

Equivalence Relations Between Deterministic and Quantum Mechanical Systems

Gerard 't Hooft¹

Received March 28, 1988

Several quantum mechanical models are shown to be equivalent to certain deterministic systems because a basis can be found in terms of which the wave function does not "spread." This suggests that apparently indeterministic behavior typical for a quantum mechanical world can be the result of locally deterministic laws of physics. We show how certain deterministic systems allow the construction of a Hilbert space and a Hamiltonian so that at long distance scales they may appear to behave as quantum field theories, including interactions but as yet no mass term. These observations are suggested to be useful for building theories at the Planck scale.

KEY WORDS: Hilbert space; massless fermions; extensive Hamiltonian; primordial observables; reversible cellular automaton; Baker-Campbell-Hausdorff expansion; discrete time.

1. INTRODUCTION

Quantum mechanics works.⁽¹⁾ In spite of many obvious objections raised to quantum mechanics when it was first proposed, it has proven to be a magnificent scheme for describing atomic and subatomic mechanics as well as for predicting new phenomena correctly. Philosophical objections purporting that there was something wrong with the logic of the theory never stood in the way of its usefulness. Nothing seems to be wrong in using quantum mechanics to describe interactions among atoms and fundamental particles.

Yet, in my view, there are reasons to believe that our present understanding of the fundamentals of quantum mechanics⁽²⁾ is incomplete,

This paper is dedicated to N. G. van Kampen.

¹ Institute for Theoretical Physics, 3508 TA Utrecht, The Netherlands.

and the presently popular ways to interpret its “logic” are not quite satisfactory.

The first is cosmological. When the *classical* trajectories of stars and galaxies are extrapolated backward in time, it is found that the earliest configurations were highly concentrated inside a tiny, nearly pointlike universe, strongly suggesting that it all started with a “big bang,” and that the initial state at $t = 0$ was simple, perhaps a fundamental singularity.

But if we regard the presently observed state of the universe as a “state in Hilbert space,” extrapolation backward according to the laws of quantum mechanics should give something entirely different. One would expect that the observables at this initial singularity cannot possibly commute with the present observables and therefore extrapolation backward in time should give some linear superposition of states with different cosmic ages, not just one single “age of the universe.” Yet this is what astrophysicists assume when they launch big bang scenarios.

If there is a “reality”⁽³⁾ beyond what is described by standard quantum mechanics, there should be a way to understand it. In this respect it is possible to add to van Kampen’s ten theorems on quantum mechanics⁽¹¹⁾ an 11th:

Quantum mechanics is not a theory about reality, it is a prescription for making the best possible predictions about the future if we have certain information about the past.

Physicists have learnt to live with the fact that these predictions are always statistical in nature. An obvious remark is that probably our information on the past was also incomplete. But whoever makes such statements is quickly put in a corner together with those other believers in “hidden variables”^(2,4) and is politely reminded of the Einstein–Podolsky–Rosen paradox⁽⁵⁾ and Bell’s theorems.⁽⁶⁾ Now, those theorems and *Gedanken* experiments show that one cannot attach labels to electrons to make their movements look deterministic. They do not prove that hidden variables inundating the entire vacuum cannot restore predictability in a formal way. Indeed, our work will show how such an idea can perhaps be made respectable.

The second reason why we might need an amendment to quantum mechanics is our inability to reconcile quantum mechanics with general relativity. In ordinary quantum field theory (which may be seen as a reconciliation between quantum mechanics and special relativity) there are infinities that can be made harmless by renormalization. But general relativity requires space-time curvature to be “quantized” and this time the infinities are much more fundamental. I am not referring to infinities that might occur when one attempts to renormalize the perturbation expansion,

because at least in principle superstring theories might have found the correct treatment for those. Much more enormous are the problems one encounters when one tries to “sum” such perturbation expansions. Because the gravitational constant (or, alternatively, the string constant) has non-vanishing dimensions, there are always phenomena for which the perturbation expansion is inapplicable. The small-distance structure in such theories is simply not understood.

Closely related to the problem of quantizing gravity is the mystery of the vanishing cosmological constant. In quantum gravity space-time can be flat only in the vacuum state. This turns the vacuum state into something very special, not just the outcome of a lengthy mathematical calculation required to find the solution of

$$H |\psi\rangle = E |\psi\rangle$$

with lowest E .

In a series of attempts to obtain more understanding in this field, I argued that the number of mutually orthogonal states in Hilbert space within a given volume (more precisely, inside a closed surface with given area) is finite⁽⁷⁾ and given by the total surrounding area. This suggests that the laws of physics at very tiny (Planckian) distance scales are *simpler* than in ordinary quantum field theories. Perhaps they are deterministic.

In this paper I will argue that a deterministic set of physical laws at tiny distance scales is not in contradiction with our present understanding of quantum mechanics.

The simplest model in which the laws of quantum mechanics agree with a deterministic “underlying” theory is the “spinning particle in a magnetic field.” This I explain in Section 2.

But the model of Section 2 is too small to exhibit one of the most essential features of quantum mechanics: the way it can be combined with thermodynamics and statistics so that the “uncertainty relation” can be seen in ordinary experiments. For this we need a system with “locality”: an experimental region can be separated from a laboratory with detectors, which can detect because they are in a metastable initial state. We need to have a Hamilton density $\mathcal{H}(x)$ which is bounded from below so that we can do thermodynamics. A model which is more interesting in this respect (the one-dimensional free massless fermion gas) is constructed in Section 3.

One might argue that also this model is too special, so I show in Section 4 how it can be generalized to the $(3+1)$ -dimensional case. Adding masses directly, however, seems to be (prohibitively?) difficult.

The most spectacular models that may combine quantum mechanics with deterministic mechanics are what I call the “deterministic reversible cellular automata.” They are defined in Section 5. The previous models

were simple, exactly soluble examples, but these are much more interesting. With a modern personal computer it was easy to verify that in most cases these automata evolve chaotically. There can be no other way to treat their long-distance behavior than by using statistics.

