Generalized Dirac structure beyond the linear regime in graphene

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Abstract

A generalized Dirac structure survives beyond the linear regime of the low-energy dispersion relations of graphene. The corresponding emergent field theory is a table-top realization of specific quantum gravity scenarios with a fundamental minimal length, whose role here is played by graphene lattice spacing. A generalized uncertainty principle of the kind compatible with this scenario is also obtained. Finally, we emphasize how this set up naturally points to certain Lorentz-violating field theories.

Keywords: Quantum Gravity Phenomenology, Generalized Uncertainty Principle, Minimal length, Graphene

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I. INTRODUCTION

Graphene is popular among high energy theorists because, at small energies, its electronic transport properties are in many respects those of a free gas of massless particles, as theoretically discovered in [1] and experimentally proved in [2]. Indeed, the dynamics of the \( \pi \) electrons of flat, unstrained, defects-free, monolayer graphene membranes, for energies up to \( \sim 3 \text{eV} \) above and below the Dirac point, is governed at a high level of accuracy by the Hamiltonian of a massless, Dirac, (2+1)-dimensional field, hence linear in the momentum, but propagating at \( v_F \sim c/300 \) rather than at \( c \) (on this see, e.g., the review [3]).

It is important for high energy theory to have found here this special relativistic-like behavior, as it gives us the opportunity to study elusive phenomena through table top experiments. Nonetheless, what is more urgent is to test theories beyond special relativity, something difficult (sometimes impossible) to do in direct experiments. The use of graphene to this latter end was proposed in [4], and elaborated in follow-up works, see, e.g., [5–8] and the review [9].

Those works rely on the linear regime of the Dirac description, hence are valid at small energies, and when curvature is considered, the energies need to be even smaller [9]. Here we move in the opposite direction, namely, we investigate what happens to the Dirac structure in a range of energy beyond the \( \pm 3 \text{eV} \). In fact, it is generally believed that already at the next step beyond the linear regime, since the standard Dirac structure is gone, with it goes also the usefulness of graphene as a lab for fundamental theories.

We show here that this is not the case, because a Dirac structure, although of a generalized kind, is present beyond the linear approximation, and it is of the kind obtained earlier in the research about generalized uncertainty principles (GUPs) [10–13] descending from quantum gravity scenarios with a fundamental minimal length (for a review see [14]). These recently proposed GUPs differ considerably from other GUPs in the literature, see, e.g. [15], and the latter GUPs would not apply here. The recent proposal is also consistent with doubly special relativity (DSR) [14], where there exists a maximum energy scale, that is the Planck energy. At that scale the smooth manifold structure of spacetime breaks down, along with the local Lorentz invariance. In graphene as well there is a maximum energy scale, at which lattice effects break the smooth manifold description. This motivates our present investigation.
FIG. 1. The honeycomb lattice of carbons making graphene. The two Bravais sublattices, $L_A$ and $L_B$, are identified by different colors (green and yellow). The three vectors connecting nearest neighbors are explicitly shown, $\vec{s}_1^{(1)} = \ell(0, -1)$, $\vec{s}_2^{(1)} = \frac{\ell}{2}(\sqrt{3}, 1)$, $\vec{s}_3^{(1)} = \frac{\ell}{2}(-\sqrt{3}, 1)$ with $\ell \approx 1.42 \text{Å}$ the carbon-to-carbon distance, whereas only one representative per $m$ of the $\vec{s}_i^{(m)}$s, till $m = 6$, is shown, along with the corresponding circle encompassing all the relevant atoms. When the color of the circle is the same of (different from) the color of the atom in the center, yellow here, the corresponding terms contribute to the diagonal (off-diagonal) part of the Hamiltonian. The less intense the color of the circle, the less important the associated terms (not is scale). The $\vec{s}_i^{(m)}$s can be expressed in terms of the $\vec{s}_i^{(1)}$, as shown in the Appendix A for $m = 2, \ldots, 6$.

II. BEYOND LINEAR APPROXIMATION AND GENERALIZED DIRAC

The honeycomb lattice in Figure 1 has two atoms per unit cell, what makes the lattice two interpenetrating Bravais lattices. The quantum state associated to such configuration is

$$|\Phi_{\vec{k}}\rangle = a_{\vec{k}}|\varphi^A_{\vec{k}}\rangle + b_{\vec{k}}|\varphi^B_{\vec{k}}\rangle$$

