

Quantum Graphenity

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Abstract

One obstacle for further progress on quantum gravity and issues like the discrete vs. continuous debate is the lack of experimental data. To a certain extent, this problem can be overcome by the simulation of models for fundamental physics by other physical systems. Here I focus on graphene as a particularly fascinating example of such a simulator and try to explain how continuous three-dimensional relativistic spacetime emerges from the discrete hexagonal crystal lattice of graphene. The potential of graphene to simulate aspects of fundamental physics is discussed.

Introduction

It is probably the most challenging open problem in theoretical physics to find a theory which comprises both general relativity describing gravity and the standard model of particle physics as limiting cases. A putative unified theory is also known as *quantum gravity*, since it is believed that such a unification requires in particular that the gravitational force acquires a quantum-mechanical description, so that all of physics would ultimately be based on quantum-mechanical principles. Among the huge number of approaches—too many to list here—one can find many which postulate a fundamental discreteness of spacetime or at least some sort of discrete structure on spacetime. The list of approaches itself may almost be continuous, so [Disc] is definitely an incomplete list; see also [Gib95b], [GP05] for more general reviews. One way to motivate this discreteness is as follows: in order to measure a very small distance Δx , Heisenberg's quantum-mechanical uncertainty relation

$$\Delta x \cdot \Delta p \geq \hbar/2$$

demands the use of probes of very high momentum uncertainty Δp , and therefore also very high energy. However now according to general relativity, if one concentrates enough energy on a very small length scale, it will self-gravitate so much that it collapses into a black hole. By doing the math, this (questionable) reasoning leads to the estimate that the smallest sensible length should be of the order of the *Planck length* $x_{\text{Pl}} \approx 1.6 \cdot 10^{-35}$ m, which compares to the size of a proton (10^{-15} m) as the size of a soccer field (10^2 m) compares to the distance of the sun to the distance to the Andromeda galaxy (10^{22} m).

Possibly another reason for the popularity of these approaches is of a more cultural nature and due to the advent of the information age. Given that digital computation and digital communication play a crucial rôle in our everyday lives, then maybe even nature herself uses similar tools? This attitude goes so far as to

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suggesting that the universe itself might be a computer [Comp]. It is tempting to interpret the very title of this essay contest along these lines. And in fact, maybe the first one to suggest that the universe is a digital computer was Konrad Zuse himself, the constructor of the first digital computer. He came up with a cellular automaton [Zus69] which simulates structures reminiscent of collisions of pointlike objects which he thought of as akin to physical particles.

As a point against the whole debate of discrete spacetime vs. continuous spacetime, and therefore also as another argument against the approaches to discrete spacetime, one may note that mathematicians have come up with many notions of geometry on spaces without points; Connes' noncommutative geometry [Con94] is possible the most prominent example. In these cases, the discrete vs. continuous dichotomy hardly even applies—thinking in terms of discrete or continuous automatically implies mental images of space which do not comprise these generalized concepts of geometry.

The lack of experimental evidence may be one of the reasons for the confusing multitude of approaches to quantum gravity. A similar diversity of opinions exists on the level of the discrete vs. continuous discussion: for example, while Forrest [For95] describes the discrete vs. continuous question as something which is in principle decidable by experiment, Floridi [Flo09] claims to show precisely this feat to be impossible.

In order to get to the point: on a totally personal level, I find it difficult to accept any of the present approaches to the quantum gravity problem as potentially promising. So instead of coming up with yet another approach—worthy of criticism at least as much as any one of the existing ones—I would like to take a step back and merely explain some of the exciting developments in a newly emerging field of research: the simulation of physical theories, in particular physical models ranging from relativistic quantum mechanics up to quantum gravity, by condensed matter systems. If there is any hint of originality in this essay, then it does not lie in its contents, but at most in their presentation.

Usually, simulating a physical system means to simulate a theoretical model of this system on a digital computer. The purpose of the simulation is to extract predictions from the model which are difficult or impossible to calculate analytically, and then compare these predictions with experiment in order to assess the correctness of the theoretical model. However in principle, a digital computer might not be the only system capable of doing this; it may also be possible to simulate the given system by another one. This would be the case, for example, if the simulant can behave in such a way that it represents both the dynamics and the observables of the simulated system (at least approximately). Of course in practice, one also requires sufficient experimental control over the simulator. As the example of the digital computer as a universal simulator shows, it is not necessary to precisely represent the dynamics of the simulated system; but arguably, the simulation becomes much more credible and realistic when the simulator also represents the dynamics as accurately as possible.