This is not an easy subject and my first attempt to understand whether and how these complicated automata mimic quantum mechanics was by using the Baker–Campbell–Hausdorff formula. This first attempt (explained in detail in Appendix A) was suggestive but not quite conclusive. I discuss a possible strategy further in Section 6.

The most interesting case would be when an effective quantum field theory emerges with a large fundamental distance scale. At large scales only renormalizable (and superrenormalizable) couplings survive, so one of the renormalizable theories should be reproduced. This possibility (and many other aspects of these results) remains to be explored.

In Appendix B I discuss why it is important to focus on models with discrete time steps.

I formulate conclusions in Section 7.

2. SPINNING PARTICLE IN A MAGNETIC FIELD

Consider an $N (=2l+1)$ -dimensional Hilbert space with Hamiltonian

$$H|m\rangle = \mu m|m\rangle, \quad m = -l, \dots, l \quad (2.1)$$

This is an ordinary quantum mechanical system known as an elementary exercise from many textbooks. In terms of the observables L_x , L_y , and L_z we surely have all aspects of quantum mechanics. The evolution operator is $U(t, t')$,

$$|m\rangle_t = U(t, t')|m\rangle_{t'} = e^{-i\mu m(t-t')}|m\rangle_{t'} \quad (2.2)$$

But now use as a basis the set

$$|g\rangle = \frac{1}{\sqrt{N}} \sum_m e^{-2\pi i m g/N} |m\rangle, \quad g = 0, \dots, N-1 \quad (2.3)$$

Suppose that we concentrate on special time intervals:

$$t - t' = 2\pi k/\mu N, \quad k \text{ integer} \quad (2.4)$$

From (2.2) we have

$$U(t-t')|g\rangle = \frac{1}{\sqrt{N}} \sum_m e^{-2\pi i m g/N - 2\pi i m k/N} |m\rangle = |g+k \pmod{N}\rangle \quad (2.5)$$

In other words, the state $|g\rangle$ evolves into the state $|g+k\rangle$ after k fundamental time intervals. If we limit ourselves to these time intervals and this basis of states, the wave function does not spread.

Conversely, we could consider a system that can be in N different states $|g\rangle$, $g=0, \dots, N-1$. At regular time intervals $2\pi/\mu N$ the system jumps from $|g\rangle$ into the next position, $|g+1\rangle$, and if it were in the state $|N-1\rangle$, it jumps back to $|0\rangle$. The evolution operator is (2.5). This system is obviously deterministic. Yet in some sense it is equivalent to our “quantum mechanically” spinning particle: no one could stop us from defining a new set of basis elements $|m\rangle$,

$$|m\rangle = \frac{1}{\sqrt{N}} \sum_g e^{2\pi i g m / N} |g\rangle, \quad m = -l, \dots, l \quad (2.6)$$

and operators L_x , L_y , and L_z . In terms of these our deterministic system may appear to be quantum mechanical. But in particular if the time intervals $2\pi/\mu N$ are extremely short, one may suspect that a macroscopic observer will not be able to distinguish the deterministic model from the quantum mechanical one.

This depends on which quantities/operators should be considered to be observables. Here in this model this is ambiguous and so the “interpretation” of the spinning electron as a deterministic system can be criticized. Now let us turn to the next model.

3. THE ONE-DIMENSIONAL FREE MASSLESS FERMION GAS

Consider the following deterministic system. We have a series of cells labeled by integers $x \in \mathbb{Z}$. The series is either infinite or periodic.² In each cell there is room for two “particles,” a left-goer (l) and a right-goer (r). So each cell can be in four states:

$$|l, r\rangle = |0, 0\rangle, \quad |1, 0\rangle, \quad |0, 1\rangle, \quad \text{or} \quad |1, 1\rangle \quad (3.1)$$

There is a clock showing time in discrete time steps which we take to be integers. After every tick of the clock every left-going particle moves from its cell to the cell at its left, and the right-goers move one cell to the right.

“Physically” this model is rather trivial and featureless. Left-goers move to the left eternally and right-goers move to the right, both with speed one. But now consider its “Hilbert space.” A basis of states is

² In the latter case, however, our analysis is not quite accurate at the boundary.

$\{\prod_x |l_x, r_x\rangle\}$, where at each x , l_x and r_x may each be either zero or one. Let the evolution operator for one unit of time be

$$U(t+1, t) \quad (3.2)$$

and the way in which it operates in our Hilbert space should be clear.

Because we have zeros and ones, it will be convenient to introduce anticommuting creation and annihilation operators. First, define

$$\begin{aligned} \sigma_l^-(x)|0, r_x\rangle &= 0 \\ \sigma_l^-(x)|1, r_x\rangle &= |0, r_x\rangle \\ \sigma_r^-(x)|l_x, 0\rangle &= 0 \\ \sigma_r^-(x)|l_x, 1\rangle &= |l_x, 0\rangle \end{aligned} \quad (3.3)$$

whereas the operation of the $\sigma_{l,r}^-$ operators does not depend on the contents of the other cells.

And then, applying a Jordan–Wigner transformation:

$$\Psi_l(x_1) = (-1)^{\sum_{x < x_1} l_x} \sigma_l^-(x_1) \quad (3.4)$$

$$\Psi_r(x_1) = (-1)^{\sum l + \sum_{x < x_1} r_x} \sigma_r^-(x_1) \quad (3.5)$$

so that

$$\begin{aligned} \{\Psi_i(x), \Psi_j(x')\} &= 0 \\ \{\Psi_i(x), \Psi_j^\dagger(x')\} &= \delta_{ij} \delta_{x,x'} \end{aligned} \quad (3.6)$$

It will be clear that

$$\begin{aligned} \Psi_l(x, t) &= \Psi_l(x+t, 0) \\ \Psi_r(x, t) &= \Psi_r(x-t, 0) \end{aligned} \quad (3.7)$$

because the ordering of the particles used in (3.4) and (3.5) is time independent.