(1)

where $\vec{k}$ labels the crystal quasi-momentum, $a_{\vec{k}}$ and $b_{\vec{k}}$ are complex functions, and $\varphi^I_{\vec{k}}(\vec{r}) = \langle \vec{r} | \varphi^I_{\vec{k}} \rangle = e^{i\vec{k} \cdot \vec{r}} \varphi^I(\vec{r})$, with $I = A, B$, are Block functions, with periodic orbital wave-functions $\varphi^I(\vec{r})$ localized at the sites of the Bravais sublattices, either $L_A$ or $L_B$. That means that the shape of the functions $\varphi^A$ and $\varphi^B$ is the same, but the support is shifted. This localization is the key ingredient of the tight binding approximation: the more the $\varphi^I(\vec{r})$ are localized, the more accurate is the approximation (see, e.g., [16]). Our goal now is to find the effective Hamiltonian that gives a good approximation of the graphene dispersion relations $E(\vec{k})$. 
From the Schrödinger equation $\hat{H}_k|\Phi_k\rangle = E(k)|\Phi_k\rangle$, multiplied from the left by $|\Phi_k\rangle$, and with $1 = \int d^2r |r\rangle\langle r|$ inserted, we have

$$\mathcal{H}_k = \langle \Phi_k | \hat{H}_k | \Phi_k \rangle = \int d^2r d^2r' \langle \Phi_k | r \rangle \langle r | \hat{H}_k | r' \rangle \langle r' | \Phi_k \rangle$$

(2)

where $\mathcal{H}_k$ is the $k$ component of a “field Hamiltonian”, that is the one that includes the wave functions. Now, we rewrite the overall interaction has sum of interactions between subsequent orders of neighbors, (including all orders this is merely a rewriting, with no approximation). Therefore, in (2) we shall use $|r\rangle = |r + s_i^{(m)}\rangle$, where the vectors $s_i^{(m)}$ join $m^{th}$-near neighbors, as indicated in Figure 1. With this the Hamiltonian splits into an onsite orbital part and an interaction potential $\langle r | \hat{H}_k | r + s_i^{(m)} \rangle \rightarrow H^{(0)}_k(r, r) + V^{(m)}_k(|r - r|)$, where $r - r = s_i^{(m)}$.

The $s_i^{(m)}$s, for any $m$ can be obtained from the $s_i^{(1)}$s that we give in caption of Figure 1 and in the Appendix A (there along with $s_i^{(m)}$s for $m = 2, ..., 6$). $V^{(m)}_k$ is the potential between atoms located at distance $|s_i^{(m)}| \equiv |s^{(m)}|$, $\forall i = 1, ..., n_m$ (in the ideal case of a perfect lattice), while $H^{(0)}_k$ is the Hamiltonian whose eigenfunctions are the orbitals $\varphi^f(r)$ with corresponding eigenvalues $\epsilon^{(0)}$ that is the onsite energy.

Putting together all this, the field Hamiltonian (2) becomes

$$\mathcal{H}_k = \sum_{m \in \text{diag}} (\epsilon^{(0)} s_m + \eta_m) \mathcal{F}_m(k)(a_k^* a_k + b_k^* b_k) + \left( \sum_{m \in \text{off}} (\epsilon^{(0)} s_m + \eta_m) \mathcal{F}_m^*(k) a_k^* b_k + \text{h.c.} \right)$$

(3)

where $s_m = \int d^2r \varphi^I(r) \varphi^J(r + s_i^{(m)})$ and $\eta_m = \int d^2r \varphi^I(r) V^{(m)} \varphi^J(r + s_i^{(m)})$ are the overlapping and the hopping parameters, respectively, and the $m$'s contribute to the diagonal terms when $I = J$, and to the off-diagonal terms when $I \neq J$. Finally $\mathcal{F}_m(k) \equiv \sum_{i=1}^{n_m} e^{ik \cdot s_i^{(m)}}$, where

$$\mathcal{F}_1 = \sum_{i=1}^{3} e^{ik \cdot s_i^{(1)}} = e^{-ik_x} \left[ 1 + 2e^{i2\ell k_y} \cos \left( \frac{\sqrt{3}}{2} \ell k_z \right) \right]$$

(4)

and $\mathcal{F}_2 = |\mathcal{F}_1|^2 - 3$. More details on the derivation of (3) and on the $\mathcal{F}_m$s are in the Appendix A.