A fascinating example of this is the simulation of black holes and their Hawking radiation in Bose-Einstein condensates [LIB⁺10], or even in the kitchen: the water splash formed in the kitchen sink upon opening the faucet contains a central part which is in some aspects formally analogous to the interior of a time-reversed black hole [JPM⁺10]! With the different ways of analyzing a physical model being analytical calculations, numerical studies, and experimental checking, such physical simulations fair in between the numerics and the experiment. In particular, these physical simulations may be helpful when there is simply no experimental data available for the system itself—as is the case for quantum gravity.

Good simulators are those systems over which one has good experimental control. One has to be able to manufacture both the kinematics and the dynamics to a suitable extent, and requires the possibility to tune some of the system parameters. Condensed-matter physics offers astonishing possibilities in this regard. Furthermore, it seems ideally suited to probe some of the models claiming the emergence of a continuous spacetime from a discrete structure: on the atomic scale, condensed-matter systems are necessarily discrete (at least in some aspects). On the other hand, this fundamental discreteness is usually not visible on the macroscopic scale, so that a continuous space has “emerged”. Nevertheless, some traits of the macroscopic

structure will depend on the microscopic physics, and hence it becomes possible to make statements about the microscopic physics from macroscopic observations. The extent to which this is possible seems a great testing ground for the discrete vs. continuous discussion.

There is one particularly astonishing example of this which I would like to explain some detail. Besides being a material where the emergent continuous spacetime is approximately relativistic (as to be discussed soon), the story of *graphene* is absolutely stunning. It is one of the many incarnations of carbon, which exists in the form of diamond, graphite, graphene, and in several others. Graphene is a two-dimensional crystal of carbon atoms situated on a hexagonal lattice (see figure 1). Graphite, on the other hand, is a three-dimensional stack of many loosely aligned graphene layers. It is the main ingredient of pencil mines, and in fact the term *graphite* stems from the ancient greek $\gamma\rho\acute{\alpha}\varphi\omega$, “I write”. Since the graphene layers in graphite can easily be torn apart, it is now known that every stroke of a pencil produces small flocks of graphene among lots of other debris. And these graphene flocks appear even though this material was thought to be unstable due to the quantum-field theoretical Mermin-Wagner theorem [GN07]!

Although it had been possible before to grow graphene layers on top of some other material functioning as a substrate, the real breakthrough came in 2004 when Geim and Novoselov developed an ingenious method for finding single-layer graphene among all the multi-layer sheets and graphite stacks which are left behind e.g. by the stroke of a pencil, or by successive tearings of graphite by Scotch tape. For this work and the ensuing experimental examination of graphene, Geim and Novoselov have been awarded the 2010 Nobel Prize in Physics. While the story of graphene itself has barely begun, my very brief account already has to end here by referring to [GN07] for more details as well as some analysis of the manifold of potential real-world applications.

The emergence of the Dirac equation

For us, the most interesting property of graphene is its potential for simulating aspects of fundamental physics. Before getting to this, a brief explanation of the to-be-simulated part of fundamental physics seems in order. According to relativistic quantum mechanics, a free electron is described by a four-component wave function depending on three space coordinates and one time coordinate, which means that it is a function of the form $\psi : \mathbb{R}^4 \rightarrow \mathbb{C}^4$. The dynamics of ψ is given by the Dirac equation [PS95] (in units with $c = 1$),

$$(i\gamma^\mu\partial_\mu - m)\psi = 0, \tag{1}$$

where the spacetime index is from the range $\mu \in \{0, 1, 2, 3\}$, the electron mass is m and the γ^μ are some 4×4 -matrices encoding the geometry of spacetime in the sense that they satisfy the

$$\text{Clifford algebra relations: } \quad \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu}. \tag{2}$$

Besides this requirement, the precise form of the γ^μ is irrelevant; but of course, for concrete calculations one needs to make a choice.

In three spacetime dimensions, the Dirac equation has precisely the same form, except that naturally the spacetime index μ has a smaller range, and also the wave function only has two components, so that $\psi : \mathbb{R}^3 \rightarrow \mathbb{C}^2$. Accordingly, the γ^μ are then only 2×2 -matrices, but are still uniquely defined by the Clifford algebra relations (2). A convenient choice is

$$\gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \gamma_1 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \quad \gamma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{3}$$

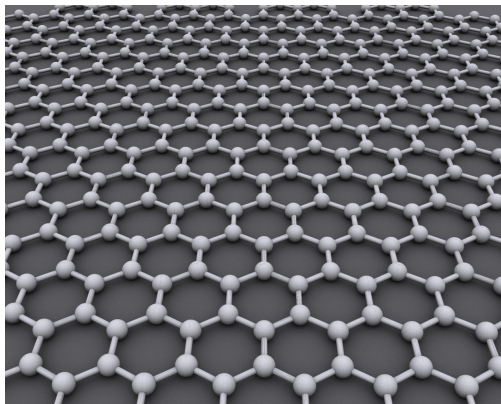


Figure 1: Graphene is a hexagonal lattice of carbon atoms. Each hexagon is chemically identical to the C_6 ring of benzene C_6H_6 . (Image from WIKIPEDIA.)