Fourier transforming

$$\Psi_i(x, t) = \frac{1}{\sqrt{L}} \sum_{k \in \mathbb{Z}_L} \hat{\Psi}_i(k, t) e^{-2\pi i k x / L} \quad (3.8)$$

where L is temporarily taken to be a finite period, and the sign of k is according to convention in quantum field theory, we have

$$\hat{\Psi}(k, t) = e^{-(2\pi i k t / L) \sigma_3} \hat{\Psi}(k, 0) \quad (3.9)$$

with

$$\sigma_3 \Psi_r = \pm \Psi_r \quad (3.10)$$

Now

$$[\hat{\Psi}_i^\dagger(-k) \hat{\Psi}_i(k), \hat{\Psi}_j(k')] = -\hat{\Psi}_j(k) \delta_{ij} \delta_{kk'} \quad (3.11)$$

Therefore, (3.9) leads to the following expression for the evolution operator:

$$U(t+1, t) = \exp \left[\frac{2\pi i}{L} \sum_k k \hat{\Psi}^\dagger(-k) \sigma_3 \hat{\Psi}(k) \right] \quad (3.12)$$

Equations (3.11) and (3.12) imply (3.9), whereas the overall sign is checked by observing that indeed

$$U(t+1, t)|0\rangle = |0\rangle \quad (3.13)$$

Therefore, if we reexpress Eq. (3.12) in terms of our original basis of the states $\prod_x |l_x, r_x\rangle$, it just reproduces the various permutations without any minus signs.

The importance of (3.12) is that this evolution operator now is generated by a Hamiltonian operator,

$$H = -\frac{2\pi}{L} \sum_k k \hat{\Psi}^\dagger(-k) \sigma_3 \hat{\Psi}(k) \quad (3.14)$$

The integer k is only defined mod L and therefore this H , in contrast with the evolution operator U of Eq. (3.12), is not unique [it is easy to verify that adding L to k does not alter (3.12)].

The infinite-volume limit of (3.14) is

$$H = -\int_{a-\pi}^{a+\pi} k \hat{\Psi}^\dagger(-k) \sigma_3 \hat{\Psi}(k) dk \quad (3.15)$$

where now

$$\Psi(x) = \frac{1}{(2\pi)^{1/2}} \int_{a-\pi}^{a+\pi} dk e^{-ikx} \hat{\Psi}(k) \quad (3.16)$$

and a is an arbitrary boundary (which could even depend on k).

In the following I choose for convenience $a=0$, but it will be important to realize that the essential features of this system will be largely independent of a , as long as

$$|a| < \pi \quad (3.17)$$

The arbitrariness of the Hamiltonian is of course related to the fact that so far we have refused to tell what the system looks like at fractional time values. It will be important to note that our Hamiltonian is not exactly the sum of local terms, because in x space it is

$$H = \sum_{x,x'} G(x-x') \Psi^\dagger(x) \sigma_3 \Psi(x') \quad (3.18)$$

with

$$G(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} k dk e^{ikx} = \begin{cases} 0 & \text{if } x=0 \\ (-1)^{x+1}/ix & \text{if } x \neq 0 \end{cases} \quad (3.19)$$

But in the continuum limit it will become hard to distinguish it from

$$H \rightarrow \int dx \Psi^\dagger(x) \left(i\sigma_3 \frac{\partial}{\partial x} \Psi(x) \right) \quad (3.20)$$

The essential point in this model now is that H is extensive: it grows with the volume of the system. In principle one could always redefine H such that its eigenvalues are all between 0 and 2π , because the original system was only well determined at integer times. We should *not* make such a redefinition though, because we wish to keep H extensive. Two portions of our model that are far apart should not be able to communicate; their Hamiltonians add up and commute mutually. This would no longer be the case if we restricted H to lie between 0 and 2π .

That our model corresponds to a free, massless fermion gas should by now be obvious. The ground state of H is what we get if all left-levels with positive k and all right-levels with negative k are occupied and the others are empty. Thus, we have a finite Dirac sea (it is finite because our cells were chosen to have a finite size, so that there is a cutoff in momentum space). Physical particles are the excitations above this lowest energy state. A single-particle state has

$$H = |k| \quad (3.21)$$

It is a left-goer or *anti-right-goer* when $k < 0$ and an *anti-left-goer* or right-goer if $k > 0$.

Note that such a particle is truly "quantum mechanical": If we try to localize it at $t=0$ by squeezing the wave function to a narrow region in our one-dimensional space, the wave function will quickly spread, because it is always a superposition of positive and negative k values.

Of course, our “vacuum” is actually a very complicated linear superposition of all possible states. All these evolve deterministically. This is why one could say that the vacuum contains “hidden variables.”

What we really need this vacuum, and the other excited states, for is to do thermodynamics. Then we can assume that at some point our system is in thermal equilibrium, which is described by a density matrix

$$\rho = e^{-\beta H} \quad (3.22)$$

It is here that we really need an extensive Hamiltonian, bounded from below by a single vacuum state and unbounded from above (in the infinite-volume limit). With (3.22) one could handle our system statistically. The problem is: the model of this section is exactly soluble and statistical treatment is rather pointless. What we need is a nontrivial model. Interacting systems will be considered in Section 5. First, let us consider a generalization of the above model to more space dimensions.

4. MASSLESS FERMIONS IN MORE DIMENSIONS

What we discovered in the previous section is that the theory of massless fermions in 1 + 1 dimensions, with a cutoff in momentum space, allows the introduction of *ever-commuting observables*. In anticipation of their possible significance to the real (quantum) world, I will from now on refer to these as “primordial” observables. They propagate in a deterministic fashion. In the model the primordial observables were the Dirac fermion occupation numbers (counting left- and right-goers separately) in all cells x . The basis generated by these primordial observables will be a set of states that I call “primordial” states. In this basis the wave function does not spread.

