# NON-COMMUTATIVE SPHERES AND NUMERICAL QUANTUM MECHANICS

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Abstract. We discuss some basic issues that arise when one attempts to model quantum mechanical systems on a computer, and we describe the mathematical structure of the resulting discretized cannonical commutation relations. The $C^*$-algebras associated with the discretized $CCRs$ are the non-commutative spheres of Bratteli, Elliott, Evans and Kishimoto.

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## 1. Introduction.

We discuss some basic issues associated with the problem of modelling quantum mechanical phenomena on a computer. Before setting out to write code for any program of this kind, one first has to recast the quantum mechanical Hamiltonian into a form appropriate for doing numerical calculations; at the same time, one has to retain the essential features of quantum mechanics (i.e., the uncertainty principle). Reflection on this problem shows that one must confront a more basic issue, namely that of "discretizing" the canonical operators $P$, $Q$ which satisfy the commutation relations

$$PQ - QP = \frac{1}{i}\mathbf{1}.$$

For simplicity, we consider one-dimensional quantum systems. We will show that there is a natural (perhaps one could say an *inevitable*) way to discretize the canonical operators $(P, Q)$ so that (a) the discretized pair conforms to the basic principles of numerical analysis, and (b) the uncertainty principle is preserved. We will see that there is a one-parameter family $(P_\alpha, Q_\alpha)$, $\alpha > 0$, of discretized canonical operators. The parameter $\alpha$ is the square of the numerical step size. For each $\alpha$, $P_\alpha$ and $Q_\alpha$ are bounded self-adjoint operators which obey an altered form of the canonical commutation relations.

If $\alpha$ is not a rational multiple of $2\pi$ then the unital $C^*$-algebra generated by $\{P_\alpha, Q_\alpha\}$ turns out to be one of the non-commutative spheres of Bratteli et al [1], [2], and hence is a simple $C^*$-algebra which has a unique tracial state. This $C^*$-algebra contains the discretized Hamiltonian, and that opens the possibility of computing its spectrum. While much remains to be learned, there are examples in which the spectrum of the discretized Hamiltonian is totally disconnected. In particular, these $C^*$-algebras contain many projections. We also show how each of these $C^*$-algebras arises as the enveloping $C^*$-algebra associated with an appropriately discretized version of the Weyl canonical commutation relations. Thus, it seems appropriate to conclude that *non-commutative spheres will arise naturally in any serious attempt to model quantum phenomena via computer.*

It is unlikely that there is a direct connection between these non-commutative spheres and the quantum spheres of Woronowicz and Podleś [6]. I should also point out that this work is in progress, and that full details will appear elsewhere. I would like to thank Paul Chernoff and Alan Weinstein for objecting strenuously to an earlier version of this paper; their constructive criticism has caused me to think more carefully about the exposition, with the result that the paper is now better than it was. Whatever deficiencies that remain are the sole responsibility of the author.

## 2. Background.

In order to tie the discussion to a specific issue, we digress briefly in order to describe the kind of computing problem which has motivated this work.

Consider the one-dimensional anharmonic oscillator. Apart from a choice of units, the relevant equation of motion is

$$\ddot{x} + x + gx^3 = 0. \tag{2.1}$$

Here, $g$ is a nonnegative constant and $x = x(t)$ is a real-valued function of time $t$. In physical terms, one has a unit mass attached to one end of a nonlinear spring, the other end being held fixed at the origin. When the spring is stretched to a

length $L$, the restoring force is $L + gL^3$. The spring is linear (i.e., it obeys Hooke's law) when $g = 0$.