Simple matrix algebra shows that this choice does indeed satisfy the Clifford algebra relations (2). For future comparison, let it be noted that the Dirac equation in 3-dimensional spacetime hence takes on the form

$$i\partial_t\psi = (-i\gamma_0\gamma_1\partial_x - i\gamma_0\gamma_2\partial_y + \gamma_0m)\psi = \begin{pmatrix} m & \partial_x - i\partial_y \\ -\partial_x - i\partial_y & -m \end{pmatrix} \psi. \quad (4)$$

To finally begin the study of charge carriers in graphene, it is necessary to take a closer look at what graphene actually is. As has already been mentioned, this material is a two-dimensional infinite crystal of carbon atoms, arranged in a hexagonal lattice (also known as “honeycomb lattice”; it has the same structure as chicken wire, see figure 1). As usually the case in condensed matter physics, the charge carriers are the *free electrons* which are those located on the outer shells of atoms and not participating in any chemical bonding to neighboring atoms. In carbon with its six electrons in total, two of these are located on the innermost orbital and hence are so tightly bound that they do not interact with anything else, while four electrons are available for chemical bonding and the formation of free electrons. Since each carbon atom in the lattice has three neighbors, three of these four available electrons are localized in chemical bonds, and therefore exactly one electron per atom remains relatively free to wander around. These free electrons are precisely the charge carriers.

We now proceed step-by-step to a heuristic (incomplete) derivation of why the wave function of the charge carriers obeys equation (4) with $m = 0$. Let’s consider a single electron hopping around the atoms of the hexagonal graphene lattice, as schematically depicted in figure 2. The approximation considered here is that of a *continuous-time quantum walk* [Kem03, III.B] on the hexagonal lattice. This means that we take the electron wave functions now to be functions $\psi : \Lambda \rightarrow \mathbb{C}$, where Λ stands for the set of atoms forming the hexagonal lattice, instead of functions $\mathbb{R}^2 \rightarrow \mathbb{C}$. Intuitively, this corresponds to the assumption that the electrons are tightly bound around the atoms. These functions form a Hilbert space denoted by $\ell^2(\Lambda)$. If $a \in \Lambda$ is an atom, let us write $|a\rangle$ for the wave function which is 1 on a and vanishes at all other atoms. This is the wave function where the electron is completely localized at atom a . Then all the $\{|a\rangle\}_{a \in \Lambda}$ taken together form a basis of $\ell^2(\Lambda)$: a state of the electron is a superposition of states localized at each atom.

Now note that the hexagonal lattice is actually a *bipartite graph*: we can partition the set of atoms into two types “ \circ ” and “ \bullet ” so that \circ -atoms are only adjacent to \bullet -atoms, and \bullet -atoms are only adjacent to \circ -atoms. Furthermore, the collection of all atoms of each type forms a parallelogrammic lattice Λ_\circ , respectively Λ_\bullet : the atoms in that parallelogrammic lattice are exactly those which can be reached from a fixed lattice

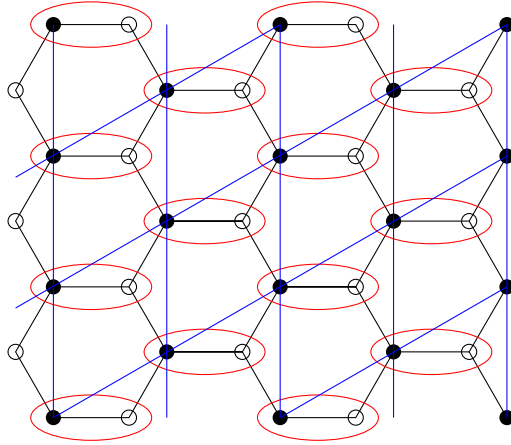


Figure 2: The carbon atoms in the hexagonal graphene lattice are considered two be of two types “ \circ ” and “ \bullet ”. The atoms of each type form a parallelogrammic sublattice, one of which is drawn with blue lines. The atoms are considered to come in pairs as indicated by the red ellipses. All this is conventional and does not influence the physics.

atom by translations of the lattice onto itself. This parallelogrammic property is useful in calculations since one can introduce a tilted cartesian coordinate system such that the lattice vectors lie exactly on the integer points of this coordinate system. The Hilbert space of wave functions $\ell^2(\Lambda)$ now decomposes into a direct sum $\ell^2(\Lambda) = \ell^2(\Lambda_\circ) \oplus \ell^2(\Lambda_\bullet)$, meaning that a wave function is determined by its components localized on Λ_\circ and Λ_\bullet .