The primordial observables in the model of Section 3 could be described in terms of the Dirac fermions, before they were allowed to fill the Dirac sea. A single Dirac fermion was deterministic because it either moves to the left or to the right with constant speed. Let us now try to find primordial observables for a single massive Dirac fermion in 3 + 1 dimensions.

Its wave function is $\psi(\mathbf{x})$ and the Hamiltonian H satisfies

$$H\psi(\mathbf{x}) = (\gamma_4 m + \alpha_i p_i) \psi(\mathbf{x}) \quad (4.1)$$

where γ_4 and α_i are anticommuting Dirac matrices. Further,

$$p_i = -i \partial/\partial x_i \quad (4.2)$$

The operators x_i , p_i , γ_4 , and α_i satisfy the equations of motion

$$\frac{d}{dt} x_i = -i[x_i, H] = \alpha_i \quad (4.3)$$

$$\frac{d}{dt} p_i = -i[p_i, H] = 0 \quad (4.4)$$

$$\frac{d}{dt} \gamma_4 = -i[\gamma_4, H] = -2i\gamma_4 \alpha_i p_i \quad (4.5)$$

$$\frac{d}{dt} \alpha_i = -i[\alpha_i, H] = 2i\gamma_4 \alpha_i m + i[\alpha_j \alpha_i] p_j \quad (4.6)$$

In the general case I was unable to select out of these noncommuting operators a complete set of primordial, commuting observables. But if $m=0$, things simplify. From now on, $m=0$.

Of course the momentum p_i is conserved [Eq. (4.4)]. Let \hat{e} be the direction of the momentum:

$$p_i = \hat{e}_i p \quad (4.7)$$

Let us choose coordinates such that \hat{e} is in the 3-direction. Then from (4.6) we find that α_3 is conserved. Its eigenvalues are ± 1 . Therefore, x_3 is also a primordial observable:

$$x_3(t) = x_3(0) + \alpha_3 t \quad (4.8)$$

Finally, γ_5 commutes with H if $m=0$. All together we now have the conserved quantities \hat{e}_i (two independent continuous degrees of freedom), $(\hat{e} \cdot \alpha)$ (one \mathbb{Z}_2 degree of freedom), and γ_5 (one \mathbb{Z}_2 degree of freedom), and the ever-commuting operator $(\mathbf{x} \cdot \hat{e})$ (one continuous degree of freedom). Together they span the complete one-particle Hilbert space, and in turn the one-particle Hilbert spaces can be multiplied to give a primordial basis in the "second-quantized" field theory.

It is interesting to see how these deterministic variables behave in space-time. For every Dirac particle we apparently only have the *direction* \hat{e} of its movement and one coordinate $(\mathbf{x} \cdot \hat{e})$ parallel to this direction. In other words: the Dirac fermion is a flat sheet, moving with the speed of light in one direction. The (fixed) variable $(\hat{e} \cdot \alpha) = \pm 1$ tells for every sheet in which of the two possible directions it goes. γ_5 is a dummy variable. Being like neutrinos, the massless Dirac fermion does not have to have both chiralities.

Some sort of cutoff in momentum space would be desirable to understand the procedure of filling up the Dirac sea. In some sense this

might correspond to dividing space into cells, just like we did in one dimension, but this is now somewhat more difficult. A consequence of dividing space into cells would be that time steps will also be discrete. I elaborate on this in Appendix B.

Adding mass is not possible within the above scheme. I suspect that a cellular automaton as described in the next section might be possible such that massive fermions are mimicked. Note that in general, mass terms will flip the direction of the movement of a sheet.

5. THE DETERMINISTIC, LOCAL, REVERSIBLE CELLULAR AUTOMATON

I generalize the models of the previous section in the following way. An infinite array of cells is arranged in a regular pattern. Each cell contains a discrete, finite variable or set of variables. Label all possible states a single cell \mathbf{x} can be in by an integer $f(\mathbf{x})$, with $0 \leq f(\mathbf{x}) < N$. There is a clock that ticks, and at every tick the system jumps from a state $f_t(\mathbf{x})$ into a state $f_{t+1}(\mathbf{x})$ according to some deterministic prescription. This makes it a deterministic cellular automaton.

The automaton is *local* if at each \mathbf{x} the new configuration $f_{t+1}(\mathbf{x})$ depends only on the values $f_t(\mathbf{x}')$ at the points \mathbf{x}' which are the immediate neighbors of \mathbf{x} or \mathbf{x} itself. The automaton is *reversible* if the mapping $f_t(\mathbf{x}) \rightarrow f_{t+1}(\mathbf{x})$ has a unique inverse, so that at any time t we can put the engine into reverse and recover the earlier configurations. If the number of cells \mathbf{x} is V , the Hilbert space spanned by the states $\{f(\mathbf{x})\}$ is N^V dimensional, and if the automaton is reversible, the evolution operator $U(t+1, t)$ in this Hilbert space is unitary.

From now on, when I use the word "automaton," I mean a deterministic cellular automaton that is reversible and local.³ Such an automaton is easy to construct. A typical example is the following construction. At every link connecting neighboring cells \mathbf{x} and \mathbf{x}' the states $(f(\mathbf{x}), f(\mathbf{x}'))$ can be in N^2 possible configurations. An evolution operator $U_{\mathbf{x}, \mathbf{x}'}$ is chosen to be an element of the permutation group $P(N^2)$. I choose to order the links $(\mathbf{x}, \mathbf{x}')$ in a certain way. The operation

$$U(t+1, t) \stackrel{\text{def}}{=} \prod_{(\mathbf{x}, \mathbf{x}')} U_{\mathbf{x}, \mathbf{x}'} \quad (5.1)$$

then defines an automaton of the kind we need.

