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The discrete Fourier transform and the quantum-mechanical oscillator in a finite-dimensional Hilbert space

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Abstract
Quantum mechanics of a linear harmonic oscillator in a finite-dimensional Hilbert space satisfying the correct equations of motion is studied. The connections to Weyl's formulation of the algebra of bounded unitary operators in finite space as well as to a truncated quantized linear harmonic oscillator are discussed. It is pointed out that the *discrete Fourier transformation* (DFT) plays a central role in determining the actual form of the position, the momentum, the number and the Hamiltonian operators. The explicit form of these operators in different bases is exhibited for some low values of the dimension of the Hilbert space. In this formulation, it is shown that the Hamiltonian is indeed the logarithm of the DFT and that by modifying Weyl's framework to include position and momentum operators with non-uniformly spaced spectra the equations of motion are satisfied.

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1. Introduction

Quantum mechanics normally deals with an infinite-dimensional Hilbert space where the self-adjoint position and momentum operators satisfy Heisenberg's *canonical commutation relation* (CCR). Quantum mechanics in finite dimensions has been found to have very important applications in quantum computing and quantum optics [12, 13]. In a finite-dimensional Hilbert space it is known that CCR cannot hold. A formulation of quantum mechanics in finite dimensions was given some years back, based on Weyl's algebra of bounded unitary

[3] This work was done while this author was on sabbatical leave at the Center for Signal and Image Processing, Georgia Institute of Technology, Atlanta, Georgia, during the Spring of 2007.

operators, where the analog of CCR was worked out. It was soon understood that when the CCR framework was applied to a linear harmonic oscillator in finite dimensions, the equations of motion became inconsistent for dimensions $n > 3$. An alternate formulation of a harmonic oscillator in finite space was to truncate the number spectrum of the oscillator.

In Weyl's form, quantum mechanics in a finite-dimensional Hilbert space is built from unitary rotations in ray space [4]. The impetus for this, however, is quantum kinematics furnished by the basic canonical commutation relation of Heisenberg and Dirac [1] and is obtained by exponentiation of the self-adjoint position and momentum operators. However, quantum dynamics requires the knowledge of the Hamiltonian and the equations of motion. Generally, as showed by Wigner [11], equations of motion will be consistent with even more general forms of the canonical commutation relation.

In this paper, we study the quantum harmonic oscillator in a finite-dimensional Hilbert space. In this case, the Hamiltonian operator has an equally spaced spectrum and thus commutes with the DFT. The main result is to show Weyl's commutation relation, unless modified to account for not-equally spaced distribution of the spectrum of the position and momentum operators, is not consistent with the equations of motion except for dimensions $n = 2, 3$ of the Hilbert space. The truncated spectrum of the number, position and momentum operators are used to demonstrate this. As is known [7], the spectrum of the truncated position operator consists of the zeros of the Hermite polynomials (not equally spaced except for dimensions 2 and 3). This resulted in the inconsistency of Weyl's form for $n > 3$ [6].

2. Standard quantum harmonic oscillator

In quantum mechanics, the harmonic oscillator obeys the equations of motion given by

$$[\mathbf{H}, \hat{q}] = -\mathrm{i}\hat{p}, \qquad [\mathbf{H}, \hat{p}] = \mathrm{i}\hat{q}, \tag{1}$$

where $\hat{p}$ and $\hat{q}$ are the self-adjoint position and momentum operators satisfying the CCR:

$$[\mathbf{q}, \mathbf{p}] = \mathrm{i}\mathbf{I}, \tag{2}$$

and the Hamiltonian operator $\mathbf{H}$ is given by

$$\mathbf{H} = \frac{\hat{p}^2 + \hat{q}^2}{2}. \tag{3}$$

$\mathbf{H}$ is in turn related to the number operator through

$$\mathbf{H} = \mathbf{N} + \tfrac{1}{2}. \tag{4}$$

The bases of the unbounded $\hat{p}$ and $\hat{q}$ operators are related through the Fourier transform via

$$|p\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(-\mathrm{i}qp)|q\rangle\,\mathrm{d}q = \mathcal{F}(|q\rangle). \tag{5}$$

As is known the Fourier transform $\mathcal{F}$ satisfies the relations:

$$\mathcal{F}^2|q\rangle = -|q\rangle, \qquad \mathcal{F}^4|q\rangle = |q\rangle. \tag{6}$$