In order to quantize this system, one passes to the Hilbert space $L^2(\mathbb{R})$ in the Schrödinger picture. Given an initial wave function $f \in L^2(\mathbb{R})$ at time zero, basic principles dictate that $f$ evolves in time according to

$$f(t) = e^{itH} f, \qquad t \in \mathbb{R},$$

where $H$ is the quantum mechanical Hamiltonian. In the case of the anharmonic oscillator, $H$ is the operator

$$\frac{1}{2}P^2 + v(Q)$$

where $P = -id/dx$, $Q$ is multiplication by $x$, and $v(x) = x^2/2 + gx^4/4$ is the potential function associated with the differential equation (2.1).

It is not hard to "draw" solutions of the classical equation (2.1) using a modern desktop computer. I have done this with good results for systems of up to 50 interacting anharmonic oscillators. For example, even with small systems (four masses, say) one can observe interesting chaotic behavior resulting from the nonlinearity of the system for $g > 0$. On the other hand, it is less clear how one might use a computer to create an interesting graphical representation of the quantized system. What I have in mind is to draw pictures of a quantized system of interacting anharmonic oscillators which resemble the pictures described above, at least insofar as that is possible.

With every quantum system there is an associated stationary stochastic process whose state space is the configuration space of the classical system ([4], [5]). Without going into the details of how this process is constructed (see section 5), let me just say that my intention is to construct "typical" sample paths for this quantum process and draw them on a computer screen. While I am not yet finished writing the code for this program, I am nevertheless convinced by the results below that it is *possible* to do it. Practical obstructions, relating to the runtime for such programs, remain to be seen.

## 3. Discretizing $P$ and $Q$.

We turn now to the specific issues that arise when one seeks to build numerical approximations to a quantum system. One must first replace the Hamiltonian

$$H = \frac{1}{2}P^2 + v(Q)$$

with an approximation to it which is appropriate for doing numerical studies. Let us first consider the momentum operator $P = -id/dx$. Letting $V$ be the one-parameter unitary group of translations

$$V_t f(x) = f(x - t),$$

then of course $P$ is the infinitesimal generator of $V$

$$V_t = e^{itP}.$$

Equivalently, we have

$$P = \lim \frac{1}{t}(V_t - \mathbf{1})$$

in an appropriate sense on the domain of $P$. Conventional wisdom indicates that $P$ should be replaced with a difference operator, the simplest one being

$$P_\tau = \frac{1}{i\tau}(V_\tau - \mathbf{1}).$$

Here, $\tau$ is the numerical step size. While this operator is certainly bounded, it is the wrong choice for two reasons. It is not self adjoint, and for small $\tau$ it approximates $P$ only to terms of order $O(\tau)$, which is not very good. Thus it is better to use the real part of the above operator, namely

$$P_\tau = \frac{1}{2i\tau}(V_\tau - V_{-\tau}).$$

This is a bounded self adjoint operator which approximates $P$ (on smooth test functions) to terms of order $O(\tau^2)$. Using the fact that $V_\tau = e^{i\tau P}$ we have the equivalent formula

$$P_\tau = \frac{1}{\tau}\sin(\tau P). \tag{3.1}$$

Considering that the function

$$f(x) = \frac{\sin(\tau x)}{\tau}$$

approximates the function $g(x) = x$ very closely in a fixed interval $-M \leq x \leq +M$ when $\tau$ is small, one can expect good numerical results from $P_\tau$ for small values of $\tau$.

We must now approximate $Q$ in a similar fashion, but in doing so we must be careful to preserve the essential features of quantum mechanics. That means the uncertainty principle. In fact, the uncertainty principle for the approximating pair $(P_\tau, Q_\tau)$ is achieved by choosing

$$Q_\tau = F^{-1}P_\tau F,$$

where F is the Fourier transform operator on $L^2(\mathbb{R})$. In order to discuss our reasons for making this choice, we digress momentarily to a more coordinate-free setting.