By setting the zero of $E(k)$ by $\epsilon^{(0)}$ the Schrödinger equation becomes (see Appendix A)

$$\psi_k^+ \hat{H}_k \psi_k = E(k) \psi_k^+ \hat{S}_k \psi_k$$

(5)
where $\psi^\dagger_k \equiv (a^\dagger_k, b^\dagger_k)$ and

$$\hat{H}_k = \begin{pmatrix} h_k^{\text{diag}} & h_k^{\text{off}} \\ h_k^{\text{off}} & h_k^{\text{diag}} \end{pmatrix}$$

and

$$\hat{S}_k = \begin{pmatrix} S_k^{\text{diag}} & S_k^{\text{off}} \\ S_k^{\text{off}} & S_k^{\text{diag}} \end{pmatrix}$$

are the Hamiltonian and the overlapping matrices respectively, with

$$h_k^{\text{diag}} = \sum_{m \in \text{diag}} \eta_m(s_m) F_m(k),$$

and

$$h_k^{\text{off}} = \sum_{m \in \text{off}} \eta_m(s_m) F_m(k).$$

Notice that

$$\hat{H}_k = h_k^{\text{diag}} \mathbf{1}_2 + \text{Re} h_k^{\text{off}} \sigma_x + \text{Im} h_k^{\text{off}} \sigma_y,$$

with

$$\mathbf{1}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$ Clearly the concurrence of a) two atoms per unit cell (doublet structure) and of b) the Hermiticity of the Hamiltonian are behind the emergence of the Pauli matrices. Nonetheless this is not enough to have a Dirac structure, as we need to focus on the dispersion relations descending from (5), that is the two solutions to the secular equation $\det(\hat{H}_k - E\hat{S}_k) = 0$ that gives an involved expression in terms of the $F_m$s, and in general there is no Dirac structure behind such dispersion relations. In fact, the values of both, the overlapping and the hopping parameters, $s_m$ and $\eta_m$, respectively, exponentially drop with $m$, as should be expected. Although there is no absolute consensus on the actual values of these phenomenological parameters, as their definition might differ depending on the model, there is general agreement on the fact that, in the ideal case of an infinite and non-deformed sheet of graphene, the values of the first few of such parameters are (see, e.g., [17] and references therein)

$$\eta_0 \simeq -0.36\text{eV}, \eta_1 \simeq -2.8\text{eV}, \eta_2 \simeq 0.12\text{eV},$$

$$s_1 \simeq 0.106, s_2 \simeq 0.001$$

from which we see that stopping at $\eta_2$ and $s_1$ is a very good approximation. Once this happens, the secular equation gives dispersion relations fully in terms of one single function $F_1$

$$E_\pm = \left(1 - s_1^2 |F_1|^2\right)^{-1} \times \left(\epsilon_0 - \epsilon_1 |F_1|^2 \pm \sqrt{(\epsilon_0 - \epsilon_1 |F_1|^2)^2 - (1 - s_1^2 |F_1|^2)(\epsilon_0 + \eta_2 |F_1|^2)^2 - \eta_1^2 |F_1|^2}\right)$$

(8)
where \( \epsilon_0 \equiv \eta_0 - 3\eta_2 \) and \( \epsilon_1 \equiv \varsigma_1\eta_1 - \eta_2 \).

Notice that at the Dirac points\(^1\), i.e. the solutions of \( \mathcal{F}_1(\vec{k}) = 0 \), \( \vec{K}_1 = \left( \frac{4\pi}{3\sqrt{3}\ell}, 0 \right) \) and \( \vec{K}_2 = \left( -\frac{4\pi}{3\sqrt{3}\ell}, 0 \right) \), we have \( E_{\pm}|_{\mathcal{F}_1=0} = \epsilon_0 \), that is the shift of the zero of the energy due to diagonal terms in the Hamiltonian. We can shift once more the zero of the energy, hence dropping this \( \epsilon_0 \) but shifting all other values accordingly, in particular \( \epsilon_1 \rightarrow \epsilon'_1 \equiv \epsilon_1 - \epsilon_0 \).

Thus, finally, dropping higher order terms \( O(\varsigma_1^2) \) and \( O(\varsigma_1\eta_2) \), we have

\[
E_{\pm} = \eta_1 \left( \pm |\mathcal{F}_1| - \tilde{A}|\mathcal{F}_1|^2 \right)
\]

(9)

where \( \tilde{A} = \epsilon'_1/\eta_1 \) is a dimensionless parameter. If we define the dimensionless vector \( \vec{P} \equiv (R\mathcal{F}_1, I\mathcal{F}_1) \) then

\[
E_{\pm} = \eta_1 \left[ \pm \frac{\hbar}{\hbar/\ell} |\vec{P}| - \tilde{A} \left( \frac{\hbar}{\hbar/\ell} \right)^2 |\vec{P}|^2 \right]
\]

(10)

\[
\equiv V_F \left( \pm |\vec{P}| - A |\vec{P}|^2 \right)
\]

(11)

where \( \vec{P} \equiv (h/\ell)\vec{P}, \ A \equiv (\ell/\hbar)\tilde{A}, \ V_F \equiv \eta_1\ell/h \) are the dimension-full quantities (recall that\(^3\) \( v_F \approx 1.5\eta_1\ell/h \)).

