\rangle^\circ := \frac{n_+^{n_+} n_0^{n_0} n_-^{n_-}}{\sqrt{n_+! n_0! n_-!}} |0\rangle^\circ,
\] (9)

with the unique ground state \(|0\rangle^\circ \equiv |0\rangle\).

*People used to the standard quantum notation can make the relations \(\eta \equiv \hat{a}\) and \(\xi \equiv \hat{a}^\dagger\).
The Cartesian and polar states thus relate through
\[
| n_x, n_y, n_z \rangle = \frac{i^{n_y} (\eta_− - \eta_+)^{n_x} (\eta_+ - \eta_+)^{n_y} \eta_0^{n_z}}{\sqrt{2^{n_x+n_y+n_z} n_x! n_y! n_z!}} | 0 \rangle
\]
\[
= i^{n_y} \sqrt{\frac{n_x! n_y!}{2^{n_x+n_y}}} \sum_{\lambda=0}^{n_x} \sum_{\mu=0}^{n_y} (-1)^\lambda
\]
\[
\times \sqrt{\frac{(\lambda+\mu)! (n_x+n_y-\lambda-\mu)!}{\lambda! \mu! (n_x-\lambda)! (n_y-\mu)!}} | \lambda+\mu, n_x, n_x+n_y-\lambda-\mu \rangle^o,
\]
and the inverse relation
\[
| n_+, n_0, n_- \rangle^o = \frac{(-1)^{n_+}(\eta_x+\eta_y)^{n_+}\eta_z^{n_0}(\eta_x-\eta_y)^{n_-}}{\sqrt{2^{n_++n_-} n_+! n_0! n_-!}} | 0 \rangle^o
\]
\[
= (-i)^{n_++n_-} \sqrt{\frac{n_+! n_-!}{2^{n_++n_-}}} \sum_{\rho=0}^{n_+} \sum_{\sigma=0}^{n_-} i^{\sigma-\rho}
\]
\[
\times \sqrt{\frac{(n_++n_-)! (n_++n_-+\rho-\sigma)!}{\rho! \sigma! (n_+\sigma)! (n_-\sigma)!}} | n_++n_-, n_++n_+\rho-\sigma, n_0 \rangle.
\]

The corresponding Schrödinger wavefunction \( \langle \vec{r} | n_x, n_y, n_z \rangle \), \( \vec{r} = (x, y, z) \), are the well-known separated Hermite-Gauss functions, a denumerable and orthonormal basis for functions in the \( L^2(\mathbb{R}^3) \) Hilbert space.

In the spherical basis, the states are determined by [5, 8, 9 Sects. I.8-9]
\[
| n, \ell, m \rangle := A_{n, \ell} (\eta^2)^{\frac{1}{2}(n-\ell)} Y_{\ell,m}(\vec{\eta}) | 0 \rangle,
\]
where \( \eta^2 := \eta_x^2 + \eta_y^2 + \eta_z^2 = \eta_0^2 - 2 \eta_+ \eta_- \) is raised to the power \( \nu := \frac{1}{2}(n-\ell) \); \( \nu \) is a non-negative integer identified as the radial quantum number. The \( Y_{\ell,m}(\vec{\eta}) \)'s are the solid spherical harmonics in the three creation operators \( \vec{\eta} \); written in polar form [6], these are [10 Sect. 3.10],
\[
Y_{\ell,m}(\vec{\eta}) = \sqrt{\frac{(2\ell+1)(\ell+m)! (\ell-m)!}{4\pi 2^m m!}} \sum_{\mu} \frac{1}{2^\mu (m+\mu)! (\ell-m-2\mu)!} \frac{\eta_+^{m+\mu}}{\eta_0^{\ell-2\mu}} \eta_-^\mu.
\]

When \( m \geq 0 \), then \( \mu \) ranges from 0 to \( \lfloor \frac{1}{2}(\ell-m) \rfloor \); when \( m < 0 \), we use \( Y_{\ell,-m}(\vec{\eta}) = (-1)^m Y_{\ell,m}(\vec{\eta})^* \). This is a polynomial of homogeneous degree \( \ell \) in the creation operators. Together with the factor \( (\eta^2)^\nu \) in (2), we have a polynomial operator of degree \( n = 2\nu + \ell \) that creates oscillator states of energy \( E_n = \hbar \omega (2\nu + \ell + \frac{3}{2}) \). Finally, the normalization coefficient in (2) is \( | \psi \rangle = A_{n,\ell} \sqrt{\frac{4\pi^{n+\ell+1} (2\nu)!}{(2\nu+2\ell+1)!!}} \).