Now as indicated by the red ellipses in figure 2, one can define a pairing between the \circ -atoms and the \bullet -atoms such that each atom of each type is paired with exactly one neighboring atom of the other type. The crucial now is to view the two atoms in a pair as two internal states of a single site. Thinking of the \bullet -atom in each pair as a representative of the pair, one can then view the state where the electron is localized on its \circ -partner as an internal excited state of the electron on the \bullet -atom. In other words, we now simply remove each \bullet -atom, but instead add to each \circ -atom an additional excited state, which gives the same Hilbert space. In this language, a wave function is a \mathbb{C}^2 -valued function on the sublattice Λ_\bullet , i.e. $\psi : \Lambda_\bullet \rightarrow \mathbb{C}^2$. let us write ψ_\bullet and ψ_\circ for its two components. Then the Schrödinger equation takes on the form

$$i\hbar\partial_t \begin{pmatrix} \psi_\bullet \\ \psi_\circ \end{pmatrix} = H \begin{pmatrix} \psi_\bullet \\ \psi_\circ \end{pmatrix}. \quad (5)$$

here, the Hamiltonian operator H is some 2×2 -matrix, whose entries are operators on $\ell^2(\Lambda_\bullet)$ which contain the hopping amplitudes between different atoms. We now assume this operator to be local, in the sense that the hopping has only a finite range, and to be symmetric in the sense that it respects all the symmetries of the hexagonal lattice, which are: translational symmetry, rotational symmetry by 120° around any atom, and reflection symmetry along the bisection of two neighboring atoms.

Now the locality assumption means that each entry of H is an operator which can be expanded as a Taylor series in the partial differential operators ∂_x and ∂_y , meaning that each matrix entry of H is of the form

$$\sum_{m,n=0}^{\infty} a^{n+m} c_{nm} \partial_x^n \partial_y^m \quad (6)$$

Appropriate powers of the lattice constant a have been inserted so that the coefficients c_{nm} become dimensionless. Recall the the partial derivatives ∂ . are, up to a factor of $-i\hbar$, exactly the momentum operators. Hence when considering physics with low enough momentum ($pa \ll \hbar$), then these operators can be approximated reasonably well by the zeroth-order and the first-order terms alone. In this case, the Schrödinger equation (5) becomes something at least reminiscent of (4): the Hamiltonian on the right-hand side will be a matrix containing constant entries and linear combinations of ∂_x with ∂_y .

Furthermore, it can actually be shown that the Hamiltonian matrix is a certain scalar multiple of

$$\begin{pmatrix} 0 & \partial_x - i\partial_y \\ -\partial_x - i\partial_y & -0 \end{pmatrix}, \quad (7)$$

which is the one from (4) with $m = 0$, is the *only* such Hamiltonian matrix consistent with the symmetries of the hexagonal lattice¹. Said scalar multiple determines the relative dimension of time t to the space coordinates x and y , and hence determines the speed of light of the simulated relativistic spacetime. A more detailed calculation [Leg10] shows that this effective speed of light is given by the Fermi velocity $v_F \approx 10^6 \frac{\text{m}}{\text{s}}$, which is way below the actual speed of light in ambient spacetime.

Finally, let it be mentioned that the Dirac equation in 2 spacetime dimensions has a nice interpretation (“Feynman’s checkerboard”) in terms of paths on a 2-dimensional lattice. Maybe a similar interpretation would be possible for the Dirac equation (4) in terms of a hexagonal lattice?

Towards Quantum Graphenity?

It has been experimentally confirmed [NKM⁺05] that the charge carriers behave indeed like Dirac particles as explained in the previous section, at least with respect to those aspects which have been experimentally accessible. Many more simulations of fundamental physics for these massless Dirac particles have already been proposed or conducted, and some of these deserve to be mentioned.

While quantum mechanics has many counterintuitive and seemingly paradoxical features, relativistic quantum mechanics in terms of Dirac particles has even more. One of these is the so-called *Klein paradox*, which states that a massless Dirac particle can tunnel through a high potential barrier easier than through a lower one [Kle29]. Although this works similarly in the massive case and is independent of the spacetime dimension, it has been impossible to put Klein’s prediction to an experimental test with actual “real” Dirac particles. Thanks to the emergence of massless Dirac particles in graphene, the Klein paradox has now been experimentally verified [KNG06]. And, as a positive indicator of the importance of such simulations, a discussion has followed, disputing these findings [Dra09].

