Does elastically deformed monolayer graphene have a curved space Dirac description?

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Undistorted monolayer graphene has energy bands which cross at protected Dirac points. It elastically deforms and much research has assumed the Dirac description persists, now in a curved space and coupled to a gauge field. We show this picture may be naive by using a real space gradient expansion to study how the Dirac equation derives from the tight binding model. Generic hopping functions give rise to large magnetic fields which spoil the truncation to the lowest derivative.

INTRODUCTION

Monolayer graphene has a band structure which contains two protected massless Dirac cones at the K and K' points. When undoped the bands are at half filling, putting the chemical potential at the Dirac points [1,2]. It can be bent beyond the linear regime [3], and when freely suspended, it naturally ripples [4,5]. When considering transport in such systems it is imperative to derive a continuum description of such distorted lattices.

Here we focus on the tight-binding model for graphene. For perturbative distortions Fourier space calculations appear to show an effective description of Dirac fields in curved space coupled to a gauge field proportional to the strain of the lattice, originally for carbon nanotubes [6] and later for graphene [7–14] [15]. It was noted early that the magnetic field scales inversely with the lattice spacing, but this is acceptable as it is suppressed by the perturbative expansion. Based on this much work has assumed a curved space Dirac description [16,22].

Here we derive an effective low energy description from the tight binding model via a real space gradient expansion, where we assume the hopping strengths vary on the tight binding model via a real space gradient expansion to study how the Dirac equation derives from the tight binding model. Generic hopping functions give rise to large magnetic fields which spoil the truncation to the lowest derivative. Perturbative corrections to the frame are of the same magnitude as higher derivative terms and so don’t survive the truncation. An alternative approach is to fine tune the magnetic field to be small. We derive the resulting differential condition that the hopping functions must satisfy, and show a continuum Dirac description in curved space with gauge field results which we derive non-linearly in the hopping functions. We consider whether mechanical effects might impose this fine tuning, but find this is not the case for a simple elastic membrane model.

THE LATTICE MODEL AND THE CONTINUUM

The tight-binding Hamiltonian for graphene is

\[ H = \sum_{n,\vec{x}} \left( t_{n,\vec{x}} + \frac{\alpha_n}{2} a_{\vec{x}A}^\dagger B_{\vec{x}B} + \text{h.c.} \right) \]  

where \( t_{n,\vec{x}} \) is the hopping strength in one of the lattice translation directions \( n, a_{\vec{x}A}^\dagger, b_{\vec{x}B}^\dagger \) are creation operators on the respective sublattices A and B and \( \alpha_n \) are the translations from site A to its neighbours, \( \vec{\ell}_1 = (\sqrt{3}/2,1/2), \vec{\ell}_2 = (-\sqrt{3}/2,1/2), \vec{\ell}_3 = -\vec{\ell}_1 - \vec{\ell}_2 \) where we have put in an explicit lattice spacing \( a \) (it is implicitly in the lattice coordinates as eg \( \vec{x}_A = a(\vec{m}A\vec{a}_1 + nA\vec{a}_2) \), \( \vec{a}_{1,2} = \vec{\ell}_{1,2} - \vec{\ell}_3 \)). Note that the \( t_n \) take values on the links, not the vertices. A general one-particle state is

\[ |\Psi(t)\rangle = \left( \sum_{\vec{y}_A} A_{\vec{y}_A}^\dagger(t)g_{\vec{y}_A} + \sum_{\vec{y}_B} B_{\vec{y}_B}^\dagger(t)g_{\vec{y}_B} \right) |0\rangle \]  

and the Schrödinger equation \( i\hbar \partial_t |\Psi\rangle = H |\Psi\rangle \) gives

\[ i\hbar \partial_t A_{\vec{x}A} = \sum_n t_{n,\vec{x}A} a_{\vec{x}A}^\dagger B_{\vec{x}B} + \text{h.c.} \]  
\[ i\hbar \partial_t B_{\vec{x}B} = \sum_n t_{n,\vec{x}B} a_{\vec{x}B}^\dagger A_{\vec{x}A} + \text{h.c.} \]  

