A Sheet of Graphene – Quantum Field in a Discrete Curved Space

Nikodem Szpak

Abstract The dynamics of electrons in a sheet of graphene can be described as a quantum field living in a discrete space – the graphene honeycomb lattice. As this space can be curved in various ways, the system offers a fascinating tool for studying and simulating the impacts of non-trivial geometries on quantum fields living in it. Local and global deformations as well as defects of the lattice can be mapped, via a discrete differential geometry, onto curvature and torsion in the continuous analog model. This allows for physical simulation and observation of quantum evolution and scattering in curved geometry and interaction with torsion. Time-dependent lattice perturbations, such as sound waves, can be interpreted as dynamical geometry and mimic gravitational waves. The immanent quantum character of the lattice structure – composed of carbon atoms – can be used for proposing a physical simulator of quantum geometry. We discuss the main ideas constituting these analogies, the latter being the topic of our ongoing project.

1 Introduction

Graphene, probably the most intensively studied material in the last decade, consists of a regular two-dimensional lattice of carbon atoms. Scientists try to produce, measure and model graphene in order to better understand its many original features. But graphene can also be seen as a laboratory offering the unique possibility of quantum simulations of relativistic phenomena which are known from particle physics but are still not accessible in experiments. Its crucial feature is the energy dispersion relation for electronic excitations which is similar to that of the relativistic Dirac equation. Thus, the excitations of the ground state of graphene behave like relativistic elementary particles and offer new insights into some ultra-relativistic processes. One

Nikodem Szpak
Faculty of Physics, University Duisburg-Essen, Germany, e-mail: nikodem.szpak@uni-due.de

of the new directions of graphene research, made possible by the newest scanning techniques, is related to the investigation of its non-flat (curvature) and non-perfect (defects) crystalline structures and their influence on its macroscopic properties [1].

The dynamics of quasi-particles hopping on the crystal lattice can be effectively described as a class of discrete Hubbard Hamiltonians [2], which have been extensively studied in the literature in the past half of the century [3]. Universality of the Hubbard class allows for matching together physical systems of very different origin but having the same mathematical description and designing new simulators in which one system mimics another. Deep connections exist between the lattice Hamiltonians and discretized fundamental relativistic field theories [4, 5, 6, 7]. In the current project, we are working to extend this analogy to curved and dynamically perturbed lattices by involving the quickly developing language of discrete differential geometry [8]. Similarly, as is the case in numerical methods based on finite difference schemes, it should allow for the approximation of the dynamics of continuous quantum fields by their evolution in discrete spaces. These relations offer a new exciting possibility of designing lattice quantum simulators for continuous quantum fields evolving in curved geometries. We plan to conduct a systematic investigation of various types of lattice perturbations and to assign them to geometric objects such as metric, connection, curvature or torsion. The advantage of this approach should be two-fold: firstly, it should provide a new elegant language for the effective description of the curved and defective structures in graphene, which should help to better understand their properties since the continuous analog field equations are mathematically much more treatable than the corresponding discrete systems. Secondly, the language should allow to interpret these types of defects as quanta of curvature or torsion and give rise to a new, very interesting type of simulators of quantum fields living in curved spaces or even of quantum geometry.

2 Discrete differential geometry from Hubbard models

The basic Hubbard Hamiltonian has the form

$$\hat{H} = \sum_{\langle n,m\rangle} T_{nm}\ \hat{\psi}_n^\dagger\ \hat{\psi}_m + \sum_n V_n\ \hat{\psi}_n^\dagger\ \hat{\psi}_n + \text{h.c.} \tag{1}$$

where $\hat{\psi}_n^\dagger$ and $\hat{\psi}_n$ stand for creation and annihilation of a (quasi)particle at site n. Usually, the first sum is carried over all neighboring pairs of sites denoted as $\langle n,m\rangle$. The hopping parameters T_{nm} represent probabilities for a (quasi)particle to jump between the sites n and m in a given time and V_n represents a local potential at site n.