In view of these involutional properties, the Fourier transform satisfies the remarkable relation:

$$\mathcal{F} = \exp\left(\frac{\mathrm{i}\pi}{2}\mathbf{N}\right) = \exp\left(\frac{\mathrm{i}\pi}{4}(\hat{p}^2 + \hat{q}^2 + \mathrm{i}[\hat{q}, \hat{p}])\right). \tag{7}$$

The eigenfunctions of the Hamiltonian $\mathbf{H}$ are the Gauss–Hermite functions defined by

$$\psi_n(q) = \langle N|q\rangle \frac{1}{\pi^{1/4}\sqrt{2^n n!}} H_n(q) \exp\left(-\frac{q^2}{2}\right), \tag{8}$$

where $H_n(q)$ is the Hermite polynomial of order n. The number operator and the Fourier operator are consequently connected through the logarithm:

$$\mathbf{N} = -\frac{2\mathrm{i}}{\pi}\log\mathcal{F}. \tag{9}$$

In the N-diagonal basis, the operator $\hat{q}$ has the symmetric tridiagonal form:

$$\hat{q} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0\ldots \\ 1 & 0 & \sqrt{2} & 0 & 0 & \ldots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \ldots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \ldots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \sqrt{5}\ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}. \tag{10}$$

These concepts are part of any standard quantum mechanics textbook [1].

3. Harmonic oscillator in finite dimensions

In a finite-dimensional Hilbert space, $\hat{q}$ and $\hat{p}$ are finite-dimensional Hermitian matrices (we use the same notation as in standard quantum mechanics), it is known that the CCR framework does not apply. The question of interest is, how close one can approach the standard harmonic oscillator that satisfies the equations of motion and the framework described in the previous section. Earlier attempts consisted in truncating the form of $\hat{q}$ in the N-diagonal form. The other approach is to use the diagonal form for $\hat{q}$ and use Weyl's algebra [4]:

$$\begin{aligned} &\mathbf{AB} = \epsilon\mathbf{BA}, \qquad \epsilon = \exp\left(\mathrm{i}\frac{2\pi}{n}\right), \\ &\mathbf{A}^n = \mathbf{B}^n = \mathbf{I}, \\ &\mathbf{A} = \exp\left(\mathrm{i}\sqrt{\frac{2\pi}{n}}\hat{p}\right), \qquad \mathbf{B} = \exp\left(\mathrm{i}\sqrt{\frac{2\pi}{n}}\hat{q}\right). \end{aligned} \tag{11}$$

When applied to the quantum harmonic oscillator, it was noted that for $n > 3$, the equations of motion become inconsistent when the spectrum of $\hat{q}$ is equally spaced. To analyze the quantum harmonic oscillator in a finite-dimensional Hilbert space, we have the following:

Theorem. *The first equation of motion given by*

$$[\mathbf{N}, \hat{q}] = -\mathrm{i}\hat{p}$$

implies the second equation of motion:

$$[\mathbf{N}, \hat{p}] = \mathrm{i}\hat{q},$$

if the following relations hold:

$$\begin{aligned} &(i) \quad [\mathbf{N}, \mathbf{S}] = \mathbf{0}, \\ &(ii) \quad \hat{p} = \mathbf{S}\hat{q}\mathbf{S}^H, \\ &(iii) \quad \mathbf{S}^2\hat{q}\mathbf{S}^2 = -\hat{q}, \\ &(iv) \quad \mathbf{S}^2\hat{p}\mathbf{S}^2 = -\hat{p}, \end{aligned} \tag{12}$$

where **S** *is the DFT matrix.*

Proof.

$$[\mathbf{N}, \hat{q}] = -\mathrm{i}\hat{p} = -\mathrm{i}\mathbf{S}\hat{q}\mathbf{S}^H.$$

Since $\mathbf{S}$ is unitary we have

$$\mathbf{S}^H[\mathbf{N}, \hat{q}]\mathbf{S} = -\mathrm{i}\hat{q}.$$

Using (i) we have

$$[\mathbf{N}, \mathbf{S}^H\hat{q}\mathbf{S}] = -\mathrm{i}\hat{q}.$$

But we have

$$\mathbf{S}^H\hat{q}\mathbf{S} = \mathbf{S}^H\mathbf{S}^H\mathbf{S}\hat{q}\mathbf{S}^H\mathbf{S}\mathbf{S} = \mathbf{S}^2\hat{p}\mathbf{S}^2 = -\hat{p}$$