Firstly we take the hopping parameters to slowly vary, so we may write, \( t_{n,\vec{x}} = t_n(\vec{x}) \) where \( t_n(\vec{x}) \) are smooth (so \( C^\infty \)) functions of the coordinates \( x^i = (x,y) \). We may then think of a continuum limit as we refine the lattice taking \( a \to 0 \). In order to derive this we write the lattice wavefunctions \( A, B \) in terms of slowly varying wavefunctions \( F,G \) and a rapidly oscillating phase \( \Phi(\vec{x})/a \),

\[ A_{\vec{x}}(t) = F(t,\vec{x})f(\vec{x})e^{i\frac{\Phi(\vec{x})+\phi(\vec{x})}{a}} \]  
\[ B_{\vec{x}}(t) = G(t,\vec{x})f(\vec{x})e^{i\frac{\Phi(\vec{x})-\phi(\vec{x})}{2a}} \]
where we assume the phases \( \Phi \) and \( \phi \), and rescaling function \( f \) are smooth functions of \( x^i \) and \( a \), so smooth in the continuum limit \( a \to 0 \). As we are interested in low energy states and the lattice theory is static, the only time dependence is seen in the slowly varying modulation functions \( F \) and \( G \). However at this stage we will not assume these are smooth in the \( a \to 0 \) limit, only that we may perform a gradient expansion in \( ad \). Now expanding in \( a \) we may write the Schrödinger equation as the continuum equation,

\[
\frac{i \hbar}{T} \gamma^a \partial_t \Psi = \gamma^a \left( u_a + i a z_a + a^2 r_a \right) \Psi - i a \gamma^a \left( w_a^i - i a q_a^i \right) \partial_i \Psi + \frac{a^2}{2} \gamma^a v_a^i \partial_i \partial_j \Psi + O(a^3) \tag{5}
\]

where \( \Psi = (F, G) \) is a complex spinor and we choose Dirac matrices \( \gamma^A = (\gamma^0, \gamma^a) = (-i \sigma^3, \sigma^1, \sigma^2) \). The quantities \( u_a, z_a, r_a, w_a^i, q_a^i, v_a^i \) are real and the ones we require here are,

\[
I^a u_a = \frac{2 i e^b \phi}{3 T} \sum_n e^{-i \phi_n} t_n, \quad I^a w_a^i = \frac{2 i e^b \phi}{3 T} \sum_n \delta_{n} e^{-i \phi_n} t_n, \quad I^a v_a^i = \frac{2 i e^b \phi}{3 T} \sum_n \delta_{n} e^{-i \phi_n} t_n, \quad I^a z_a = \frac{1}{2 \sqrt{f}} \partial_i \left( \frac{u_a x_i}{J^0} \right) \tag{6}
\]

with \( I^a = (1, i) \). We introduce the energy scale \( T \) and think of \( t_n(\vec{x}) = T \) as the undeformed model.

### Attempting to Truncate to Dirac

We will now truncate this continuum Schrödinger equation to first derivative order acting on \( \Psi \). We should be suspicious about whether such a truncation is valid, but for now we will interpret \( \Phi \) to order \( O(a) \) as a curved space Dirac equation coupled to a gauge field. We compose spacetime coordinates \( x^\mu = (t, x^i) \) and define the metric,

\[
d s^2 = g_{\mu \nu} dx^\mu dx^\nu = -v^2 dt^2 + g_{ij}(\vec{x}) dx^i dx^j \tag{7}
\]

Here \( v \) will be the Fermi velocity for the undeformed model, \( t_n(\vec{x}) = T \). This may be written in terms of a frame \( e^\mu_i \), and its dual \( e^\mu_A \), where,

\[
e^\mu_0 = \frac{1}{v}, \quad e^\mu_a = e^\mu_0 = 0, \quad g_{\mu \nu} = \eta_{AB} e^\mu_i e^\nu_j \tag{8}
\]

with \( \eta_{AB} = \text{diag}(-1, +1, +1) \). We fix

\[
f = \sqrt{\det e^\mu_i} = |g|^{1/4} \tag{9}
\]

which ensures that the \( U(1) \) charge density of the Dirac theory is that of the original electrons,

\[
J^0 = \sqrt{g} \Psi^\dagger \gamma^0 \Psi = (A, B)^\dagger \cdot (A, B) \tag{10}
\]

This is equivalent to ensuring the lattice anti-commutators \( \{a^\mu_{\tilde{x}}, a^\nu_{\tilde{y}}\} = \{\tilde{b}^\mu_{\tilde{x}}, \tilde{b}^\nu_{\tilde{y}}\} = \delta_{\tilde{x} \tilde{y}} \) imply the correct curved space anti-commutator \( \{\Psi^\dagger(\vec{x}), \Psi(\vec{y})\} = \frac{1}{\sqrt{f}} \delta^{(2)}(\vec{x} - \vec{y}) \).