The simplest example of a relation between the Hubbard model and a field dynamics is the scalar field $\phi_n = \phi(x_n)$ in one dimension discretized on a non-uniform lattice $x_n = (n+\varepsilon_n)\ell$ where ε_n parameterize small displacements of the regular grid. The Laplace-Beltrami operator Δ_g, defined in a Riemannian geometry with metric

g_{ij}, has the continuous representation

$$\Delta_g = \frac{1}{\sqrt{|g|}}\partial_i\left(\sqrt{|g|}g^{ij}\partial_j\phi\right), \tag{2}$$

where $|g| = |\det g_{ij}|$. Going from the continuum to the lattice, as is also done in numerical calculations, one needs a discrete scheme for calculating derivatives, e.g. $\bar{\partial}_x\phi_n = (\phi_{n+1} - \phi_n)/a_n$ where $a_n = x_{n+1} - x_n = (1 + \varepsilon_{n+1} - \varepsilon_n)\ell$ is the distance between two neighboring lattice sites. Then, a discretized Laplacian on the lattice reads

$$\bar{\Delta}\phi_n = \frac{1}{a_n\ell}\bar{\partial}_x\left(\frac{1}{a_n\ell}\bar{\partial}_x\phi_n\right). \tag{3}$$

The dynamics of a quantum particle satisfying the nonrelativistic Schrödinger equation $H\phi = -\Delta\phi + V\phi$ can be thus approximated on the lattice by a Hubbard Hamiltonian (1) with the hopping parameters $T_{n,n+1} \equiv J_n = [-1 + 2(\varepsilon_{n+1} - \varepsilon_n)]/\ell^2$ and $V_n = [2 - 2(\varepsilon_{n+1} - \varepsilon_{n-1})]/\ell^2$. Since the latter describes crystalline systems in solid state physics it allows for the construction of a class of analog models in which lattice systems with given J_n and V_n can mimic quantum physics in curved space with the effective metric $(g_{11})_n = (a_n)^2 = (1 + \varepsilon_{n+1} - \varepsilon_n)^2\ell^2$.

In higher dimensions the situation is more complex – in addition to parameters representing distances between the neighbors the angles between the lattice links also enter the formula for the discretized Laplace-Beltrami operator. The language of non-orthonormal frames, in which the metric $g_{(a)(b)} = \mathbf{e}_{(a)} \cdot \mathbf{e}_{(b)}$ is related to the co-frame $\mathbf{e}_{(a)}$ spanned by the links attached to each lattice vortex, is then more suitable. In this approach, perturbations of the metric correspond to the strain tensor $\delta g_{(a)(b)} = \varepsilon_{ab} = \frac{1}{2}(\partial_a u_b + \partial_b u_a)$ where u_a is the deformation field describing perturbations of the lattice. The same strain tensor appears in models describing electrons in deformed crystals [9], whenever the dispersion relation is quadratic at low energies, i.e. $E(\mathbf{k}) \sim \delta_{ab}k^a k^b$. It allows for the construction of analog models in which the lattice strain ε_{ab} gives rise to curved geometry with an effective metric $g_{ab} = \delta_{ab} + \varepsilon_{ab}$.

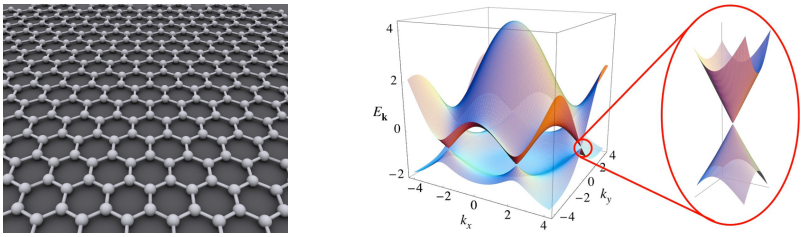

Fig. 1 The hexagonal lattice of graphene (left) and the dispersion relation for the Hubbard model with one Dirac cone magnified (right).