Suppose that one has a pair of one-parameter unitary groups $U$, $V$ which act on the same Hilbert space $H$ in such a way that $V_s U_t = e^{ist}U_t V_s$, and such that the set of operators $\{U_t\} \cup \{V_s\}$ is irreducible. Then the self-adjoint generators $P$, $Q$ of these two groups

$$V_t = e^{itP}, \qquad U_t = e^{itQ}$$

obey the commutation relation cited in the introduction. Choose a unit vector $f$ in the underlying Hilbert space $H$. Then the probability measure associated with the observable $Q$ and the state $f$ is the probability measure defined (on the Borel subsets of $\mathbb{R}$) by

$$q(S) = < E_Q(S)f, f >, \qquad S \subseteq \mathbb{R}$$

where $E_Q$ is the spectral measure of $Q$. Similarly, the probability distribution associated with $P$ and $f$ is

$$p(S) = < E_P(S)f, f >, \qquad S \subseteq \mathbb{R}$$

The uncertainty principle for the pair of observables $(P, Q)$ makes the following qualitative assertion: if a wave function $f$ represents a physical state such that the measure $q$ appears highly concentrated near a point, then the measure $p$ must appear "spread out". A similar assertion applies, of course, with $p$ and $q$ interchanged.

It is not hard to reformulate this somewhat vague assertion entirely in terms of the Fourier transform operator. To see this, notice first that there is a unitary operator $F \in \mathcal{B}(H)$ such that

$$P = F^{-1}QF, \qquad -Q = F^{-1}PF, \tag{3.2}$$

Indeed, since the pair $(P', Q')$ defined by $P' = -Q$, $Q' = P$ is irreducible and satisfies the same commutation relation (equivalently, $U_{-s}V_t = e^{ist}V_tU_{-s}$, $s, t \in \mathbb{R}$), the Stone-von Neumann theorem implies that the two pairs $(P, Q)$ and $(P', Q')$ are unitarily equivalent, and $F$ may be chosen as a unitary operator implementing this equivalence. Moreover, because of the irreducibility hypothesis $F$ is uniquely defined by (3.2) up to a scalar multiple of absolute value 1. It follows from the relation $P = F^{-1}QF$ and elementary functional calculus that

$$E_P(S) = F^{-1}E_Q(S)F, \qquad S \subseteq \mathbb{R},$$

and hence the formula for the measures $p$ and $q$ can be rewritten in terms of $F$ as follows

$$\begin{aligned} q(S) &= < E_Q(S)f, f > \\ p(S) &= < E_Q(S)Ff, Ff >, \qquad S \subseteq \mathbb{R}. \end{aligned}$$

Applying the Stone-von Neumann theorem once again, we may assume (after replacing $(P, Q)$ with a unitarily equivalent pair) that $H = L^2(\mathbb{R})$, $P = -id/dx$, $Q =$ *multiplication by* $x$, and that $f$ is a normalized function in $L^2(\mathbb{R})$. Notice too that, after this change of coordinates, $F$ must be a scalar times the usual Fourier transform operator. Indeed, for this choice of $P$ and $Q$ acting on $L^2(\mathbb{R})$, the Fourier transform operator $F_0$ is well-known to satisfy (3.2), i.e.,

$$F_0P = QF_0, \qquad F_0Q = -PF_0.$$

Hence by irreducibility we must have $F = \lambda F_0$ where $\lambda$ is a complex number of absolute value 1. Thus in these coordinates the preceding formulas for $p$ and $q$ become

$$\begin{aligned} q(S) &= \int_S |f(x)|^2 \, dx \\ p(S) &= \int_S |\hat{f}(x)|^2 \, dx, \qquad S \subseteq \mathbb{R} \end{aligned}$$

$\hat{f}$ denoting the Fourier transform of the function $f$.

At this point, one can recognize the uncertainty principle as reflecting a familiar property of the Fourier transform. Indeed, if the measure $q$ is highly concentrated near a point $x_0$ then so is the wave function $f$; hence its Fourier transform $\hat{f}$ is highly spread out (approximating a constant multiple of the pure exponential $x(\lambda) \to \exp(ix\cdot\lambda)$) and thus the measure $p$ is highly dispersed.

