Math. Struct. in Comp. Science (2007), *vol.* 17, *pp.* 177–183.
doi:10.1017/S0960129507005956 Printed in the United Kingdom

Discrete–continuous and classical–quantum

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Received 21 November 2006

We present a discussion concerning the opposition between discreteness and the continuum in quantum mechanics. In particular, it is shown that this duality was not restricted to the early days of the theory, but remains current, and features different aspects of discretisation. In particular, the discreteness of quantum mechanics is key for quantum information and quantum computation. We propose a conclusion involving a concept of completeness linking discreteness and the continuum.

1. Discrete–continuous in the old quantum theory

Discreteness is obviously a fundamental aspect of quantum mechanics. When you shine white light, which is a continuous spectrum of colours, into a monatomic gas, you get back precise line spectra, and only quantum mechanics can explain this phenomenon. In fact, the birth of quantum physics involved discretisation rather more than discreteness: in Max Planck's famous paper of 1900, and even more explicitly in the 1905 paper by Einstein on the photo-electric effect, what they really do is just what a computer does, in that an integral is replaced by a discrete sum, with the discretisation length given by Planck's constant.

During the 1910's, Niels Bohr then applied this idea to the atomic model, which represents another form of discretisation. It is now astonishing to observe how long it took for the *atomic hypothesis* to be accepted (Perrin 1905). Nevertheless, Bohr proposed a quantum atomic model: the atom is a classical one, that is, a nucleus with electrons 'orbitting' it, but, instead of considering the continuous family of possible trajectories, Bohr proposed to select only those for which the action (the enclosed area inside the planar trajectory) was a multiple of Planck's constant. The differences between the corresponding energies divided by Planck's constant then give precisely the frequencies of the spectral lines of the hydrogen atom that were observed experimentally.

Extending this 'algorithm' to a more general (non-integrable) situation gave rise, through the work of Born, Heisenberg and Schródinger, to the birth of quantum mechanics (Paul 2006), which was a much more conceptual and fundamental theory, and from which the old Bohr theory can be deduced in the limit where Planck's constant $\hbar \to 0$. However, the old 'phenomenological' theory remains accurate even nowadays for systems for which quantum mechanics has difficulty in predicting numbers. In chemistry or atomic physics, for example, the large number of degrees of freedom often makes quantum mechanics difficult to use explicitly: solving Schrödinger equation is hard, and its semi-cassical approximation (see below) is difficult to handle when the system is not integrable. Roughly speaking, we can say that there is a strong temptation to apply Bohr's old rule, that is, to make any quantity that looks 'like' an action discrete (and a multiple of an effective small Planck's constant), and although there is no real justification for this approach, the results can sometimes be very good.

In fact, the old quantum rules are a little bit like a visa† permitting entry to the quantum world, but on condition that one stays close to the classical border. But this visa is not just a computational aid, it is often the only way to get effective computations, and is even now a great source of inspiration for those who want to understand the semi-classical limit of non-integrable systems.

It is worth noting that quantum theory appeared as a *discretisation* of the classical situation in two ways during this (pre-quantum mechanics) period: the atomic hypothesis as a discretisation of continuous matter, and the Bohr theory as a discretisation of continuous classical mechanics.

We conclude this introduction by mentioning that discreteness is one of the two key ingredients in quantum computation (the other being the superposition principle). The fact that a single particle (qubit) can support binary information is typically quantum. Moreover, modern experiments in atomic physics reveal more and more that quantum discreteness can be observed in real situations. Indeed, it was long considered that the smallness of the Planck constant and the large number of particles involved in experiments meant that discreteness would rarely be observed in nature (a little bit like the way statistical – discrete – phenomena are usually handled well if they are treated as continuous). However, modern physics can now provide real situations where there are very few atoms and quantum discreteness can be observed. This should inspire different ways of thinking about the discrete/continuous opposition, at least in its relationship to the natural sciences.

2. Discrete–continuous and the Heisenberg–Schödinger pictures

Quantum mechanics may be said to have had two births (the earlier developments are referred to as quantum theory) – the first being due to Heisenberg; the second, only a few months later, being due to Schrödinger – and these separate developments, from our point of view, echo the discrete–continuous opposition. Heisenberg's matrix theory represented a radical change of paradigm (although it is also founded on a discretisation of perturbation theory (Paul 2006)), with all the classical quantities becoming matrices, that is, discrete. The Schrödinger vision seems more 'classical', as the Schrödinger equation is a partial differential equation, which certainly also explains the success of this theory. It also reflects the contrast between the young Heisenberg and the already well-established Schrödinger. An analysis of how these two points of view penetrated the scientific community during the twentieth century would certainly form a very interesting historical study.