In contrast, in hexagonal lattices like graphene, the dispersion relation is linear at low energies (Fig. 1), i.e. $E(\mathbf{k}) \sim \pm|k|$, and the effective discrete field behaves like a Dirac spinor and the metric does not couple directly to it. As is known from the continuous Dirac equation defined on a curved space, the covariant derivative appearing in the 2+1-dimensional massless Dirac equation

$$i\partial_t \Psi = \bar{c}\, \sigma^{(a)} e^{\ i}_{(a)} (\partial_i - \Gamma_i)\Psi$$

contains the spin connection $\Gamma_i = \frac{1}{8}\omega_i^{(a)(b)}[\gamma_{(a)}, \gamma_{(b)}]$ with coefficients $\omega_i^{(a)(b)} = e^{(a)}_{\ j}(\partial_i e^{(b)j} + \Gamma^j_{ik} e^{(b)k})$ obtainable from the frame field $e^{\ i}_{(a)}$ only. $\bar{c}$ is the effective velocity of light in graphene, about 300 times smaller than the speed of light in vacuum c.

There also exists a mechanism generating mass in the Dirac field based on breaking the hexagonal symmetry. The so called Kekule perturbations [10] modify the hopping parameters in such a way that the energy spectrum splits into two gapped bands and the Dirac points disappear leaving relativistic dispersion relation for massive particles $|E(\mathbf{k})| \approx \pm\sqrt{m^2 + \mathbf{k}^2}$ at low energies. The mass of the excitations can be freely tuned by the strength of the Kekule perturbation.

This language enables for the description of several types of plastic deformations of graphene like strain, ripples or folding by means of external curvature from embedding in the third dimension and has been applied to study the electronic properties of curved graphene (for a review see Vozmediano, Katsnelson and Guinea [11] and the references therein).

3 Curvature and torsion from lattice defects

All lattice deformations discussed so far have had a character of small perturbations, not changing its global structure. However, it is virtually impossible to have real crystals with macroscopic curvature without structural defects. Therefore, in our current project, we focus on lattice irregularities that have an impact on the long range lattice structure. This requires an extension of the current approach by the description of structural defects like dislocations and disclinations. These effects can introduce effective curvature and torsion fields, giving rise to Riemann-Cartan geometries in which the simulated quantum fields can evolve.

Geometrization of the defects has been initiated by Kleinert [12] and applied to graphene by Vozmediano, Katsnelson, Guinea *et al* [11]. Extending the geometric language based on non-orthonormal frames allows for a direct interpretation of defects in terms of (a discrete) differential geometry: disclinations appear to be quanta of curvature while dislocations appear to be quanta of torsion [12, 13].

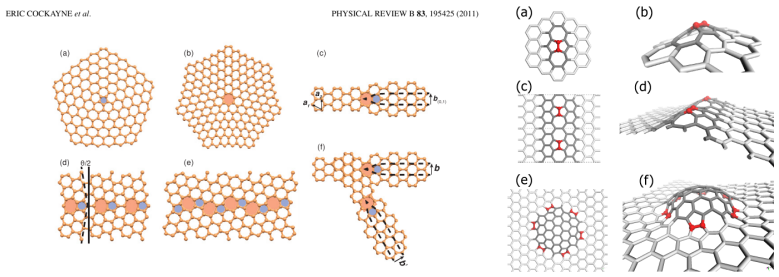

Fig. 2 Flat (left) and bumpy (right) graphene defects.

4 Open problems

The elegant geometric language has one drawback, presenting an obstacle in applications to physical systems. The framework proposed so far assumes that the frame field $e^{i}_{(a)}$, defined directly by the lengths and angles between the lattice links, gives rise to a natural connection $\Gamma^{(a)}_{(b)(c)} = e^{(a)}_{i}\partial_{(b)}e^{i}_{(c)}$ which defines parallelism on the lattice (cf. [14]). These connection coefficients tell the particles moving in the curved geometry which lines are straight and which are bent. While in the discretized differential geometry that approach seems to be quite natural, when applied to physical crystals it appears inaccurate. Electrons in crystals satisfy a fundamental *ab initio* quantum description and the notion of parallelism (straight lines) must derive from its properties, not from the geometry of the lattice links only. In other words, it is an idealizing assumption that the effective continuous geometric fields (frame, metric, curvature, torsion) are identical to those of the underlying lattice geometry. However, in the quantum simulators these are the Hamiltonians that have to match, not the geometries. Therefore, we see an urgent need to improve the current state-of-the-art by developing methods for deriving the real connection coefficients from the underlying quantum physical models.