Hence it follows that

$$[\mathbf{N}, \hat{p}] = \mathrm{i}\hat{q}.$$

The problem thus boils down to solving for $\hat{q}$ satisfying the equation:

$$[\mathbf{N}, \hat{q}] = -\mathrm{i}\mathbf{S}\hat{q}\mathbf{S}^H. \tag{13}$$

The particular form of $\hat{q}$, however, is very sensitive to the basis chosen. If we choose $\mathbf{N}$ and $\mathbf{S}$ to be diagonal, they have the form:

$$\mathbf{N} = \mathrm{diag}(0, 1, 2, \ldots, n-1), \qquad \mathbf{S} = i^{\mathbf{N}} = \exp\left(\frac{\mathrm{i}\pi}{2}\mathbf{N}\right). \tag{14}$$

We can now solve for $\hat{q}$ satisfying equation (13) as follows:

$$\begin{aligned} &\mathbf{N}_{rs} = (r + (n-1)/2)\delta_{rs} \\ &\mathbf{S}_{rs} = \exp\left(\frac{\mathrm{i}\pi}{2}\mathbf{N}_{rs}\right), \qquad |r| \leqslant (n-1)/2 \\ &\hat{q}_{rs}[(r-s) + i^{r-s+1}] = 0 \quad \Rightarrow \quad (r-s) = \pm 1. \end{aligned} \tag{15}$$

This specifically implies that the operator $\hat{q}$ would have a tridiagonal form in the $\mathbf{N}$ and $\mathbf{S}$ diagonal basis. The eigenvalues of $\hat{q}$ are thus related to the zeroes of special functions. In particular, if we require $\mathbf{N}$ to have the form:

$$\mathbf{N} = \tfrac{1}{2}(\hat{p}^2 + \hat{q}^2 + \mathrm{i}[\hat{q}, \hat{p}]) \tag{16}$$

then the eigenvalues of $\hat{q}$ are the zeroes of the Hermite polynomials and $\hat{q}$ and $\hat{p}$ have the truncated form given by

$$\begin{aligned} \hat{q} &= \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0\ldots \\ 1 & 0 & \sqrt{2} & 0 & 0 & \ldots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \ldots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \ldots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \sqrt{5}\ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}, \\ \hat{p} &= \frac{-\mathrm{i}}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0\ldots \\ -1 & 0 & \sqrt{2} & 0 & 0 & \ldots \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & 0 & \ldots \\ 0 & 0 & -\sqrt{3} & 0 & \sqrt{4} & \ldots \\ 0 & 0 & 0 & -\sqrt{4} & 0 & \sqrt{5}\ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \end{aligned} \tag{17}$$

which is just the truncated form of $\hat{p}$, $\hat{q}$ from the standard harmonic oscillator. The zeros of the Hermite polynomials are not equally spaced except for $n = 2, 3$. The equations of motion and other properties except, of course, for the CCR are obeyed. A change of basis will not affect the equations of motion and the particular forms of the operators involved will be different. We give the forms of these matrices in three different basis: (a) N diagonal, (b) **S**-centralized and (c) $\hat{q}$ diagonal scenarios. To proceed from the **N** diagonal to the **S** centralized basis we require the matrix of eigenvectors of **S**. As is known [9], the analytic form for the eigenvectors of **S** is not known. We present in the following section the form of these matrices for $n = 3, 4, 5$. For the purposes of analysis, we define the centralized DFT [9] as

$$\mathbf{S}^{(c)}_{rs} \equiv \frac{1}{\sqrt{n}} \exp\left(-\mathrm{i}\frac{2\pi}{n} rs\right) = \mathbf{U}\mathbf{S}_{\mathrm{diag}}\mathbf{U}^{H}, \qquad |r, s| \leqslant \frac{n-1}{2}, \tag{18}$$

where $\mathbf{U}$ is the matrix of eigenvectors of $\mathbf{S}^{(c)}$ and $\mathbf{S}_{\mathrm{diag}} = \mathrm{diag}(1, i, i^2, \ldots, i^n)$. □