† We have borrowed this image form a talk by J. M. Levy-Leblond.

The way in which Heisenberg's picture can be included in the Schrödinger one is interesting in itself, as it shows a situation where the *continuum* generates the *discrete*†. To understand this, we may consider the analogy between quantum mechanics and a drum. A drum is a vibrating membrane: the vibrations are encoded in a partial differential equation (wave equation). A partial differential equation is a way of going from the local to the global: knowing the position of the membrane within a very tiny piece of the surface determines the position everywhere thanks to the propagation driven by the PDE. But in addition to the PDE, the motion of the drum is constrained by the boundary, on which the vibration must cancel. If one gives an initial position, in the given tiny part, and propagates it using the PDE, the result is that the vibration will never cancel at the boundary, apart, that is, for a discrete set of initial positions for which the *miracle* will happen. This discrete set is called the spectrum of the drum and is an example of the discreteness generated by the continuity of the PDE. The drum selects, from amongst the continuum of vibrations, those that will cancel on the border. And, whatever kick you give to the drum, the spectrum is (almost) the same.

The Heisenberg theory appears from Schrödinger's in the same way: a PDE embedded in the continuum gives rise to discreteness thanks to the boundary condition. But in this case the set of *frequencies* is more complicated, less harmonic than was the case for the drum (from this point of view it would be amusing to analyse carefully the analogy between this loss of harmonicity, and the almost contemporary birth of non-tonal music), but the idea is the same: *the continuum generates discreteness.*

In saying this we are abusing language a little. Indeed, if it were true that the PDE lives definitively in the continuum, the eigenvalue problem for the Schrödinger equation would be a little more tricky. Indeed the way the spectrum exhibits itself is a mixture of:

1 the PDE (Schrödinger equation);
2 the boundary condition (border of a box); and
3 the space of solutions in which one looks to solve the problem.

This last part took some time to be established carefully (by von Neumann). The solution space nowadays has the magic name of Hilbert space. And a Hilbert space can be thought of as a limit of finite dimensional spaces together with a concept of *completeness* (this view seems old-fashioned now, but one can find it in textbooks until the late 40s): the quantum continuum is indeed a passage to infinity with completeness, and this is crucial when recovering the (discrete) spectrum. We will discuss this fact later.

3. Discrete–continuous and the Bohr–Sommerfeld semi-classical formula

The big success of Heisenberg and Schrödinger was to recover the spectrum of simple systems (such as the Hydrogen atom or oscillators) in accordance with the old Bohr theory (actually the biggest success was to predict the $\frac{\hbar}{2}$ of the harmonic oscillator, which was not given by Bohr). But exact solutions are rare, and semi-classical methods soon gave

† We may note here that in his original paper Schrödinger thanks Hermann Weyl for help concerning the resolution of his eigenvalue equation.

https://doi.org/10.1017/S0960129507005956 Published online by Cambridge University Press

rise to results for which the old Bohr law was recovered from the Schrödinger equation in the limit $\hbar \to 0$. The so-called WKB method used here was inherited from optics (the semi-classical limit is equivalent to the passage from physical to geometrical optics) and gives a precise prescription for *ordering* the spectrum by the set of naturals. However, labelling, in a natural and explicit way, an (*a priori* unordered) discrete set by integers is a very ambitious task, so it is not surprising that it works only for a few systems (the ones called integrable), and one can say that the extension of such a procedure to the non-integrable situation is still not fully understood.

The principal reason that the WKB–Bohr–Sommerfeld theory does not work in general is that it relies on the existence of so-called invariant (by the classical flow) tori, which are geometrical objects that cease to exist for non-integrable systems. However, if one gives up the ambition to associate a natural number (given by classical mechanics) with EACH eigenvalue, but considers globally the set of eigenvalues (the spectrum), there is a natural discrete set of objects that does always exist: the set of periodic trajectories. We will see the link between these two discrete sets in the next section.