*Please note that Chacón and de Llano use “\( \nu \)” for the total quantum number \( n \), while we use it for the radial quantum number in expressions where it simplifies notation.
We use the principal quantum number \( n \), rather than the radial \( \nu \), for our notation of bra-kets and coefficients (in contradistinction to [4] and [?]) because it simplifies many analytical and numerical consideratios. With \( n = 2\nu + \ell \), the spherical kets (2)–(2) can be written in terms of the polar ones (9) as [5]

\[
|n, \ell, m\rangle = \frac{(-1)^\nu}{2^\ell \ell!} \sqrt{\frac{(2\ell+1) 2^m (\ell-m)!}{(n-\ell)!! (n+\ell+1)!!}} \times \sum_{s=0}^{\ell} \sum_{r=0}^{\nu+s} (-1)^{r+s} 2^r \binom{\ell}{s} \binom{\nu+s}{r} \frac{(2\ell-2s)!}{(\ell-2s-m)!} \\
\times |r+m, n-2r-m, r\rangle,
\]

for \( m \geq 0 \), while for \( m < 0 \), the expression for \(|n, \ell, -m\rangle\) in (15) will exchange \(|n_+, n_0, n_-\rangle\) \( \mapsto |n-, n_0, n_+\rangle\). The Schrödinger wavefunctions \( \langle \vec{r} | n, \ell, m \rangle \), are well known to be separated into a power and associated Laguerre-Gauss function of the radius, times a spherical harmonic of the direction of \( \vec{r} \); these form also a denumerable and orthonormal basis for \( L_2^r(\mathbb{R}^3) \). We use round kets for the spherical basis to distinguish them when labeled with numerical values.

In [5] the overlap between the Cartesian and spherical bases, (10) and (2) is reported. It is nonzero only when they belong to the same energy level and have the same parity in the \( x-y \) plane, i.e.,

\[
n_x + n_y + n_z = n, \quad \text{and} \quad n_x + n_y \pm m \text{ is even}.
\]

Their expression, with \( \nu = \frac{1}{2}(n-\ell) \), can be written as

\[
\langle n_x, n_y, n_z | n, \ell, m \rangle = i^{n_y} (-1)^{\nu+\frac{1}{2} [(n_x-n_y) \pm m]} 2^{-\ell} \binom{\nu}{\frac{1}{2}[n_x+n_y+m]} \\
\times \sqrt{\frac{(2\ell+1) (\ell-m)!}{(\ell+m)! (n-\ell)!! (n+\ell+1)!!}} \times \sum_{r=0}^{\ell} \sum_{s=0}^{n_x} \binom{\ell}{s} \binom{\nu+r}{r} \frac{(2\ell-2s)!}{(\ell-2s-m)!} \binom{\nu+r}{r} \binom{(n_x-s)!}{r!} \binom{(n_x-n_y+m)!}{r!} \binom{(\frac{1}{2}[n_x+n_y+m]-s)!}{r!} \\
\times \binom{\frac{1}{2}[n_y-n_x-m]+s}{r!} \binom{\frac{1}{2}[n_y-n_x-m]+s}{r!},
\]

for \( m \geq 0 \), while for \( m < 0 \),

\[
\langle n_x, n_y, n_z | n, \ell, m \rangle = (-1)^{n_z} \langle n_x, n_y, n_z | n, \ell, -m \rangle.
\]

Note that all factorials in (17) are applied to integer numbers due to (2).

The overlap coefficients (17) transform unitarily between the \( \tau_n \) Cartesian states within each energy level \( n \), which form a basis for a completely symmetric irreducible representation of \( SU(3) \), and the spherical states which reduce into \( SO(3) \) angular momentum multiplets, and which sum the same number of states, \( \sum_{\ell \in L(n)} (2\ell+1) = \)
For each \( n \in \{0, 1, 2, \ldots \} \), the transformation relations between bases are
\[
| n, \ell, m \rangle = \sum_{n_x+n_y+n_z=n} | n_x, n_y, n_z \rangle \langle n_x, n_y, n_z | n, \ell, m \rangle,
\]
\[
| n_x, n_y, n_z \rangle = \sum_{\ell \in L(n), m \in M(\ell)} | n, \ell, m \rangle \langle n, \ell, m | n_x, n_y, n_z \rangle.
\]
(19)

Now, in the spherical basis, 3D rotations \( R \in \text{SO}(3) \) are transformations that only act within the angular momentum multiplets
\[
R : | n, \ell, m \rangle = \sum_{m' \in M(\ell)} | n, \ell, m' \rangle \langle n, \ell, m' | R | n, \ell, m \rangle = \sum_{m' \in M(\ell)} | n, \ell, m' \rangle D^\ell_{m',m}(R),
\]
(20)
where \( D^\ell_{m',m}(R) \) are the well known Wigner big-D rotation matrices, usually expressed in Euler angles \( R(\phi, \theta, \psi) \).