Automata are ideal targets for personal computers and with some simple programs I tested many examples. It is important to restrict

³ One could use the acronym "CARL," but I prefer to avoid acronyms.

consideration to reversible ones. In the majority of cases I found that even the simplest initial states rapidly evolve chaotically.⁴ This suggests that if any of these correspond to a quantum mechanical system in the way the model of the previous section does, then this should be extremely complicated, comparable to an interacting quantum field theory.

How do we construct the corresponding Hamiltonian? A formal solution is easy to construct. The evolution operator (5.1) is a special element of the permutation group $P(N^V)$. Any element of $P(N^V)$ can be written as a product of cyclic elements,

$$U(t+1, t) = \prod_i P_c(N_{(i)}); \quad \sum_i N_{(i)} \leq N^V \quad (5.2)$$

We have

$$P_c^{N_{(i)}} = 1 \quad (5.3)$$

One derives that the evolution operator (5.2) has N^V (possibly degenerate) eigenvalues

$$\begin{aligned} e^{-2\pi i k / N_{(1)}} \quad (0 \leq k < N_{(1)}) \\ e^{-2\pi i k / N_{(2)}} \quad (0 \leq k < N_{(2)}); \quad \text{etc.} \end{aligned} \quad (5.4)$$

By formally diagonalizing $U(t+1, t)$, one finds an H_0 with

$$U(t+1, t) = e^{-iH_0} \quad (5.5)$$

where H_0 has eigenvalues E_0 at

$$2\pi k / N_{(1)}; \quad 2\pi k / N_{(2)}; \quad \text{etc.} \quad (5.6)$$

all satisfying

$$0 \leq E_0 < 2\pi \quad (5.7)$$

This is, however, *not* a suitable Hamiltonian. In terms of this our system does not even remotely resemble a conventional quantum mechanical system. Because of our freedom to add or subtract multiples of 2π to or from E , we have no way to distinguish these energy levels from each other, and to declare that one of these is the "vacuum" would be totally senseless.

⁴ In many cases "chaos" only sets in at time scales longer than the size of the system, so that disturbances had the opportunity to bounce several times against the boundary, or run around periodic ones. In many other models, however, extremely simple initial states start to evolve chaotically immediately, independent of faraway boundaries.

The point is that we need another Hamiltonian H , with

$$U(t+1, t) = e^{-iH} \quad (5.8)$$

in such a way that H is extensive, and can be written as

$$H = \sum_{\mathbf{x}} \mathcal{H}(\mathbf{x}) \quad (5.9)$$

where $\mathcal{H}(\mathbf{x})$ is (more or less) local. Certainly when \mathbf{x}_1 and \mathbf{x}_2 are far apart we must be able to see that this system is local:

$$[\mathcal{H}(\mathbf{x}_1), \mathcal{H}(\mathbf{x}_2)] \rightarrow 0 \quad (5.10)$$

How does one construct a Hamiltonian satisfying (5.9) and (5.10) [and therefore certainly *not* (5.7)]? Note that if $\mathcal{H}(\mathbf{x})$ acts in a finite-dimensional subspace of Hilbert space, this Hamiltonian will have a unique ground state (and “upper state,” which is of less interest). In the “continuum limit” the system should resemble a respectable quantum field theory. But does $\mathcal{H}(\mathbf{x})$ exist?

6. CONSTRUCTING THE HAMILTONIAN

Given a cellular automaton with a unitary evolution operator $U(t+1, t)$ that is “local,”

$$U = \prod_{\mathbf{x}} U_{\mathbf{x}} \quad (6.1)$$

$$[U_{\mathbf{x}}, U_{\mathbf{x}'}] = 0 \quad \text{if } |\mathbf{x} - \mathbf{x}'| > d \quad (6.2)$$

for some $d > 0$; can one write down a Hamiltonian H such that the following are satisfied?—

$$U = e^{-iH} \quad (6.3)$$

$$H = \sum_{\mathbf{x}} \mathcal{H}(\mathbf{x}) \quad (6.4)$$

$$[\mathcal{H}(\mathbf{x}), \mathcal{H}(\mathbf{x}')] = 0 \quad \text{if } |\mathbf{x} - \mathbf{x}'| > d' \quad (6.5)$$

Equations (6.1) and (6.2) represent a generalization of (4.1). Most automata that can be constructed must be of this form. They guarantee locality, and a maximum speed d with which information can be transmitted. Intuitively, we would assume a Hamiltonian obeying (6.3)–(6.5) to exist. But what is d' ?

Closer inspection shows that a finite d' is probably impossible, and that (6.5) must be replaced by a less stringent condition, for instance,

$$|[\mathcal{H}(\mathbf{x}), \mathcal{H}(\mathbf{x}')]| < f(|\mathbf{x} - \mathbf{x}'|) \quad (6.6)$$

with

$$\lim_{x \rightarrow \infty} f(x) = 0 \quad (6.7)$$

One possible construction goes as follows. Write

$$U_x = \exp[-iA(\mathbf{x})] \quad (6.8)$$

Now let us divide the operators U_x into "commuting classes." If V is the set of points or links x at which the U_x are defined, then

$$V = V_1 \cup V_2 \cup \dots \quad (6.9)$$

with, if possible, only a finite number of nonoverlapping subsets V_i , such that if \mathbf{x}_1 and \mathbf{x}_2 are in the same subset V_a , then

$$[U_{\mathbf{x}_1}, U_{\mathbf{x}_2}] = 0 \quad (\mathbf{x}_1 \in V_a, \mathbf{x}_2 \in V_a) \quad (6.10)$$

For example, in a one-dimensional chain, V_1 could be the set of even points and V_2 the set of odd points.

We can then write (if necessary after some further transformations)

$$U = U_1 \cdot U_2 \dots \quad (6.11)$$

with

$$U_a = \exp \left[-i \sum_{x \in V_a} A(\mathbf{x}) \right] \equiv \exp(-iA_a) \quad (6.12)$$

Now we can use the Baker–Campbell–Hausdorff expansion

$$\begin{aligned} e^A e^B = \exp \{ & A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] + \frac{1}{12}[[A, B], B] \\ & + \frac{1}{24}[[A, [A, B]], B] \pm \dots \} \end{aligned} \quad (6.13)$$

a series containing only commutators. In the simplest case, Eq. (6.11) only contains two terms, so that (6.13) must be used only once; otherwise, we just repeat it several times.