4. Form of the operators in $\hat{q}$-diagonal basis

(1) For $n = 3$ we have

$$\hat{q}_d = \sqrt{\frac{3}{2}}\mathrm{diag}(-1, 0, 1)$$

$$\Omega_3 = \mathbf{S}_{\text{q-diag}} = \frac{1}{6}\begin{pmatrix} -1+3\mathrm{i} & 4 & -1-3\mathrm{i} \\ 4 & 2 & 4 \\ -1-3\mathrm{i} & 4 & -1+3\mathrm{i} \end{pmatrix}$$

$$\mathbf{M}_3 = \frac{1}{6}\begin{pmatrix} 7 & -4 & 1 \\ -4 & 4 & -4 \\ 1 & -4 & 7 \end{pmatrix}.$$

(2) For $n = 4$ we have

$$\hat{q}_d = \mathrm{diag}\,\underbrace{(-1.651, -0.525, 0.525, 1.651)}_{\text{Zeroes of } H_4}$$

$$\Omega_4 = \begin{pmatrix} -0.488 & 0.288+0.5\mathrm{i} & -0.288+0.5\mathrm{i} & -0.408 \\ 0.288+0.5\mathrm{i} & 0.488 & -0.408 & 0.288-0.5\mathrm{i} \\ -0.288+0.5\mathrm{i} & -0.408 & 0.488 & -0.288-0.5\mathrm{i} \\ -0.408 & 0.288-0.5\mathrm{i} & -0.288-0.5\mathrm{i} & -0.488 \end{pmatrix}$$

$$\mathbf{M}_4 = \begin{pmatrix} 1.908 & -0.788 & -0.212 & -0.092 \\ -0.788 & 1.092 & 0.908 & 0.212 \\ -0.212 & 0.908 & 1.092 & 0.788 \\ -0.092 & 0.212 & 0.788 & 1.908 \end{pmatrix}.$$

(3) For $n = 5$ we have

$$\hat{q}_d = \mathrm{diag}\,\underbrace{(-2.02, -0.959, 0, 0.959, 2.02)}_{\text{Zeros of } H_5}$$

$$\mathbf{M}_5 = \begin{pmatrix} 2.694 & -0.887 & 0.245 & 0.113 & 0.061 \\ -0.887 & 1.639 & -1.088 & -0.272 & -0.113 \\ 0.245 & -1.088 & 1.333 & 1.088 & 0.245 \\ 0.113 & -0.272 & 1.088 & 1.639 & 0.887 \\ 0.061 & -0.113 & 0.245 & 0.887 & 2.694 \end{pmatrix}.$$

It can be easily verified that all the equations of motion are satisfied and that the Hamiltonian has the same structure as for the standard harmonic oscillator and is indeed the logarithm of the DFT. For the equations of motion to be satisfied in the $\hat{q}$ diagonal basis, the form of $\hat{q}$ cannot have uniformly spaced elements since the basis change from the **N**-diagonal basis is a similarity transformation. This fact is consistent with earlier results in QFMD [5, 6], where the equations of motion were violated for $n > 3$, when the elements of $\hat{q}$ were chosen to be equally spaced. Furthermore the form of the DFT in the $\hat{q}$-diagonal basis cannot be the centered version of the DFT used in [5, 6], but rather the similarity transformed version of the diagonal version of the DFT in the **N**-diagonal basis, accomplished using the eigenvectors of the tridiagonal $\hat{q}$.

5. Centralized DFT basis

(1) For $n = 3$ we have

$$\mathbf{S} = \frac{1}{\sqrt{3}}\begin{pmatrix} -0.5+\mathrm{i}\frac{\sqrt{3}}{2} & 1 & -0.5-\mathrm{i}\frac{\sqrt{3}}{2} \\ 1 & 1 & 1 \\ -0.5-\mathrm{i}\frac{\sqrt{3}}{2} & 1 & -0.5+\mathrm{i}\frac{\sqrt{3}}{2} \end{pmatrix}.$$

$$\hat{q} = \begin{pmatrix} 1.213 & 0.119 & 0 \\ 0.119 & 0 & -0.119 \\ 0 & -0.119 & -1.213 \end{pmatrix}.$$

$$\mathbf{N} = \mathbf{I} + \frac{1}{2\sqrt{3}}\begin{pmatrix} 1 & -2 & 1 \\ -2 & -2 & -2 \\ 1 & -2 & 1 \end{pmatrix}.$$