3 Importation of \( \text{SU}(3) \) symmetry on the finite 3D oscillator model

The gist of the 1D finite oscillator model is to replace the Heisenberg-Weyl (HW) Lie algebra of raising (\( \eta \)) and lowering (\( \xi \equiv \eta^\dagger \)) operators
\[
\{ \eta, \xi, 1 \} \in \text{span} \ HW, \quad [\xi, \eta] = 1,
\]
(21)
with an \( \text{su}(2) \) algebra of generators \( \{ J_k \}_{k=1}^3 \) in a fixed representation \( j \), of dimension \( N = 2j + 1 \), and classify the basis states with the unit-spaced eigenvalues of either position or mode, as
\[
\text{position } q: \quad J_1 | j, q \rangle = q | j, q \rangle |
\]
mode \( n \):
\[
J_3 | j, n \rangle = (n-j) | j, n \rangle |
\]
(22)
\[
N^{-1}.
\]

There are thus only \( N \) mode eigenstates \( n \in \{0, 1, \ldots, N-1\} \) in the 1D finite oscillator model \cite{1}. The \( \text{su}(2) \) commutation relations are the usual ones \cite{10},
\[
[J_3, J_1] = iJ_2, \quad [J_3, -J_2] = iJ_1, \quad [J_1, J_2] = iJ_3.
\]
(23)

The first two are the geometric and dynamic Hamilton equations of the quantum oscillator, while the third distinguishes between the finite oscillator from the continuous model. The overlaps between the position and mode bases constitute the finite oscillator eigenstates found across the related literature \cite{11},
\[
\Psi^{(j)}_n(q) := | j, q | j, n \rangle = d^n_{j-n,q} \left( \frac{1}{2\pi} \right)
\]
\[
= \frac{(-1)^n}{2^n} \sqrt{\binom{2j}{n}} \binom{2j}{j+q} K_n(j+q; \frac{1}{2}; 2j),
\]
(24)
where $d_{m,m'}^{j}(\frac{1}{2}\pi)$ are the Wigner little-$d$ functions [10] for the $\frac{1}{2}\pi$ angle between $J_1$ and $J_3$, and $K_n(j+q;\frac{1}{2};2j)$ are the symmetric Kravchuk polynomials of degree $n$ in $q_{-j}^{j}$. When $j \to \infty$ in an appropriate limit, the Kravchuk functions [3] become the Hermite-Gauss eigenfunctions of the continuous quantum oscillator.

In the three dimensions that we now study, we have three sets of commuting $su(2)$ generators, $i \in \{x, y, z\}$, each giving position and mode [22] along the three space axes. We are here interested in the case where $j_x = j_y = j_z = j$ so that we have a total of $N^3 = (2j + 1)^3$ states that we can represent as points in a cube of side $N$, which we picture in Fig. 1 (above). Modifying slightly the notation in (3) where subscripts denotes the related basis, we write the discrete and finite position states as $|q_x, q_y, q_z\rangle^{(N)}_1$. On the other hand, the discrete mode states, correspondingly written as $|n_x, n_y, n_z\rangle^{(N)}_3$ with $n_i \in [0, N-1]$, are pictured in Fig. 1 (below left-right) with the total mode number $n = n_x + n_y + n_z$ along the vertical axis, which ranges from $n = 0$ at the bottom vertex, up to $n = 3(N-1) = 6j$ at the top vertex. A basis of $N^3$ discrete Cartesian wavefunctions is built from the 1D model in (3) simply as the direct product of the individual one-dimensional wavefunctions

$$\Psi_{n_x,n_y,n_z}^{(j)}(q_x,q_y,q_z) := \langle n_x,n_y,n_z|q_x,q_y,q_z\rangle^{(N)}_3 = \Psi_{n_x}^{(j)}(q_x)\Psi_{n_y}^{(j)}(q_y)\Psi_{n_z}^{(j)}(q_z).$$

These are orthonormal and complete bases for the $N^3$ space of ‘3D images’, ‘voxels’, ‘signals’ or states on the discrete cube of Fig. 1. These act as unitary transformation matrix elements between the two bases depicted in that figure, i.e.,

$$|n_x,n_y,n_z\rangle^{(N)}_3 = \sum_{q_x,q_y,q_z=-j}^{j}|q_x,q_y,q_z\rangle^{(N)}_1\langle q_x,q_y,q_z|n_x,n_y,n_z\rangle^{(N)}_3,$$

$$|q_x,q_y,q_z\rangle^{(N)}_1 = \sum_{n_x,n_y,n_z=0}^{2j}|n_x,n_y,n_z\rangle^{(N)}_3\langle n_x,n_y,n_z|q_x,q_y,q_z\rangle^{(N)}_1.$$  

where we remark that the basis for the modes $n_i$ is not so intuitive for visual representation, despite it has the same exact information that the basis of position $q_i$.