Each term in (6.13) is now of the desired form (6.4), (6.5), as one can easily see. But each commutator connects points \mathbf{x} and \mathbf{x}' that are a

distance d apart, and it follows that terms of order n in A_a, A_b , will yield contributions to $\mathcal{H}(\mathbf{x})$ that obey (6.5), but with

$$d' = nd \quad (6.14)$$

Therefore, (6.6) and (6.7) correspond to requiring a sufficient degree of convergence of the Baker–Campbell–Hausdorff series. One can prove that if

$$e^A e^B = e^F \quad (6.15)$$

then the series for F converges uniformly only if the eigenvalues of F lie within an interval smaller than 2π (see Appendix A). What this really means is that each term in (6.13), when commuted with one of the others, should have eigenvalues not further than 2π apart. This, unfortunately, is not good enough for us. By construction, F will be extensive, and its eigenvalues should grow proportionally with the volume.

Note that there is some arbitrariness in this construction because one may add or subtract multiples of 2π to the eigenvalues of each of the operators $A_a(\mathbf{x})$. This freedom corresponds to the freedom to choose the relative phases of the primordial states when combined to give the eigenstates of H .

Now the first few coefficients of the BCH series seem to converge rather rapidly and one might hope that these, possibly improved by some resummation procedure, will already give quite good approximate expressions for an extensive Hamiltonian. But since its eigenvalues will be further apart than 2π , we expect no absolute convergence, so we searched for a better way to relate quantum field theories with cellular automata.

We found a Hamiltonian with constraint that can reproduce the automaton described by (5.1) directly if x space is one-dimensional and the pairs (x, x') are nearest neighbors only. Take the one-dimensional massless fermion gas of Section 3, but now allow the right- and left-goers each to come in N varieties. Left-goers are constrained in the initial state to stay further apart than some limiting distance d , and so are the right-goers. We now impose that whenever a left-goer at x' meets a right-goer at x , with $|x' - x| < d' \ll d$, then both transform according to the permutation $U_{x,x'}$, while at the same time they continue their paths.

The distances between all pairs of left-goers will stay constant, and so the constraint that they stay further apart than d will be obeyed at all times, and *idem ditto* for the right-goers.

A Hamiltonian that reproduces this law of evolution can be written as

$$H = H_0 + H_1 \quad (6.16)$$

with [as in Eq. (3.20)]

$$H_0 = \int dx \sum_i \Psi_i^\dagger(x) i\sigma_3 \frac{\partial}{\partial x} \Psi_i(x) \quad (6.17)$$

$$H_1 = \int dx dx' \sum_{ijkl} \Psi_i^\dagger(x) P_- \Psi_k(x) W_{ijkl} f(x-x') \Psi_j^\dagger(x') P_+ \Psi_l(x') \quad (6.18)$$

with

$$f(x-x') = 0 \quad \text{if } |x-x'| > d' \quad (6.19)$$

and W to be specified later. P_\pm are projection operators projecting out left-goers and right-goers, respectively.

Remember that we have not (yet) filled the Dirac sea, so Ψ^\dagger always creates a particle and Ψ annihilates. This, with the constraint, allows us to solve the Schrödinger equation exactly. Consider a right-goer approaching a left-goer. They are in a state

$$\psi(i, x, j, x') = \phi(i, j, t) A(x-t) B(x'+t) \quad (6.20)$$

where i, x refer to the right-goer and x', j to the left-goer. Lower-case ψ is a wave function, not an operator field. For the functions A and B we will later substitute Dirac delta functions.

The Schrödinger equation,

$$\partial\psi/\partial t = -iH\psi$$

implies

$$\left[\frac{\partial}{\partial t} \phi(i, j, t) \right] AB = \sum_{kl} W_{ijkl} f(x-x') \phi(k, l, t) AB \quad (6.21)$$

Now choosing

$$A = \delta(x-t); \quad B = \delta(x+t) \quad (6.22)$$

we get

$$\frac{\partial}{\partial t} \phi(i, j, t) = \sum_{kl} W_{ijkl} f(2t) \phi(k, l, t) \quad (6.23)$$

After the small interval during which the particles cross ($f \neq 0$) the state $\phi(ij)$ transforms into $U\phi(ij)$, where the $N^2 \times N^2$ transformation matrix U is determined by

$$U = \exp \left[W \int_{-\infty}^{\infty} f(2t) dt \right] \quad (6.24)$$

which we take to be our deterministic U .

Thus, if (6.24) is satisfied, *and* the constraint mentioned earlier, then (6.16) is the Hamiltonian for our automaton. Now, if we want to consider it as a quantum mechanical Hamiltonian, we need to know its ground state. This only exists if we discretize x space (as in Section 3), using meshes with length d'' ($0 \ll d'' \ll d' < d$). Our discretized Hamiltonian will reproduce the cellular automaton approximately but not exactly, because contrary to (3.20), Eq. (3.18) is nonlocal.

7. CONCLUSIONS

We have constructed various models illustrating an aspect of quantum mechanics that seems to have received little attention: the possibility to have a set of ever-commuting observables that algebraically generate the entire Hilbert space. The construction in Section 6 shows that this possibility may even persist in quantum field theories with interactions such as the four-fermion interaction. The possible existence of such observables is of little relevance for interpreting the laws of quantum mechanics at the level of atoms, molecules, or even elementary particles. The “paradoxical” properties of electrons and hydrogen atoms remain, but may become a little more acceptable.⁽³⁾ We know that *macroscopic* observables such as the position of a pointer on a scale, the state of a particle counter, etc., all commute, a statement that does not contradict the standard rules because these observables are extremely incomplete. We now conjecture that they also commute with the primordial variables.