Now the Schrödinger equation \( \Phi \), truncated to first derivatives on spinors, can be written as,

\[
a i e^a_i \gamma^a D_\mu \Psi = O(a^2) \tag{11}
\]

where we have taken \( v = 3 a T/(2 \hbar) \), and the covariant derivative is given in terms of a magnetic gauge field \( A_{\mu} = (0, A_i) \) and spin connection, parameterized here by the spatial 1-form \( \Omega_i \),

\[
D_i \Psi = \partial_i \Psi, \quad D_i \Psi = \left( \partial_i - i A_i + \frac{i}{2} \sigma_i \Omega_i \right) \Psi \tag{12}
\]

and the frame and gauge field to this order \( O(a) \) are,

\[
e^i_a = w^i_a, \quad A_i = -\frac{1}{a} e^i_a u_a \tag{13}
\]

Using the relations \( \Omega \) and our choice of \( f \) we find,

\[
\Omega^i = e_{ab} e^i_a \partial_j e^j_b \tag{14}
\]

which is precisely the torsion free spin connection that follows from the frame \( e^i_a \). While we might expect that in the absence of lattice defects torsion vanishes in a continuum description, it is pleasing to see this explicitly emerge.

We may understand the local freedom of shifting the phases of the two lattice fields \( A \) and \( B \) in equation \ref{eq:14} as a local frame rotation freedom,

\[
\phi \rightarrow \phi + \delta \phi \implies \left\{ \begin{array}{l}
e^i_a \rightarrow e^i_a - \delta \phi e_{ab} e^i_b \\
A_i \rightarrow A_i + \frac{i}{2} \sigma_i \partial_j \delta \phi
\end{array} \right. \tag{15}
\]

for an infinitesimal \( \delta \phi \), together with a local gauge transform on the vector \( A_a = e^i_a A_i \),

\[
\Phi \rightarrow \Phi + \delta \Phi \implies \left\{ \begin{array}{l}
A_a \rightarrow A_a - \frac{1}{a} \partial_\nu e^\nu_a \\
e^i_a \rightarrow e^i_a - v^i_j \partial_j \delta \Phi
\end{array} \right. \tag{16}
\]

for infinitesimal \( \delta \Phi \).

Now we ask whether this truncation to first derivatives can be generally valid. We argue that for generic \( t_n \) it is not, as contributions from the Dirac terms come at the same order as those from higher derivative terms in equation \ref{eq:11}. This may be seen in two ways;

- The gauge field in equation \ref{eq:14} goes as \( A_i \sim 1/a \). The spinor \( \Psi \) responding to this will then generally have variation on scales that vanish as \( a \to 0 \), hence ruining the gradient expansion. We will discuss this explicitly for perturbative deformations.

- The local phase symmetry in \ref{eq:16} is a gauge transformation for \( A_a \), but \( e^i_a \) transforms too and this is inconsistent with its interpretation as a frame which should be invariant.
On the latter issue there should be a continuum formulation of \( \delta \) written to manifest these local symmetries where the derivative expansion will be in covariant derivatives with respect to the gauge and frame symmetry. Consider a putative two derivative term to match that in \( \delta \). It will have the form \( a^2 \gamma^a v_a^{ij} \bar{D}_i \bar{D}_j \Psi \) where \( \bar{D}_i \) are covariant. Note that their gauge and spin connections need not be the same as those of the leading Dirac theory. However, by taking the gauge field to scale as \( \sim 1/a \) then we see this term contains a contribution,

\[
a^2 \frac{\gamma^a v_a^{ij} \bar{D}_i \bar{D}_j \Psi}{2} \leftrightarrow -ia^2 \gamma^a v_a^{ij} B_i \partial_j \Psi
\]  

(17)

for some gauge connection \( B_i \). Then \( \delta \) gains a new term, \( w_a^i = e_a^i + av_a^{ij} B_j \), and now if \( B_i \) transforms as \( v_a^{ij} B_i \rightarrow v_a^{ij} B_j - \frac{1}{a} v_a^{ij} \partial_j \Phi \), then we indeed see that \( e_a^i \) is invariant with \( B_i \) accounting for the transformation of \( w_a^i \). However, then the gauge fields mix the contribution of covariant derivative terms between the partial derivative orders.

**TWO TRUNCATIONS TO DIRAC**

In order to give a consistent truncation of our theory to the leading Dirac term we must tame the lattice scale gauge field by requiring \( aA_i \rightarrow 0 \) as \( a \rightarrow 0 \). There are two approaches.