In the two-dimensional case examined in Refs. [2, 3], the position states are placed on an $N \times N$ square pixelscreen as shown in Fig. 2 (instead of the cube in Fig. 1), and the mode states are arranged in an $N \times N$ rhombus whose vertical axis is the total mode number $n = n_x + n_y$ and the horizontal axis is the mode difference $n_x - n_y$. The horizontal rungs in the rhombus, characterized by $n_0^{2N-2}$, contain each $n + 1$ members in the triangle that is the lower half of the rhombus $0 \leq n \leq N-1 = 2j$, while the upper triangle $N \leq n \leq 2N-2 = 4j$ contains the high-mode components, whose members reflect the lower triangle. At this point, the importation of the $su(2)$ symmetry consists in taking these sets of $n+1$ states to be $su(2)$ multiplets, $|\lambda,\mu\rangle$, of angular momentum $\lambda = \frac{1}{2}n$ and distinguished by the mode difference $\mu = \frac{1}{2}(n_x - n_y)$, $\mu|\lambda\rangle$. This holds for the states in the triangle in the lower half of the rhombus; the upper triangle is treated in the same way for $n \to 4j - n$. Thereby, plane rotations
Figure 1: Above: States of the 3D Cartesian finite oscillator wavefunctions $\Psi_{n_x,n_y,n_z}^{(N)}(q_x,q_y,q_z)$ in (25), of points $q_x,q_y,q_z|^j_{-j}$, arranged into a cube of side $N = 2j + 1$. Below: Eigenstates of mode number, arranged by axes $(n_x,n_y,n_z)$, with mode numbers $n_{i0}^{N-1}$. The diagonal axis crossing the cube distinguishes the total modes $n = \sum_i n_i$, the right-down vertex is $n = 0$ and the left-top vertex corresponds to $n = 3(N-1) = 6j$. Below-left. Triangular planes are drawn between the lower (inverted) pyramid $n_{i0}^{2j}$, and the upper pyramid $n_{4j}^{6j}$. Below-right. Hexagonal planes are drawn for the intermediate region $n_{2j+1}^{4j-1}$.  

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Figure 2: *Left:* States of a two-dimensional finite oscillator represented as points (or pixels) on a square $N \times N$ screen ($N = 2j+1$). *Right:* Mode states of the 2D finite oscillator, $|n_x, n_y\rangle_3, n_x, n_y^{(2)}$, and $n_x + n_y = n|^{(3)}_0$ arranged into a rhombus. The horizontal lines join the imported $\text{su}(2)$ multiplets $|\lambda, \mu\rangle$ of angular momenta $\lambda = \frac{1}{2}n \in \{0, \frac{1}{2}, 1, \ldots, j\}$ in the lower (and correspondingly in the upper) half of the rhombus, distinguished by $\mu = \frac{1}{2}(n_x - n_y)|^{\lambda}_{-\lambda}$.

by $\alpha$ in the $x$-$y$ plane of the pixellated screen are obtained from the well-defined rotations of the $|\lambda, \mu\rangle$ basis states, which are only multiplied by $\exp(i\alpha\mu)$.

Returning to the three-dimensional case examined here, we must import the continuous oscillator $\text{su}(3)$ symmetry algebra onto the finite oscillator mode states at each total mode level $n = n_x + n_y + n_z$ of Fig. 1 and then use its $\text{so}(3)$ subalgebra to define states which transform properly under rotations as in Eq. (20). In this case we have to slice the rhomboid-cube of modes into $n$ = constant planes and see if and how we can accommodate them into $\text{so}(3) \subset \text{su}(3)$ multiplets. In slicing the cube in this way, we have now three regions to examine, instead of the two triangles of the 2D rhombus in Fig. 2.

Consider first the mode levels in the range $0 \leq n \leq N - 1$ where the slices of the cube yield triangular arrangements of $\tau_n$ points of side $n + 1$, such as that shown in Fig. 1. These form completely symmetric (or bosonic) irreducible representations of $\text{su}(3)$, containing the multiplet of the states $|n_x, n_y, n_z\rangle$ of an ordinary quantum oscillator with $n$ energy quanta. These quanta can be shifted among the three axes by means of the nine $u(3)$ generators. These generators, $C_i^j, i, j \in \{x, y, z\}$, are built in terms of three commuting sets of boson creation and annihilation operators, $\eta_i, \xi_j$, fulfilling the commutators

$$C_i^j := \eta_i \xi_j, \quad [C_i^j, C_k^l] = \delta_{j,k} C_i^l - \delta_{l,i} C_k^j, \quad (C_i^j)^\dagger = C_j^i. \quad (27)$$

In the vector space of these nine generators there is the invariant of total mode

$$C := \sum_i C_i^i = \eta_x \xi_x + \eta_y \xi_y + \eta_z \xi_z = \eta_+ \xi_+ + \eta_0 \xi_0 + \eta_- \xi_-, \quad (28)$$
which is at the center in the decomposition \( u(3) = u(1) \oplus su(3) \) that determines this completely symmetric (bosonic) representation of \( su(3) \) to be characterized by the single non-negative integer \( n \).