More generally, if one starts with *any* bounded self-adjoint operator $P_1$ in the von Neumann algebra generated by all translation operators on $L^2(\mathbb{R})$, then one can expect some form of the uncertainty principle for the pair of operators $(P_1, FP_1F^{-1})$, at least for bounded operators $P_1$ which are reasonable approximations to $P$. In more detail, we first find a bounded real valued Borel measurable function $\phi$ such that $P_1 = \phi(P)$. Standard functional calculus implies that $Q_1 = FP_1F^{-1} = F\phi(P)F^{-1} = \phi(Q)$. Thus if $f$ is any normalized function in $L^2(\mathbb{R})$ then we have

$$< E_{Q_1}(S)f, f) = < E_Q(\phi^{-1}S)f, f >, and$$
$$< E_{P_1}(S)f, f) = < E_P(\phi^{-1}S)f, f >=< E_Q(\phi^{-1}S)Ff, Ff >$$

for any Borel set in $\mathbb{R}$, $\phi^{-1}S$ denoting the inverse image of the set $S$ under $\phi$. It follows that the probability measures associated with the observables $Q_1$, $P_1$ and the state defined by $f$ are given by

$$q_1(S) = \int_{\phi^{-1}S} |f(x)|^2\, dx$$
$$p_1(S) = \int_{\phi^{-1}S} |\hat{f}(x)|^2, dx, \qquad S \subseteq \mathbb{R}$$

In the most degenerate cases where $\phi$ is nearly constant, these formulas have little content. However, if $|\phi(x) - x|$ is small for all $x$ in a very large interval, then these two measures closely approximate the measures $p$, $q$ of the preceding paragraphs, and hence they can be said to obey the uncertainty principle.

Returning now to the problem of approximating $Q$, we conclude from these observations that in order to preserve the uncertainty principle for the approximating operators $(P_\tau, Q_\tau)$, one should set

$$Q_\tau = FP_\tau F^{-1},$$

where $F$ is the usual Fourier transform. Notice that *there is no arbitrariness in the choice of* $Q_\tau$; once we have settled on a discretized approximant $P_\tau$ to $P$, $Q_\tau$ is forced upon us by requiring that the uncertainty principle should be preserved.

Equivalently, the definition of $Q_\tau$ is

3.3 $$Q_\tau = \frac{\sin(\tau Q)}{\tau}.$$

In terms of the one-parameter group of multiplication operators

$$U_t f(x) = e^{itx} f(x),$$

this definition can also be written

$$Q_\tau = \frac{1}{2i\tau}(U_\tau - U_{-\tau}),$$

$\tau$ being the same step size used for $P_\tau$.

Thus for every $\tau > 0$, we have a pair of bounded self adjoint operators $(P_\tau, Q_\tau)$. We will write $C^*(P_\tau, Q_\tau)$ for the unital $C^*$ algebra generated by $P_\tau$ and $Q_\tau$.

Finally, our approximation to the original Hamiltonian is defined as

$$H = \frac{1}{2}P_\tau^2 + v(Q_\tau).$$

We abuse notation slightly here, but since we will have no need to refer back to the original unbounded Hamiltonian it will cause no problem. $H$ is a bounded self adjoint operator for every continuous real-valued function $v$, and it obviously belongs to $C^*(P_\tau, Q_\tau)$.

$$\gamma_t(a) = e^{itH}ae^{-itH}$$

defines a uniformly continuous one-parameter group of inner automorphisms of this $C^*$-algebra.

Let us now recall the definition of non-commutative spheres $\mathcal{B}_\alpha$ [1], [2]. Let $\alpha \in \mathbb{R}$ and let $U$, $V$ be a pair of unitary operators which satisfy

$$VU = e^{i\alpha}UV.$$

The $C^*$-algebra $\mathcal{A}_\alpha$ generated by $U$ and $V$ is well known to be independent of the particular choice of $U$ and $V$, is simple, and has a unique tracial state.