The only distinction, then, between a quantum theory and a deterministic “primordial” theory is that in the quantum system we decided to consider nonprimordial observables, i.e., observables that mix different primordial states. The fundamental theory that I propose in this paper is that, for describing the real world, a complete set of such primordial observables can be found, in terms of which we can formulate the fundamental laws of physics, and that the nonprimordial observables are not essential. They are needed *only* to enable physicists to make statistically significant predictions of the future at large distance scales, where the microscopic primordial observables are by far too complicated and change much too rapidly (chaotically?) to be directly observed. It is quite conceivable that these microscopic primordial observables are only relevant at the Planck scale (of course, our description of the “spinning particle” should be seen as a model, not as a theory for the primordial variables describing real electrons in some magnetic field).

This theory implies a statement about “reality.” It is tempting to suggest that this will be the only acceptable answer to the cosmology

problem mentioned in the introduction: the observables describing the very first picoseconds of the universe were primordial observables. They commute with the present macroscopic observables, and hence are uniquely measurable by careful observations today, in principle.

But many conceptual problems are still mysterious. One conceptual difficulty in our theory that we will have to learn to understand is that a density matrix $e^{-\beta H}$ describes "chaos" at all values of β , including 0 and ∞ . It then becomes a mystery how β can be determined from a given solution of the cellular automaton. I leave many such questions open, but I am convinced that they will not invalidate the theory.

One might wonder, as I did, how phase factors and interference phenomena can be explained in such a theory. I now suspect that indeed phase factors are arbitrary, but as soon as one introduces an extensive Hamiltonian to describe the evolution in a way that we are used to, one of the eigenstates of the evolution operator will play the role of the "vacuum." If we made no assumption about the existence of any Hamiltonian at all and did not know which is its lowest eigenstate, then we would not know if our "experiments" are surrounded by a "vacuum," and we would have no way to talk about "interference."

It should be possible to verify the statement that the present "standard model" describing all known interactions among elementary particles, including gravity, can ultimately be written in terms of primordial observables only. To think that a $(3+1)$ -dimensional world can be described in terms of primordial observables only is not crazy, as I did demonstrate.

Quantum gravity remains as difficult as ever. Since energy is now a rather ambiguous concept in the present theory, it is even harder to understand how it can act as a source of space-time curvature. But I claim that it is the entire Hamiltonian one should look at, which is the one that includes the gravitational forces. It describes the quantum evolution of space-time and matter together, and we know that the Einstein-Hilbert action is one of the very few possibilities left by demanding general relativistic invariance. So I suggest that one should try to construct just any deterministic cellular automaton that allows space-time to be not flat. Lattices such as the ones discussed in ref. 8 could work, but it seems to be extremely difficult to design any law of evolution at all that avoids the paradoxes that arise from gravitational collapse.

It may be remarked that primordial variables are particularly easy to find in one space and one time dimension (the massless bosonic case can be handled in a way similar to the fermionic case). So I suggest that the presently popular superstring theories might lead the way to primordial variables for the real world.

Finally, the present observations may possibly lead to applications in

more conventional particle physics: perhaps a cellular automaton can be found that has QCD as its thermodynamic limit, so that it can be used as a *three-dimensional* computer model for numerical simulations.

APPENDIX A. CONVERGENCE OF THE BAKER-CAMPBELL-HAUSDORFF SERIES

Consider two operators A and B , which in general will be assumed to act in an infinite-dimensional Hilbert space, but we are especially interested in the case that they can be written as

$$A = \sum_x A(\mathbf{x}); \quad B = \sum_x B(\mathbf{x}) \quad (\text{A.1})$$

where $A(\mathbf{x})$ and $B(\mathbf{x})$ act only in a finite-dimensional subspace and are bounded from below and above. We are interested in an operator $F(\lambda)$ satisfying

$$e^{F(\lambda)} = e^A e^{\lambda B} \quad (\text{A.2})$$

where λ is a complex variable.

$F(\lambda)$ is not uniquely determined by (A.2), because changing one of its eigenvalues by a multiple of $2\pi i$ leaves (A.2) unaltered. But we can in addition to (A.2) require

$$F(0) = A \quad (\text{A.3})$$

and choose a path in λ space that avoids possible singularities of F . The question is whether such a path exists that connects $\lambda=0$ with $\lambda=1$ and whether $F(1)$ is indeed determined by the Baker-Campbell-Hausdorff series.

We have

$$\frac{d}{d\lambda} e^{F(\lambda)} = \int_0^1 dx e^{(1-x)F} \frac{dF}{d\lambda} e^{xF} = e^F B \quad (\text{A.4})$$

and

$$\begin{aligned} e^{-xF} G e^{xF} &= G + x[G, F] + \frac{x^2}{2!} [[G, F], F] \\ &+ \frac{x^3}{3!} [[[G, F], F], F] + \dots \end{aligned} \quad (\text{A.5})$$

to be found by repeated differentiation in x .

Let us introduce the short-hand notation

$$"[G, F^n]" \equiv [[\dots [G, F], F], \dots], F] \quad (\text{A.6})$$

and rewrite (A.5) as

$$e^{-xF} G e^{xF} = "[G, e^{xF}]" \quad (\text{A.7})$$

where the function inside the "[.]" symbols is to be expanded in a power series.

We then have

$$\left[\frac{dF}{d\lambda}, \int_0^1 dx e^{xF} \right] = \left[\frac{dF}{d\lambda}, \frac{e^F - 1}{F} \right] = B \quad (\text{A.8})$$

so that

$$\frac{dF}{d\lambda} = \left[B, \frac{F}{e^F - 1} \right] \quad (\text{A.9})$$

Now,

$$\frac{F}{e^F - 1} = 1 - \frac{1}{2}F + \frac{B_2}{2!}F^2 + \frac{B_4}{4!}F^4 + \dots \quad (\text{A.10})$$

where $B_2 = 1/6$, $B_4 = -1/30, \dots$, are the Bernoulli numbers. So, one finds

$$\begin{aligned} \frac{dF}{d\lambda} = & B - \frac{1}{2} [B, F] + \frac{B_2}{2!} [[B, F], F] \\ & + \frac{B_4}{4!} [[[[B, F], F], F], F] + \dots \end{aligned} \quad (\text{A.11})$$

from which the Baker–Campbell–Hausdorff series (6.13) can now easily be constructed.