Within the set of \( su(3) \) generators \([3]\) we find the subset that generates the rotation subalgebra \( so(3) \subset su(3) \) of self-adjoint operators

\[
\begin{align*}
\mathcal{L}_x &:= -i(C^z_x - C^y_x) = \frac{1}{\sqrt{2}}[(\eta_+ + \eta_-)\xi_0 + \eta_0(\xi_+ + \xi_-)], \\
\mathcal{L}_y &:= -i(C^x_z - C^z_y) = -i\frac{1}{\sqrt{2}}[(\eta_+ - \eta_-)\xi_0 - \eta_0(\xi_+ - \xi_-)], \\
\mathcal{L}_z &:= -i(C^y_x - C^x_y) = \eta_+\xi_+ - \eta_-\xi_-,
\end{align*}
\]

whose commutation relations are \([\mathcal{L}_i, \mathcal{L}_j] = -i\mathcal{L}_k \) (with \( i, j, k \) a cyclic permutation of \( x, y, z \)). The usual raising and lowering operators in \( so(3) \) are

\[
\mathcal{L}_+ := \mathcal{L}_x + i\mathcal{L}_y = \sqrt{2}(\eta_+\xi_0 - \eta_0\xi_-), \\
\mathcal{L}^- := \mathcal{L}_x - i\mathcal{L}_y = \sqrt{2}(\eta_-\xi_0 - \eta_0\xi_+),
\]

with \( (\mathcal{L}_+)^\dagger = \mathcal{L}_- \), and commutators \([\mathcal{L}_z, \mathcal{L}_\pm] = \pm \mathcal{L}_\pm \) and \([\mathcal{L}_+, \mathcal{L}_-] = -2\mathcal{L}_0 \equiv -2\mathcal{L}_z \).

The invariant Casimir operator is

\[
\mathcal{L}^2 = \mathcal{L}^2_x + \mathcal{L}^2_y + \mathcal{L}^2_z = \mathcal{L}_\pm \mathcal{L}_\mp + \mathcal{L}_0(\mathcal{L}_0 \pm 1).
\]

The three commuting generators

\[
C^x_x = \eta_x\xi_x, \quad C^y_y = \eta_y\xi_y, \quad C^z_z = \eta_z\xi_z,
\]

yield the three labels of the \( \tau_n \) Cartesian states \( |n_x, n_y, n_z\rangle \), while the invariant \( \mathcal{C} \) in \([3]\), \( \mathcal{C}^2 \) in \([3]\), and \( \mathcal{C}_z \) in \([29]\) determine the labels of the spherical basis \( |n, \ell, m\rangle \) with the ranges specified in \([2]\) and shown in Fig. 1. The \( + -- \) mode difference \( m := n_+ - n_- \), as in the \( 2D \) case, will have the role of angular momentum projection along the \( z \)-axis, provided that the \( \tau_n \) points in set can be fitted into complete \( so(3) \subset so(2) \) multiplets characterized by ranges \( m|\ell, -\ell \rangle \), i.e., those given by \([2]\).

Figure 1 also provides a geometric proof that shows that there are complete \( so(3) \) multiplets in any one of the levels \( n|N - 1 \rangle \) in the lower ‘inverted pyramid’ of finite-cube states. The lowest two rungs in the triangle of the figure contain \( n + 1 \) and \( n \) points respectively; when projected, on the \( m = \frac{1}{2}(n_x - n_y) \) axis they sum \( 2n + 1 \) points equidistant by unity, as if they were a multiplet of highest angular momentum \( \ell = n \). Then come the next higher two rungs of \( n - 1 \) and \( n - 2 \) points, that project on \( 2n - 3 \) equidistant points, as if they belonged to a multiplet \( \ell = n - 2 \). In the triangle of Fig. 1 the process continues with every two rungs yielding \( \ell = n - 4, n - 6, \) etc., ending with \( \ell = 1 \) if \( n \) is odd or, when \( n \) is even, the projection of the single apex point, \( m = 0 \) of \( \ell = 0 \). Of course, only the two extreme pairs of points \( \pm \mu = \ell = n \) and \( \pm (m - 1) \) are single and belong to that highest \( \ell \); all other \( m \)'s will be linear combinations of the \( \ell \)'s that we projected out geometrically in this figure.
The symmetry importation on $0 \leq n \leq N - 1 = 2j$ consists in using the coefficients that bind the quantum harmonic oscillator Cartesian and spherical states; namely, the coefficients (17) given explicitly by Chacón and de Llano [5]. The slices in the upper pyramid of the cube of modes, for $4j = 2(N - 1) \leq n \leq 3(N - 1) = 6j$, yield reflected multiplets of ‘anti’-states, for which we may expect extra phases.

Figure 3: Mode states of the 3D finite oscillator, $|n_x, n_y, n_z\rangle_3, n_i^{N-1}(N = 2j+1)$, for total mode $n = \sum_i n_i$, form triangles of side $n + 1$ and irregular hexagons that depends on the level $n$ reached. This slices the cube in Fig. 1. a) At the lower levels $n \in \{0, 1, \ldots, 2j\}$ of that figure and, b) rotating by $180^\circ$ those within the highest range, $n \in \{4j, 4j+1, \ldots, 6j\}$. When we import the $\mathfrak{su}(3) \supset \mathfrak{so}(3)$ symmetry contained in (3)–(29), we project out complete multiplets $|\ell, m\rangle$ of $L^2$ and $L_z$, where $\ell$ and $m$ have the ranges (2).