**Perturbative deformation**

The lattice scale of the gauge field has been previously emphasised in \( \delta \). In the derivation of curved space Dirac of \( \delta \) and following work this was addressed using a perturbative expansion where,

\[
t_n = T(1 + \epsilon \delta t_n)
\]  

(18)

with \( |\epsilon| \ll 1 \). Let us expand about the K Dirac point,

\[
\Phi = \frac{4\pi}{3\sqrt{3}} x + \epsilon \chi(x).
\]  

(19)

The gauge field is then,

\[
A_i = -\frac{\epsilon}{a} \left( \frac{2}{3} \sum_n \epsilon_{ij} \delta_{n}^i \partial_{n} \delta_{n}^j + \partial_i \chi \right)
\]  

(20)

and we see \( \chi(x) \) parameterizes the gauge freedom. While this goes as \( \sim 1/a \), the perturbative expansion in \( \epsilon \) controls this. The geometry depends on this gauge, the frame leading to the metric,

\[
g_{ij} = \delta_{ij} - \frac{4}{3} \epsilon \sum_n (\delta_{n}^i \delta_{n}^j + \epsilon K^{ijk} \epsilon^{kl} \partial_l \chi)
\]  

(21)

which has Ricci scalar curvature

\[
R = \frac{4}{3} \sum_n (\delta_{ij} - \delta_{n}^i \delta_{n}^j) \partial_i \partial_j \delta_n + \epsilon K^{ijk} \epsilon^{kl} \partial_i \partial_j \partial_l \chi
\]  

(22)

where we have defined \( K^{ijk} = -\frac{4}{3} \sum_n \ell_{n}^i \ell_{n}^j \ell_{n}^k \). Taking the \( K' \) Dirac point corresponds to taking \( \Phi \rightarrow -\Phi \), \( e_a^i \rightarrow -e_a^i \) and \( A_i \rightarrow -A_i \), and the metric is invariant. For \( \chi = 0 \) these reproduce the results of \( \delta \) (when we consider the physical metric, rather than the Weyl rescaled one \( \delta \)). Previously these results have been taken to show the perturbatively deformed tight binding model is described by a curved space Dirac equation. However we explicitly see here the gauge freedom \( \chi \) gives a physical contribution to the curvature. Noting that 2-d geometry is locally characterized by the Ricci scalar, in fact we can then choose any geometry, including a flat one, with an appropriate gauge choice \( \chi \). The second concerning feature highlighted in \( \delta \) is that while we have controlled \( A_i \sim \epsilon/a \), we have done this at the cost of the spin connection being parametrically smaller, \( \Omega_i \sim \epsilon \), as \( a \rightarrow 0 \). There they posit that the spin connection should be ignored, and one has only a varying frame and gauge field.

Here we argue the previous discussions are incorrect, and this perturbative deformation is only consistent taking a flat unperturbed frame. We will show in the simplest example that the corrections to the frame have the same order as the two derivative term. Consider in some region of size \( L \) the perturbative deformation to be \( \phi = \chi = \delta t_3 = 0 \) and \( \delta t_1 = -\delta t_2 = x^2 \). This yields \( A_i = (0, \frac{2}{\pi L}, \frac{4\pi}{3\sqrt{3}} x) \), a Landau gauge magnetic field \( B = \frac{1}{\ell_B} \) with \( \ell_B = \sqrt{aL/\epsilon} \) the magnetic length which diverges as \( a \rightarrow 0 \) but may be parametrically larger than the lattice scale. At leading order \( O(\epsilon) \) and \( a \ll L \) this may be solved by Landau levels. Here we focus on the lowest level wavefunction, taking \( \Psi = \left( 0, e^{-\frac{x^2}{2\ell_B^2}}, \frac{4\pi}{3\sqrt{3}} x \right) \). Now we can evaluate the Dirac term on this leading solution and compare this to the two derivative term. Then at \( O(\epsilon) \) we have \( v_a^{ij} = \frac{\epsilon}{2L} \delta_{a}^{ij} K^{kmn} \epsilon_{mnj} \), and find,

\[
\imath a e_a^i \gamma^a \nabla_i \Psi = -\frac{\imath a e}{4L} \gamma^1 \Psi, \quad \gamma^2 \gamma^a v_a^{ij} \partial_i \partial_j \Psi = -\frac{\imath a e}{2L} \gamma^1 \Psi
\]  

(23)

so both go as \( \sim \epsilon c/L \). We emphasize that the Dirac term is non-zero here due to the varying frame at \( O(\epsilon) \). Thus this simple example demonstrates that the perturbative contribution to the frame in the Dirac term is the same order as higher derivative terms, and it is therefore inconsistent to consider it in isolation.

We note it is consistent to truncate to Dirac if we ignore corrections to the frame as then for \( a \ll L \) these terms are small corrections to the flat gauged Dirac term.