4. Discrete–continuous and the trace formula

The helium atom is a 3-body system, but unlike the celestial 3-body problem, it is not perturbative. What matters for the Schrödinger equation are the charges and not the masses, and the charge of each electron is half of that of the nucleus, and thus of the same order. Therefore, after the initial great success of quantum mechanics, the helium atom has remained a challenging system, a system for which the regular methods of computing eigenvalues fail (and this is true more generally for all quantum systems that are far from integrable).

The situation changed radically in 1971 when Gutzwiller published a fascinating paper, whose contents is now called the Gutzwiller trace-formula. The idea is that the trace of the resolvent at energy E of the Schrödinger operator is determined semi-classically by the set of periodic orbits of the classical system of energy E. Mathematically, it reads

$$\sum_j \frac{1}{E_j - E} \quad \sim \sum_{\gamma \ of \ energy \ E} T_\gamma \frac{e^{i\frac{S_\gamma}{\hbar}+\sigma_\gamma}}{\sqrt{\mathrm{Det}(1-\mathrm{P}_\gamma)}}$$

where $\{E_j\}$ is the set of eigenvalues, γ is a periodic orbit, T_γ is its period, and S_γ, σ_γ and P_γ are its action, Maslov index and Poincaré mapping, respectively. Note that the left-hand side is purely *quantum* and the right-hand side is purely *classical*.

The situation here has radically changed from the Bohr theory: first, one does not associate a single eigenvalue to each periodic trajectory, but the spectrum to the set of periodic orbits. In fact, the formula written in this way is not mathematically correct since the left-hand side, as written, does not exist (for example, if the spectrum contains E, the formula explodes); but, fortunately, the right-hand side does not make sense either. Indeed, the number of periodic orbits of period less than a given number increases exponentially as the number diverges, thus removing any hope of the convergence of the sum. This (typical) situation in physics where a formula takes the form of a link between quantities that do not really exist usually gives rise to a *regularised* formula in mathematics. When expressed rigorously, the Gutzwiller formula has to be read as a means of expressing our knowledge of the spectrum, given a certain *precision* ΔE, as a sum of quantities involving periodic orbits, of period less than a certain number ΔT. Note that ΔE and ΔT are related by the (time-energy) Heisenberg principle:

$$\Delta E \times \Delta T \sim \hbar,$$

thus relaxing the precision gives rise to a general formula.

But there is a more conceptual difference between the Gutzwiller result and the Bohr theory (or, equivalently, the semi-classical one). The Bohr prescription consists of selecting from a *continuum* of invariant tori those satisfying a certain topological ($\hbar$ **dependent**) condition (the actions have to be multiples of $\hbar$). In the Gutzwiller formula, one deals directly with a *discrete* (and $\hbar$ **independent**) set (of periodic orbits). In the Bohr case, the continuum is predominant; in the Gutzwiller one, discreteness is predominant. One builds discreteness (of the spectrum) directly from discreteness (of periodic orbits).

Moreover, although one can think of the periodic trajectories as a subset of all the trajectories, a periodic trajectory is the solution (and the only solution) of a given problem consisting precisely of computing the periodic trajectories. Note that this is analogous to the construction of the Hilbert space for quantum mechanics, in the sense that they have a precise ontological status, as do the eigenvalues in quantum mechanics. Finally, let us mention the importance of periodic trajectories for dynamical systems, as had already been noticed by Poincaré, especially when one looks at long periods.

To conclude this section, it is amusing to note that a knowledge of the periodic trajectories of a classical system does not in itself, in principle, determine it, but it does determine the corresponding quantum system, which then, taking the limit $\hbar \to 0$, determines the classical one.

5. Persistence of quantum coherence in the classical limit

In this section we want to show, using a simple, but physically relevant, example, how the discreteness of the quantum setting can lead to phenomena for which quantum effects remain valid in the classical limit.

Consider a quantum particle moving freely in a circle. Its Hamiltonian is the Laplacian on the circle times $\hbar^2$, and the evolution is explicitly solved in terms of Fourier expansion.

Let $\psi^0(\theta) := \sum c_n e^{in\theta}$ be the initial condition. A very easy computation shows that at time t the wave function is

$$\psi^t(\theta) = \sum c_n e^{itn^2\hbar} e^{in\theta}.$$

Therefore

$$\psi^{k2\pi/\hbar} = \psi^0$$

for each integer k.