Equation (A.11) can also be used to study convergence of the series. As long as (A.11) converges, the function $F(\lambda)$ will be a well-defined analytic function of λ . Suppose we have a basis in which $F(\lambda)$, for certain λ , is diagonal:

$$F |f\rangle = f |f\rangle \quad (\text{A.12})$$

Then (A.11) reads

$$\langle f_1 | \frac{dF}{d\lambda} | f_2 \rangle = \frac{\Delta f}{e^{\Delta f} - 1} \langle f_1 | B | f_2 \rangle; \quad \Delta f = f_2 - f_1 \quad (\text{A.13})$$

The expansion in Δf converges if

$$|\Delta f| = |f_2 - f_1| < 2\pi \quad (\text{A.14})$$

This certainly holds if all eigenvalues of F are within an interval of length 2π , but this is precisely what we did not want: F was supposed to become the Hamiltonian, an extensive operator, whose eigenvalues may at best be within bounds that grow proportionally with the volume.

Since (A.14) is probably a necessary condition for the Baker–Campbell–Hausdorff series to converge, we must impose that in the f basis the only nonvanishing matrix elements of B must be ones satisfying (A.14) as a selection rule. I do not know whether it is possible to obey this rule exactly or only approximately. It should hold on a curve in λ space from 0 to 1. Note that we do not have to insist that $F(\lambda)$ be a continuous function of λ . Its eigenvalues could flip by multiples of 2π , so that (A.14) can be recovered if the f values in large matrix elements of B would tend to float apart.

The condition can also be written as

$$|\langle f_1 | [F, B] | f_2 \rangle| < 2\pi |\langle f_1 | B | f_2 \rangle| \quad (\text{A.15})$$

APPENDIX B. CONTINUOUS VERSUS DISCRETE TIME STEPS

Suppose we have a deterministic set of equations determining the evolution of a physical system as a function of time. Let us first take time to be continuous, and assume the equations to be first-order differential equations. Let the parameters be described by some finite or infinite set of numbers q_i , with

$$dq_i/dt = f_i\{q\} \quad (\text{B.1})$$

We can always decide to define a Hilbert space spanned by the states $\{|q_1, q_2, \dots\rangle\}$, and define the associated momenta

$$p_i = -i \partial/\partial q_i \quad (\text{B.2})$$

The quantum mechanical “Hamiltonian” generating (B.1) is then

$$H = \sum_i f_i\{q\} p_i \quad (\text{B.3})$$

Thus, every deterministic system is equivalent to a quantum system with Hamiltonian (B.3). The snag is, the Hamiltonian (B.3) is not the usual energy and it certainly is not bounded from below, whatever the functions

f_i are. So, *no* deterministic system with continuous time corresponds to a physically acceptable quantum world. Now the model of Section 4 may seem to be an exception, but it is not, because we had to fill up a Dirac sea to find the "bottom" of the Hamiltonian. This procedure is only finite if we introduce some cutoff in momentum space, which in turn will be equivalent to introducing some minimal length of time.

If time steps are discrete, we must replace (B.1) by

$$q_i(t+1) = f_i\{q(t)\} \quad (\text{B.4})$$

which now allows a finite-dimensional Hilbert space of states $|q\rangle$. In terms of these we can write the "quantum mechanical" evolution operator

$$U(t, t+1)|q\rangle = |f(q)\rangle \quad (\text{B.5})$$

and it is certainly possible to write U as

$$U = e^{-iH} \quad (\text{B.6})$$

where H is bounded from below. In principle one could choose all energy eigenvalues to be between 0 and 2π , but the requirement that H be extensive in general leads to eigenvalues that are much further apart.

NOTE ADDED IN PROOF

The role of cellular automata in the fundamental laws of physics has been speculated on before. I thank E. Fredkin for further discussions and suggesting further references.⁽⁹⁾

REFERENCES

1. N. G. van Kampen, Ten theorems about quantummechanical measurements, Utrecht preprint THU-88-3.
2. M. Jammer, *The Conceptual Development of Quantum Mechanics* (McGraw-Hill, 1966).
3. J. S. Bell, Talk given at the Schwinger Symposium, UCLA, March 12, 1988.
4. J. M. Jauch, *Foundations of Quantum Mechanics* (Addison-Wesley, 1968).
5. A. Einstein, B. Podolsky, and N. Rosen, *Phys. Rev.* **47**:777 (1935).
6. J. S. Bell, *Physics* **1**:195 (1964).
7. G. 't Hooft, On the quantization of space and time, in *Proceedings of the Moscow Seminar on Quantum Gravity* (Academy of Sciences of the USSR, 1987), Utrecht preprint 1987.
8. G. 't Hooft, in *Recent Developments in Gravitation*, M. Lévy and S. Deser, eds. (Plenum, New York); C. J. L. Mannion and J. G. Taylor, *Phys. Lett.* **100B**:261 (1981); T. D. Lee, Physics in terms of difference equations, Talk given at the Niels Bohr Centenary Symposium, Copenhagen, October 1985; L. Bombelli *et al.*, Spacetime as a causal set, Syracuse, preprint, March 1987; P. Menotti and A. Pelissetto, *Phys. Rev. D* **35**:1194 (1987).
9. E. Fredkin and T. Toffoli, *Int. J. Theor. Phys.* **21**:219 (1982); T. Toffoli, *Int. J. Theor. Phys.* **21**:165 (1982); R. P. Feynman, *Int. J. Theor. Phys.* **21**:467 (1982).