**Fine tuning**

In order to preserve curvature we are forced to fine tune the gauge field so that \( aA_i \rightarrow 0 \) as \( a \rightarrow 0 \), which implies the condition \( u_a \rightarrow 0 \) in this limit. The condition
A natural choice of lattice phase is then just a translation in momentum space \( \vec{k} \to \vec{k} - \vec{K}/a \), via \( \Phi = \vec{k} \cdot \vec{x} \). In the inhomogeneous case we can define a spatially varying wavevector \( \vec{K}(\vec{x}) \) by using exactly the same expression as for the homogeneous case, but now with spatially varying \( t_n(\vec{x}) \). Calculating the curl of this vector we find

\[
F_{xy} = \partial_x A_y - \partial_y A_x = \frac{1}{a} (\partial_x K_y - \partial_y K_x)
\]

so up to a gauge transformation then \( K_i/a \) gives the gauge field \( A_i \). The condition (24) is the requirement that \( \nabla \times \vec{K} \) vanishes to leading order, yielding a finite magnetic field as \( a \to 0 \).

**FINE TUNING AND EMBEDDING**

Can this fine tuning of equation (25) arise from mechanical considerations? Consider an almost flat embedding into \( \mathbb{R}^3 \) with coordinates \( (X^i, Z) \) given by,

\[
X^i = x^i + e v^i(\vec{x}) \quad , \quad Z = \sqrt{\epsilon} h(\vec{x})
\]

with height function \( h \) and strain field \( v^i \). Linearizing in \( \epsilon \) the induced metric of this embedding is,

\[
g_{ij}^{(\text{ind})} = \delta_{ij} + 2 \epsilon \sigma_{ij} \quad , \quad \sigma_{ij} = \frac{1}{2} (\partial_i v_j + \partial_j v_i + \partial_i h \partial_j h)
\]

with indices lowered/raised using \( \delta_{ij} \) and \( \sigma_{ij} \) is the strain tensor. Assuming the hopping parameters depend on bond length and not angle \( \ell_n \), then to \( O(\epsilon) \),

\[
t_n \approx T \left( 1 - \epsilon \beta \sigma_{ij} \ell_i^a \ell_j^a \right)
\]

where \( \beta \) can be estimated for graphene as \( \beta \approx 3.3 \) \( [28] \). We may neatly express our fine-tuning condition (26) as,

\[
K^{ij} \partial_k \sigma_{ij} = 0
\]

Consider the canonical elastic energy,

\[
E_{\text{mech}} = \int d^2 \vec{x} \left( \frac{\kappa}{2} \beta^2 h^2 + \mu \sigma_{ij}^2 + \frac{\lambda}{2} \sigma_{ij}^2 \right)
\]

with bending rigidity \( \kappa \) and Lamé coefficients \( \mu \) and \( \lambda \). Varying the strain field \( v^i \) yields, \( \mu \partial_i \sigma_{ij} + \frac{\lambda}{2} \partial_i \sigma_{ij} = 0 \). Assuming \( \mu, \lambda > 0 \) then this is generally incompatible with the previous fine tuning condition. Thus this membrane energetics does not impose the necessary constraint on strain for a curved space Dirac description.

In the event that the constraint is satisfied the perturbation to the electrometric is \( g_{ij} \approx \delta_{ij} + 2 \epsilon \beta \sigma_{ij} \). As emphasized in \( \{10, 22\} \) this is not the same as the induced metric in equation (33). Non-perturbatively the \( t_n(\vec{x}) \) will be a functional of the induced metric \( g_{ij}^{(\text{ind})}(\vec{x}) \), and the map to the electrometric is given by equation (25).

**CONCLUSION**

We have argued that contrary to previous assertions such as \( \{7\} \), the tight binding model with generic slow
variation of the hopping functions does not have a curved space Dirac description coupled to a gauge field. We find a continuum spinor description, but this is generally obstructed from truncating to first spinor derivatives by large magnetic fields. Making the $t_n$ vary perturbatively cannot solve this, although it does allow a consistent flat space gauged Dirac description. Thus we argue the spatial variation of the Fermi light cone is generically irrelevant. One may obtain a curved space Dirac description if one fine tunes the variation of the hopping functions. However this fine tuning appears unnatural and we have shown simple membrane energetics will not impose it. Thus we believe it is unlikely that elastically deformed graphene monolayers have a curved space Dirac description. Likewise, optical lattice constructions of graphene-graphene monolayers have a curved space Dirac description. Thus we believe it is unlikely that elastically deformed graphene monolayers have a curved space Dirac description.

Acknowledgments

This work was supported by STFC Consolidated Grant ST/T000791/1.

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