This phenomenon of periodicity in time (the reconstruction of the wave packet) is precisely due to the discreteness of the sum involved in the initial state. No such reconstruction would appear if we replaced the sum by an integral. Note also that

https://doi.org/10.1017/S0960129507005956 Published online by Cambridge University Press

the period of reconstruction is proportional to $\frac{1}{\hbar}$, and is thus pushed to infinity in the semi-classical limit.

This reconstruction of the wave packet is very important in the physics of quantum computing and quantum information (the Kerr phenomenon). It has been observed experimentally (Stoler and Yurke 1986) and is one of the most striking appearances of quantum coherence in the experimental physics of simple systems. One can find a precise mathematical analysis of a more general situation related to this in Paul (2006).

6. Conclusion: the discrete, the continuum, the infinite and completeness

So far we have discussed a number of different situations for which the discrete/continuous opposition has applied: Bohr's quantum theory (selection of discreteness from the continuum); the Heisenberg/Schrödinger quantum mechanics (matrix theory as opposed to a differential equation); the return to Bohr conditions in constructing quantum solutions in the classical limit; and finally, the trace formula, where the intrinsic quantum discreteness is built up from the intrinsic discrete structure of the classical periodic orbits.

Let us concentrate again on the Schrödinger/Heisenberg polarity and be a bit more precise about the concept of Hilbert space. A Hilbert space is a Banach space for which the norm is given by a scalar product. A Banach space is a *complete* metric space. Of course, for a finite dimensional space, this completeness plays no part, but the important case is the infinite dimensional case, which is obtained from the finite one by completion in a way that leaves no hole. The set $\mathbb{Q}$ of rational numbers with the usual distance is not complete. Quantum mechanics uses the passage to infinite closest to the finite. The trace of this is evident: the orthonormal bases are countable, and all (separable, infinite dimensional) Hilbert spaces are unitary equivalent, that is, there is only one. In a certain sense, the duality between Heisenberg (matrix theory) and Schrödinger (PDEs) is not so heterogeneous: the continuum of Schrödinger (corresponding to a differential equation sitting in a Hilbert space) is, in fact, an economical extension of the finite dimension matrices of Heisenberg. It might suffice to understand this to read the preface of the book Halmos (1949), where Halmos explains how the link between matrix and Hilbert space is not so obvious†, and he writes a full book on it, more precisely, on the finite dimensional case.

The continuum used in quantum mechanics is certainly a well-adapted one, being 'equivalent' to the discreteness of the quantum theory.

The *true continuum*, that of the classical theory, is recovered only when the Planck constant vanishes. In this limit: the spectra of operators become continuous; the Bohr–Sommerfeld condition loses all its substance; the cut-off in the maximal period of periodic orbits in the trace formula diverges, letting the set of periodic orbits (and even just the maximal period one) occupy all the space; and the oscillations become so fast that the concept of discreteness itself is smoothed, like looking through the wrong spectacles. Seen

† 'That Hilbert space theory and elementary matrix theory is intimately associated came as a surprise to me and colleagues of my generation....'

like this, the classical world, and its obvious partner the continuum, may be thought of as a 'dirty' rough approximation.

Finally, we should note that what we call discreteness here is to be taken in a slightly different sense from the normal usage: the spectrum is discrete and the Hilbert space 'countable', but the continuum appears within the structure itself through the ring structure of the theory – although a vector is specified by a *discrete* set of numbers, these numbers themselves take *continuous* values (in $\mathbb{R}$ or $\mathbb{C}$). Nevertheless, one can think of this product by the reals as representing a trace of the (underlying) classical theory. In principle, atoms are in eigenstates of Hamiltonians, which are the only stationary states. If one considers linear combinations of such states, one has to perform a quantum operation on them; but a quantum operation driven by classical considerations. And this is really one of the difficulties in understanding this classical–quantum entanglement: in general one acts on atoms through an electromagnetic field, but this field is classical, being governed by a classical generator, and a human being turns the handle to regulate the intensity. An isolated quantum system either remains in a stationary state or makes a transition from one state to another, and what is observed is the set of line spectra, not the wave function. One of Heisenberg's key ideas was to concentrate on *observable* quantities (which became a key idea for all quantum physics: for example, renormalisation in quantum field theory). Through the transition between states, differences between eigenvalues are observable, and are fully discrete. Perhaps we have to consider that the actual quantum mechanics setting is in fact something like *quantum* $\otimes$ *classical*, and that the introduction of real or complex numbers arises from this tensorial operation, this entanglement between the 'quantum and classical'.

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