The 3D case is more complicated than the 2D one, because we also have to consider the intermediate range of total modes $N = 2j + 1 \leq n \leq 4j - 1 = 2N - 3$. There, the $n$-slices of the mode cube are hexagons of generally unequal sides. We indicate by $(B, T)$ a hexagon with $B$ points on the base and $T$ points on the top. In particular, the $N$ triangles in the bottom pyramid ($n \in \{0, 1, \ldots, N-1\}$) are $(n+1, 1)$ in Fig. 1 and the $N$ inverted triangles in the top pyramid $(1, 6j - n + 1)$. The $N - 2$ intermediate hexagons are thus $(N - 1, 2), (N - 2, 3), \ldots, (3, N - 2), (2, N - 1)$. We have thus to ask whether the sets of points $(n_x, n_y, n_z)$ in this intermediate region can be linearly combined into complete angular momentum multiplets, as those in the pyramid of Fig. 1—or not. In Fig. 1 we show these intermediate slices for $N = 7$ (a cube of $7^3 = 343$ voxels) that form the hexagons $(6, 2)$ and $(5, 3)$ for $n = 6$ and 7; the next two hexagons, $(3, 5)$ and $(2, 6)$ for $n = 8$ and 9, can be seen rotating the figure by $180^\circ$. We note that we can indeed project out complete multiplets $|\ell, m\rangle$ of eigenstates where $m = \frac{1}{2}(n_x - n_y)|\ell, \ell\rangle$, with linear combinations of $\ell \in \{5, 4, 2\}$ in the first hexagon and $\ell \in \{5, 4, 3\}$ in the second. As long as $N$ is even, we can scale up the figures to see that beyond the $(N, 1)$ triangle at total mode $n = N - 1$, in the first intermediate hexagon $(N - 1, 2)$ for $n = N$, the projected points will accommodate themselves into angular momentum multiplets $\ell \in \{N - 1, N - 2, N - 4, \ldots, 2\}$. For mode $n = N + 1$, the hexagon
Figure 4: Hexagonal slices of the mode state space $|n_x, n_y, n_z\rangle_3$ of the 3D finite oscillator: a cube of $N = 7$ points on the side (corresponding to $j = 3$) and having $7^3 = 343$ points. a) For total mode numbers $n = 8, 9$ we show the hexagon (6, 2) and b) (5, 3). For $n = 11, 12$ the hexagons (3, 5) and (2, 6) are 180°-rotated versions of these. Notice that $n = 10$ has (4, 4), because we are dealing with an odd number of points, there exist a middle symmetrical hexagonal plane $(N - 2, 3)$ will contain so(3) multiplets $\ell \in \{N - 1, N - 2, N - 3, N - 5, \ldots, 3\}$, and generally for $n = N + M$, the hexagon $(N - M + 1, M)$ will contain $\ell \in \{N - 1, N - 2, \ldots, N - M\} \cap \{N - M - 2, N - M - 4, \ldots, M\}$.

### 4 Analysis of rotations

In Figure 5 we show the composition of rotations for a “volumetric pixelated image”. The example presented is based on the analytic expression for the coefficients (17) and the rotation kernel (20). There we have a double-T, that is, a figure resembling the letter “T” facing opposing directions. From left to right, we concatenate rotations around axes $q_1$ and $q_2$, simultaneously; we choose steps $\Delta = \pi/16$, from 0 to $\pi/2$. In this configuration, the Euler angles $\alpha = \beta$ and $\gamma$, define a spiral-like path around $q_3$, transitioning from vertical to horizontal position, and rotating the legs of the double-T. At $\alpha = \beta = \pi/4$ the rod points toward the direction vector $n = (1, 1, 1)$ of the pixelated cube.

The voxels show false color since the amplitude of every one of them has been scaled to be within the range [0, 1], using methods previously reported [12], where the principal voxels that form the body of the rod are presented in a bluish tone, and the voxels with orangish tone are pixels appearing due the “discrete Gibbs-like phenomena” of the sharp edges in the transformation. We want to remark that, since the transformation is unitary when the rotation is performed, every one of the voxels acquires some amplitude value; but the voxels ranging below a threshold far from the body of the rod are treated as residues, and thus they are not shown in the figure, although they are taken into account when the transformation is sequentially performed.
Figure 5: Rotation of a \textit{double-T}, that is, a T on top and bottom facing opposite directions. The three-dimensional space has dimension of $9^3$ voxels. The rotation is done around the $q_1$ and $q_2$ axes simultaneously, from 0 to $\pi/2$, using the coefficients (17) and the rotation kernel (20). Here we see a spiral-like path from a vertical to a horizontal position of the volumetric figure.