Another phenomenon, already predicted by Schrödinger in 1930 [Sch30], is the so-called *Zitterbewegung* (jittery motion) of Dirac particles. Upon calculating the expectation value of the particle’s position operator and looking at its time dependence, one finds that this expectation value can move in a wobbly-jittery way, including changing the direction by a half turn. While this effect has also not yet been detected in actual spacetime, there have been concrete proposals for experiments on graphene [RZ09]. It has already been observed in another simulating system, a trapped ion [GKZ⁺10].

So far, the discussion has mostly been about *free* Dirac particles only, i.e. those whose wave function satisfies the simple wave equation (4). While this has been fascinating, it surely cannot be a good simulation, since actual particles interact! So, is it possible to modify the graphene lattice in such a way that some sort of interactions are simulated as well? Maybe even interactions which resemble those which we know from fundamental physics, namely gauge theories and gravity? Indeed, in works of Cortijo and Vozmediano [CV07] it is proposed that this is the case. The basic ideas are somewhat like this: an actual crystal will usually not

¹Details of this will appear elsewhere, if they have not yet appeared elsewhere.

be perfect, but contain disorder and irregularities. For example, it may so happen that some of the hexagons in the hexagonal lattice are not actually hexagons, but, say, pentagons or heptagons. Only a single such defect dramatically changes the geometry of the crystal; for example in the presence of a single pentagon defect, it makes the lattice wrap up into a conical structure with the pentagon at its tip. This has two effects: firstly, it destroys the nice pairing of the two sublattices of figure 2, and secondly, it creates an effective curvature on the graphene sheet, precisely localized at the tip of the cone. While the former problem can be regarded as the influence of an effective $SU(2)$ -gauge field which interchanges \circ -states and \bullet -states upon traversing a loop around the tip, the latter kind of curvature has been likened to the effect of cosmic strings [?].

Besides topological defects, another observation is that the graphene lattice is actually not flat at all, but rather naturally crumpled [FLK07]. It seems plausible that the resulting curvature of the graphene sheet results in a curvature of the Lorentzian metric determining the Dirac equation (4). If this is indeed the case, then a crumpled graphene sheet naturally models Dirac particles on a crumpled background spacetime, i.e. a background spacetime with gravity! Even better, the graphene ripples themselves are subject to thermal fluctuations—in terms of the simulated spacetime, this means that the geometry of the spacetime itself is subject to fluctuations! At very low temperatures, and under very isolated conditions guaranteeing coherence, it may even be possible that the dynamics of the ripples is governed by quantum fluctuations. In this case, the graphene sheet may possibly be a simulator of three-dimensional quantum gravity, emergent from a discrete lattice: **quantum graphenity**. Whether this makes any sense at all remains to be seen. When one's understanding becomes so shallow that one's writing drifts off into wild speculation, it is time to stop.

Conclusion

The basic tenet of this essay is that physical systems can simulate each other to some extent, even if they are radically different in nature. Given that one of the troubles with fundamental physics is the practical impossibility of experimentally testing most theoretical proposals, I have tried to enunciate the idea that this can partly be circumvented by said simulations. Graphene crystals offer essentially unique possibilities in this regard due to the simulability of relativistic fermion physics. Not only can counterintuitive phenomena from relativistic quantum mechanics be demonstrated in graphene, it also functions as a toy model for the emergence of continuous relativistic spacetime from an underlying discrete spatial lattice.

So what is left to be done? Obviously one should look both for further simulators of fundamental physics models and for further fundamental physics phenomena which can be simulated by experimentally accessible systems. Besides this, there is an interesting abstract direction waiting to be explored: what does it precisely mean to simulate a physical system by another one? To what extent does a digital computer simulate a physical system, even though its components have totally different dynamics? This is where notions from computer science and the mathematical field of category theory might enter the game, since the concepts of (bi-)simulation and behavioral equivalence have long been investigated in this context and the connection to physics is beginning to get explored [Abr09]. Doing this also means that one will have to define precisely what a physical system is and which *category* of physical systems one wants to consider.

In any case, I hope that you, Dear Reader, have gained some insight and understanding from this essay, even if I did not have any new models of physics to embark upon and cannot provide any convincing argument for either side of the *discrete vs. continuous* debate. Sometimes it is necessary to take a few steps back before being able to advance.

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