5 Applications

The presented language opens the way for the modeling and simulation of very interesting effects in which quantum fields interact with curvature and torsion either distributed across the lattice or in the form of localized singularities. Once it has been fully developed, specific examples of quantum fields and their coupling to curvature can be considered. The simplest examples which can be studied are graphene sheets with point or line defects. Already a single dislocation defect (quantum of a torsion in the analog model) is theoretically very interesting. In some sense, it corresponds to a vortex on which the scattering of quantum fields poses a very complex problem with many surprises, e.g. recently discovered bound states [15, 16]. The

vortex background is also related to rotating black-hole spacetimes (e.g. the Kerr black hole) for which many conjectures about the field behavior (energy conservation, boundedness) remain open.

Line defects in two dimensions correspond to grain boundaries and occur commonly in graphene. They can be simulated in the analog models with extended torsion density (cf. [17]) and bear some similarities to cosmic strings.

Further, the so called "5-7" defects introduce significant elastic distortions in the lattice around [18], bending the nearby "straight lines". Especially interesting are the defects giving rise to the global angle defects, such as the "5" or "7"-rings (Fig. 2), which correspond to a curvature quanta in the analog model. They bend the "geodesic" lines around the curvature centers in a way corresponding to gravity or anti-gravity (positive or negative mass, respectively).

Similar ideas to those described here, have been also proposed for optical lattices – another discrete system with very promising features as an analog system for quantum fields. Analogs of cosmological spacetimes [19] or torsion [20] have been discussed but have not been realized yet.

6 Outlook

Graphene also allows quantum simulators with dynamical geometries mimicking the evolution of (quantum) fields in the presence of passing gravitational waves to be considered. Sound waves in graphene, causing tiny changes in the carbon atom positions, can represent time-dependent perturbations of the lattice geometry and mimic the metric waves. This idea seems especially attractive since it aims to provide a simulator with truly time-dependent geometry as we know it only from General Relativity.

Another very attractive idea appearing to be within reach is the simulation of quantum geometry. Considering slightly displaced atoms in a crystal as a base for the effective geometry in which the valence electrons live and treating the atoms themselves as quantum objects should lead to some form of quantum geometry (cf. spin net and spin foam models [21, 22]) – a very hotly discussed topic in Quantum Gravity. The phenomenon of defect dynamics, in which defects slowly propagate on the lattice, change type or disappear, adds another perspective for studying dynamical quantum geometries.

7 Conclusions

Graphene is a very flexible material with rich geometric possibilities. It provides an ideal model for implementing both types of curvature appearing in the lattice models: (a) the extrinsic curvature present due to folding and embedding of the two-dimensional graphene sheets in three dimensions and (b) the intrinsic curvature and

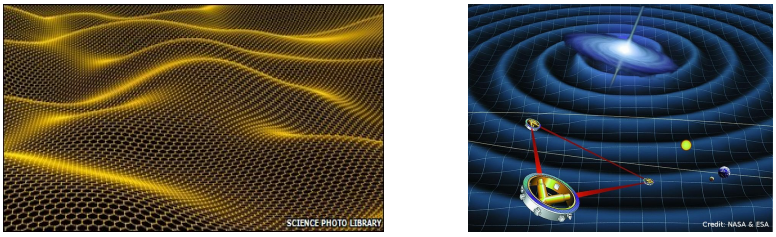

Fig. 3 Graphene ripples (left) compared to gravitational waves modifying space geometry (right).

torsion coming into play due to structural defects. Moreover, graphene allows for the design of closed surfaces with nontrivial topologies, as is the case for fullerenes, nanotubes and similar structures.

Configurations in which the effective Hamiltonians, in the continuous limit, correspond to quantum fields interacting with curvature or torsion open up the possibility of designing a new type of quantum simulators with some hope of proposing the first physical simulator of quantum geometry for quantum fields. It needs to be mentioned that the problem of the evolution of quantum fields in the presence of curvature and torsion still poses some fundamental questions of a theoretical nature and as such has never been observed in any laboratory experiment. Any access to such systems would be highly desirable.

The increasing interest in the technological applications of graphene requires the development of an efficient and easy-to-use geometric language (toolbox) for the classification and modeling of various types of graphene geometries as well as the prediction, description and study of new phenomena appearing in defective graphene structures. Understanding the implications of defects on its physical properties and purposive usage of the defects can be another big step in the engineering of new materials.

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