(2) For $n = 4$ we have

$$\hat{q} = \begin{pmatrix} 0.377 & -1.037 & 0.561 & 0 \\ -1.037 & -0.282 & 0 & -0.561 \\ 0.561 & 0 & 0.282 & 1.037 \\ 0 & -0.561 & 1.037 & -0.377 \end{pmatrix}$$

$$\mathbf{N} = \begin{pmatrix} 2.153 & -0.653 & 0.271 & -0.229 \\ -0.653 & 0.847 & -0.771 & 0.271 \\ 0.271 & -0.771 & 0.847 & -0.653 \\ -0.229 & 0.271 & -0.653 & 2.153 \end{pmatrix}.$$

(3) For $n = 5$ we have

$$\hat{q} = \begin{pmatrix} -0.721-0.079\mathrm{i} & 0.344-0.022\mathrm{i} & 1.007-0.07\mathrm{i} & 0.095-0.066\mathrm{i} & 0.022+0.079\mathrm{i} \\ 0.344+0.079\mathrm{i} & 0.819-0.045\mathrm{i} & -0.899-0.036\mathrm{i} & -0.011 & -0.108-0.079\mathrm{i} \\ 0.981 & -0.871 & 0 & 0.871 & -0.981 \\ 0.108+0.079\mathrm{i} & 0.011 & 0.899+0.036\mathrm{i} & -0.819+0.045\mathrm{i} & -0.344-0.079\mathrm{i} \\ -0.022-0.079\mathrm{i} & -0.095+0.066\mathrm{i} & -1.007+0.07\mathrm{i} & -0.344+0.022\mathrm{i} & 0.721+0.079\mathrm{i} \end{pmatrix}$$

$$\mathbf{N} = \begin{pmatrix} 1.787 & 0.044-0.151\mathrm{i} & -0.536-0.243\mathrm{i} & 0.569-0.151\mathrm{i} & -1.064 \\ 0.099 & 1.835+0.085\mathrm{i} & 1.004+0.138\mathrm{i} & 0.685+0.085\mathrm{i} & 0.624 \\ -0.447 & 0.916-0.106\mathrm{i} & 2.757-0.171\mathrm{i} & 0.916-0.106\mathrm{i} & -0.447 \\ 0.624 & 0.685+0.085\mathrm{i} & 1.004+0.138\mathrm{i} & 1.835+0.085\mathrm{i} & 0.099 \\ -1.064 & 0.569-0.151\mathrm{i} & -0.536-0.243\mathrm{i} & 0.044-0.151\mathrm{i} & 1.787 \end{pmatrix}.$$

As with the $\hat{q}$-diagonal basis representation, it can be verified that the equations of motion are satisfied and that the form of the Hamiltonian is invariant to the basis change. In the earlier work on QMFD, the equations of motion were satisfied for $n \leqslant 3$, however, the number operator did not have the desired form in equation (16).

6. Conclusions

Quantum mechanics of a linear harmonic oscillator in a finite-dimensional Hilbert space, where the equations of motion are completely satisfied has been worked out. The inconsistencies in the truncated form of the oscillator in the **N** (and hence **S**) diagonal form that were prevalent in the Weyl's form and in earlier attempts at the same can be traced back to (a) the fact that the spectrum of the operator $\hat{q}$ is not uniformly spaced in the **q**-diagonal basis, and (b) incorrect use of the centralized DFT in the different bases. The equations of motion will still be satisfied in any basis as long as the appropriate version of the DFT is used. If we prefer to retain the form of the Hamiltonian, i.e., quadratic in the position and momentum operators in the different representations, the corresponding $\hat{q}$ has to be tridiagonal in the **N**-diagonal form and its spectrum is simply the zeroes of the Hermite polynomials. With this framework the discrete Hamiltonian maintains the same logarithmic connection to the DFT that the Gauss–Hermite differential operator has with the Fourier operator $\mathcal{F}$. The limiting process, where one desires convergence to the second-order Gauss–Hermite differential operator, also holds well with this framework.

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