5 Conclusions

The use of the Cartesian-to-spherical transformation coefficients of Bargmann and Moshinsky has been applied in optics before, by Pei and Liu [13] for the purpose of efficiently approximating 3D Cartesian data through solid spherical harmonics under various cutoffs; subsequent work has used them to estimate rotation angles between Cartesian data [14].

Here we extend the three-dimensional rotations previously reported at [15], were due to a limitation of the group of rotations importation, there was no way to freely rotate a set of voxels under concatenation. In this work, this limitation is overcome by the coupling between Cartesian and spherical basis, whose conjecture is proved to be accurate, since the composition of the transformation is truly unitary. Moreover, we don’t need to perform some previous treatment to the original data, like smoothing or filtering, to overpass the limitations discussed above. In the sense of unitarity, as the set of previous works always stated, this method is extremely slow since every voxel depends on all the others, thus we are facing a computational cost of $O(N^6)$.

Finally, the Fourier group is but a subgroup of the most general group $U(N^D)$ of unitary transformations among the $N^D$ pixel elements of images $f_{m_1,\ldots,m_D} \in \mathcal{C}^{N^D}$. This is the ‘aberration group’ described in Ref. [16] for 1D finite signals. At present we see no compelling application for this group beyond the two-dimensional case. Yet it would further the understanding of the structure of all transformations that conserve information in finite discrete systems, from the same viewpoint where linear and nonlinear canonical transformations conserve the structure of Hamiltonian geometric optics.
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A Counting modes in the cube
Here we give the detailed number of modes in each plane of the space \( n_x + n_y + n_z = n \). This shows the completeness of the method developed in this work since at the end, we must have the same number of points \( N^3 \) when we count the coplanar modes.

For the sake of clarity, we present three tables, the first and second are worked examples for \( N = 5, 7 \), and the third is a generalization for \( N = \#\text{odd} \). The first column is the counting mode \( n \in \{0, 3N - 3\} \), and the second column shows the number of modes in the planes depicted as the base \( B \) and tops \( T \) in the pair \((B, T)\), the third column shows the number of angular momentum \( \{\ell\} \) in the plane, and in the final column, we give the total number of modes that are coplanar at each level \( n \).

Conjecture 1 The number of angular momenta over the whole cube is
\[
\{\ell\}^N \{\ell_{\text{max}} - 1\}^N \cdots \{1\}^N, \text{ with } \ell_{\text{max}} = N - 1, \text{ and } \{\ell\}^N := N(2\ell + 1).
\]

From this last, we can calculate the total number of points in the cube in terms of the angular momenta as
\[
\sum_{\ell=0}^{N-1} \{\ell\}^N = N(2N + 1) + N(2N - 3) + \cdots + 3N + N
\]
\[
= N \sum_{M=1}^{N} (2N - 2M + 1)
\]
\[
= 2N^3 - 2N \sum_{M=1}^{N} (M + N^2)
\]
\[
= 2N^3 - 2N \left( \frac{1}{2} N(N + 1) \right) + N^2
\]
\[
= N^3.
\]
\[
N = 5
\]

| \( n \) | \((B, T)\) | \{\(\ell\)\} | \(\sum (2\ell + 1)\) |
|--------|-------------|--------------|----------------|
| 0      | (1, 1)      | \{0\}        | 1              |
| 1      | (2, 1)      | \{1\}        | \(2 + 1 = 3\) |
| 2      | (3, 1)      | \{2, 0\}     | \(3 + 3 = 6\) |
| 3      | (4, 1)      | \{3, 1\}     | \(4 + 6 = 10\) |
| 4      | (5, 1)      | \{4, 2, 0\}  | \(5 + 10 = 15\) |
| 5      | (4, 2)      | \{5, 3\}     | \(15 + 3 = 18\) |
| 6      | (3, 3)      | \{6, 4, 2\}  | \(18 + 1 = 19\) |
| 7      | (2, 4)      | \{5, 3\}     | \(15 + 3 = 18\) |
| 8      | (1, 5)      | \{4, 2, 0\}  | 15             |
| 9      | (1, 4)      | \{3, 1\}     | 10             |
| 10     | (1, 3)      | \{2, 0\}     | 6              |
| 11     | (1, 2)      | \{1\}        | 3              |
| 12     | (1, 1)      | \{0\}        | 1              |
|        |              |              | Total : 125 = \(5^3 = N^3\) |