Noting that the pair $(U^{-1}, V^{-1})$ satisfy the same commutation relations as $(U, V)$, we can define a unique $*$-automorphism $\sigma$ of $\mathcal{A}_\alpha$ by requiring

3.4 $$\sigma(U) = U^{-1}, \qquad \sigma(V) = V^{-1}.$$

We have $\sigma^2 = id$, and hence $\sigma$ defines a $\mathbb{Z}_2$-action on $\mathcal{A}_\alpha$. When $\alpha$ is *not* a rational multiple of $\pi$, $\mathcal{B}_\alpha$ is defined as the fixed subalgebra

$$\mathcal{B}_\alpha = \{a \in \mathcal{A}_\alpha : \sigma(a) = a\}.$$

**Theorem 3.5.** *For every positive $\tau$ such that $\tau^2/\pi$ is irrational, $C^*(P_\tau, Q_\tau)$ is isomorphic to $\mathcal{B}_{\tau^2}$.*

*Remarks.* In case $\alpha/\pi$ is irrational, it is well known that the unique trace on $\mathcal{A}_\alpha$ gives rise to a representation of $\mathcal{A}_\alpha$ which generates the hyperfinite $II_1$ factor $R$, and one can show that the weak closure of the $\sigma$-fixed subalgebra is a subfactor of $R$ having Jones index 2. Recalling that such subfactors of $R$ are unique up to conjugacy (see [3], pp.1–2 for more detail), we can recognize this as a very stable invariant for the embedding of $C^*(P_\tau, Q_\tau)$ in $\mathcal{A}_{\tau^2}$ at the level of von Neumann algebras. Thus, we may think of $C^*(P_\tau, Q_\tau)$ as being isomorphic to an "index two" $C^*$-subalgebra of the irrational rotation algebra $\mathcal{A}_{\tau^2}$.

We also remark that since the step size $\tau$ must be chosen to be a small rational number in any realistic computational setting (for example, $\tau = 10^{-4}$ is typical for me), the $C^*$-algebras $C^*(P_\tau, Q_\tau)$ that actually arise will always satisfy the hypothesis of Theorem 3.5.

Let $tr$ be the tracial state of $C^*(P_\tau, Q_\tau)$. Then for every $\beta > 0$ there is a KMS state $\omega_\beta$ associated with the group $\gamma$ and the value $\beta$. $\omega_\beta$ is defined on $C^*(P_\tau, Q_\tau)$ by

$$\omega_\beta(a) = \frac{tr(e^{-\beta H}a)}{tr(e^{-\beta H})}.$$

The GNS construction applied to $\omega_\beta$ leads to a representation of $C^*(P_\tau, Q_\tau)$ which

**4. The discretized $CCR$ algebra..**

We now give an alternate description of $C^*(P_\tau, Q_\tau)$ as the universal $C^*$-algebra associated with a discretized version of Weyl's form of the canonical commutation relations. Significantly, it is this realization of $C^*(P_\tau, Q_\tau)$ that is most useful for doing numerical calculations. Fix $\alpha > 0$, not a rational multiple of $\pi$. Consider the discrete abelian group $G = \mathbb{Z} \times \mathbb{Z}$, and let $\omega : G \times G \to \mathbb{T}$ be the bi-character defined by

$$\omega((m,n),(p,q)) = e^{i(np-mq)\alpha/2}.$$

By a representation of the *discretized canonical commutation relations* we mean a uniformly bounded family $\{D_x : x \in G\}$ of bounded *self adjoint* operators on a Hilbert space which satisfy

$$D_x D_y = \omega(x,y) D_{x+y} + \omega(y,x) D_{x-y}. \tag{4.1}$$

*Remarks.* Formula 4.1 is a generalization of the elementary trigonometric identity

$$2\cos A \cos B = \cos(A+B) + \cos(A-B),$$

in which phase shifts have been added via the cocycle $\omega$. For example, the real-valued function $D : G \to \mathbb{R}$ defined (for $\sigma$ and $\phi$ fixed) by

$$D(m,n) = 2\cos(m\sigma + n\phi)$$

satisfies 4.1 for the trivial cocycle $\omega = 1$. It is also clear that 4.1 is closely related to Weyl's formulation of the canonical commutation relations. Finally, it can be shown that any bounded family of self-adjoint operators satisfying 4.1 must in fact obey $\|D_x\| \leq 2$; thus *there is a natural construction which produces a universal enveloping $C^*$-algebra $C^*(G,\alpha)$ for the relations 4.1.*

It can also be shown that the original operators $P_\tau$, $Q_\tau$ serve to define a unique $*$-representation $\pi$ of $C^*(G,\tau^2)$. $\pi$ is specified uniquely by requiring that

$$\pi(D(1,0)) = 2\tau P_\tau, \qquad \pi(D(0,1)) = 2\tau Q_\tau. \tag{4.2}$$

While a fairly explicit formula can be given for each of the operators $\pi(D(m,n))$ in terms of $P_\tau$ and $Q_\tau$, we shall not do so here. Now we are in position to formulate the second characterization of $C^*(P_\tau, Q_\tau)$.

**Theorem 4.3.** *The representation $\pi$ defined by 4.2 gives rise to an isomorphism of $C^*$-algebras*

$$C^*(\mathbb{Z} \times \mathbb{Z}, \tau^2) \cong C^*(P_\tau, Q_\tau).$$

**5. The canonical stochastic process.**

We now indicate how one can construct a stochastic process using the discretized operators $P_\tau$, $Q_\tau$ from section 3. Let $v$ be any continuous real-valued potential function, and set

$$H = \frac{1}{2}P_\tau^2 + v(Q_\tau).$$

**Theorem 5.1.** *Let $f_0, f_1, \ldots, f_n$ be nonnegative continuous functions of a real variable, and let $t_1, t_2, \ldots, t_n \geq 0$. Let $tr$ be the tracial state on $C^*(P_\tau, Q_\tau)$. Then*

$$tr(f_0(Q_\tau)e^{-t_1 H} f_1(Q_\tau)e^{-t_2 H} \ldots e^{-t_n H} f_n(Q_\tau)) \geq 0.$$

Using Theorem 5.1, we can make use of apparatus developed by Klein and Landau [4] as follows. Let $\alpha \geq 0$ and let $tr$ be the tracial state of Theorem 5.1.

**Theorem 5.2.** *Fix $\beta > 0$. There is a real-valued stochastic process $\{X_t : 0 \leq t \leq \beta\}$ which is defined by the conditions*

$$E(f_1(X_{t_1})f_2(X_{t_2}) \ldots f_n(X_{t_n})) = \frac{tr(e^{-t_1 H} f_1(Q_\tau)e^{-(t_2-t_1)H} f_2(Q_\tau) \ldots e^{-(t_n-t_{n-1})H} f_n(Q_\tau))}{tr(e^{-\beta H})}$$

*for every $0 \leq t_1 \leq t_2 \leq \cdots \leq t_n = \beta$, every $f_1, f_2, \ldots, f_n \in C_0(\mathbb{R})$, and every $n = 1, 2, \ldots$.*

*Remarks.* This process $\{X_t : 0 \leq t \leq \beta\}$ is stochastically continuous and periodic with period $\beta$ in that $X_\beta(\omega) = X_0(\omega)$ almost surely. Moreover, if one extends it in the obvious way to a periodic process (with period $\beta$) defined for all $t \in \mathbb{R}$, the resulting process is stationary and obeys a form of reflection-positivity (i.e., Osterwalder-Schrader positivity) which is appropriate for periodic processes.

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