Table 1: For \(N = 5\), we have a total of \(N^3 = 125\) points in the cube. For every coplanar level \(n\), we have a subset of points that has symmetrical reflection around \(n = 6\), where \((B, T) = (3, 3)\). The sum of the total angular momentum \(l\) leads to the total number of points \(N^3\).
| $n$ | $(B,T)$ | $\{\ell\}$ | $\sum(2\ell + 1)$ |
|-----|---------|-------------|------------------|
| 0   | (1,1)   | \{0\}       | 1                |
| 1   | (2,1)   | \{1\}       | 2 + 1 = 3        |
| 2   | (3,1)   | \{2,0\}     | 3 + 3 = 6        |
| 3   | (4,1)   | \{3,1\}     | 4 + 6 = 10       |
| 4   | (5,1)   | \{4,2,0\}   | 5 + 10 = 15      |
| 5   | (6,1)   | \{5,3,1\}   | 6 + 15 = 21      |
| 6   | (7,1)   | \{6,4,2,0\} | 7 + 21 = 28      |
| 7   | (2,6)   | \{5,3,1\}   | 5 + 28 = 33      |
| 8   | (3,5)   | \{8,6,4,2\} | 3 + 33 = 36      |
| 9   | (4,4)   | \{9,7,5,3\} | 1 + 36 = 37      |
| 10  | (3,5)   | \{8,6,4,2\} | 3 + 33 = 36      |
| 11  | (2,6)   | \{5,3,1\}   | 5 + 28 = 33      |
| 12  | (1,7)   | \{6,4,2,0\} | 28               |
| 13  | (1,6)   | \{5,3,1\}   | 21               |
| 14  | (1,5)   | \{4,2,0\}   | 15               |
| 15  | (1,4)   | \{3,1\}     | 10               |
| 16  | (1,3)   | \{2,0\}     | 6                |
| 17  | (1,2)   | \{1\}       | 3                |
| 18  | (1,1)   | \{0\}       | 1                |

|   | Total : | 343 = 7^3 = N^3 |

Table 2: For $N = 57$, we have a total of $N^3 = 343$ points in the cube. For every coplanar level $n$, we have a subset of points that has symmetrical reflection around $n = 9$, where $(B, T) = (4, 4)$. The sum of the total angular momentum $l$ leads to the total number of points $N^3$. 
\[N = \text{odd}\]

| \(n\) | \((B, T)\) | \(\{\ell\}\) | \(\sum(2\ell + 1)\) |
|-------|-------------|----------------|--------------------|
| 0     | (1, 1)      | \{0\}          | 1                  |
| 1     | (2, 1)      | \{1\}          | \(2 + 1 = 3\)     |
| ...   | ...         | ...            | ...               |
| \(n\) | \((n + 1, 1)\) | \{\(n, n - 2, ..., 0\) or \(1\)\} | \(\tau_n = \frac{1}{2}(n + 1)(n + 2)\) |
| ...   | ...         | ...            | ...               |
| \(N - 2\) | \((N - 1, 1)\) | \{\(N - 2, N - 4, 0\)\} | \(\tau_{N-2}\) |
| \(N - 1\) | \((N, 1)\)   | \{\(N - 1, N - 3, 1\)\} | \(\tau_{N-1}\) |
| \(N\)  | \((N - 1, 2)\) | \{\(N - 1, N - 2, ..., 2\)\} | \(\frac{1}{4}(N^2 + 3N + 2)\) |
| \(N + 1\) | \((N - 2, 3)\) | \{\(N - 1, N - 2, ..., 3\)\} | \(\frac{1}{2}(N^2 + 5N - 6)\) |
| ...    | \(\frac{3}{2}(N - 1)\) | \{\(N - 1, N - 2, ..., \frac{N - 1}{2}\)\} | \(\frac{1}{4}(3N^2 + 1)\) |
| ...    | \(2N - 4\)  | \{\(N - 1, N - 2, ..., 3\)\} | \(\frac{1}{2}(N^2 + 5N - 6)\) |
| ...    | \(2N - 3\)  | \{\(N - 1, N - 2, ..., 2\)\} | \(\frac{1}{2}(N^2 + 3N + 2)\) |
| \(2N - 2\) | \((1, 7)\)  | \{\(N - 1, N - 3, 1\)\} | \(\tau_{N-1}\) |
| \(2N - 1\) | \((1, 6)\)  | \{\(N - 2, N - 4, 0\)\} | \(\tau_{N-2}\) |
| ...    | ...         | ...            | ...               |
| \(3N + 3 - n'\) | \((1, n' + 1)\) | \{\(n', n - 2, 1\) or \(0\)\} | \(\tau_{n'}\) |
| ...    | ...         | ...            | ...               |
| \(3N - 4\) | \((1, 2)\)  | \{1\}          | 3                  |
| \(3N - 3\) | \((1, 1)\)  | \{0\}          | 1                  |
| \(\text{Total :}\) | \(N^3\)    |                |                    |

Table 3: Generalization for the counting modes when we deal with a cube of \(N^3\) odd number of points. We see that, in the same fashion as the 2D case for integer representation size \(j\), we have a central mode at \(\frac{3}{2}(N - 1)\). For semi-integer \(j\), there exist two middle points at \(\frac{3}{2}(N - 2)\) and \(\frac{3}{2}(N - 1)\).
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