Henceforth, considering \( \vec{P} \) as a momentum, we can use the customary Dirac prescription \( |\vec{P}| \rightarrow \vec{\sigma} \cdot \vec{P} \) that gives

\[
H \equiv \sum_{\vec{k}} \mathcal{H}_{\vec{k}} = V_F \sum_{\vec{k}} \psi^\dagger_{\vec{k}} \begin{pmatrix} P - A & P \ P \ P \end{pmatrix} \psi_{\vec{k}}
\]

(12)

as the effective Hamiltonian corresponding to the dispersion relations \( |\vec{P}| \rightarrow \vec{\sigma} \cdot \vec{P} \) and we used the properties of the Pauli matrices, \( \sigma_i\sigma_j = \delta_{ij}1_2 + i\epsilon_{ijk}\sigma^k \), that give \( \vec{P} \vec{P} = |\vec{P}|^2 1_2 \). This is precisely the form of the Hamiltonian obtained earlier when generalizing the Dirac Hamiltonian to allow for a GUP with a minimal fundamental length \([11,13]\), here clearly given by the carbon to carbon distance \( \ell \). To see this we just need to introduce a “high energy momentum”

\[
\vec{Q} \equiv \vec{P}(1 - A|\vec{P}|)
\]

(13)

that clearly gives \( H = V_F\vec{Q} \) as the effective Hamiltonian governing the physics of graphene within a range of energies much wider than the one where the linear approximation holds.

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\(^1\) In this paper, since no defects, nor deformations of the membrane are considered, we can safely focus on a single Dirac point, say \( \vec{K}_1 \equiv \vec{K}_D \). This we do from now on.
Here the Lorentz (rotation) symmetric structure is preserved by construction by both expressions for $H$. Although Lorentz invariant, the structure for $A \neq 0$ exhibits a particle-antiparticle (electron-hole) asymmetry, that would correspond to the matter-antimatter asymmetry in the quantum gravity scenarios.

On the other hand, when $[x_i, P_j] = i \hbar \delta_{ij}$ then

$$[x_i, Q_j] = i \hbar \left[ \delta_{ij} - A \left( Q \delta_{ij} + \frac{Q_i Q_j}{Q} \right) \right]$$

as is easily seen by following [11–13], and Lorentz violating terms $\frac{Q_i Q_j}{Q}$ appear.

### III. LOW-ENERGY MAPPING

Let us now make contact with the standard Dirac picture of graphene. This means to express $P_i$, therefore $\mathcal{F}_1(\vec{k})$ in (4), in terms of $p_i$, where $\vec{k} = \vec{K}^D + \vec{p}$. In fact, the structure in (12) is only apparently $O(\ell)$, because $\vec{P}$, as it stands, contains all orders in $\ell$.

The expansion gives the following dispersion relations, up to $O(p^3)$ (see (11))

$$E_{\pm} = V_F \left( \pm \frac{3}{2} p^2 + \frac{3}{8} \ell p^2 \cos(3\theta) \mp \frac{3}{64} \ell^2 p^3 \cos^2(3\theta) \right. \left. - A \left( \frac{9}{8} p^2 + \frac{9}{8} \ell p^3 \cos(3\theta) \right) \right)$$

$$= v_F \left( \pm \frac{3}{2} p^2 + \frac{3}{4} \ell p^2 \cos(3\theta) \mp \frac{3}{32} \ell^2 p^3 \cos^2(3\theta) \right. \left. - \frac{3}{2} \ell \epsilon_{11} \left( \frac{3}{2} \eta_1 \right) p^2 + \frac{3}{2} \ell \epsilon_{11} \left( \frac{3}{2} \eta_1 \right) p^3 \cos(3\theta) \right), \quad (15)$$

where $p = |\vec{p}|$, $\tan \theta = p_y/p_x$, $v_F \equiv 3/2V_F$, and $\hbar = 1$.

Lorentz violating terms appear in the dispersion relation (15). We stress here that, as customary in Lorentz violating scenarios (see, e.g, [18, 19]), the orientation of the vectors is important. Here all vectors will be referred to the honeycomb lattice orientation, and it is very important to mention explicitly our axis choice, which is as shown in Figure 1.

Accordingly the corresponding $O(p^3)$ Hamiltonian is

$$H = v_F \sum_{\vec{p}} \psi_{\vec{p}}^\dagger \left[ \begin{array}{c} \sigma_x \left( p_x - \frac{\ell}{4} (p_x^2 - p_y^2) - \frac{\ell^2}{8} p_x (p_x^2 + p_y^2) \right) \\
\sigma_y \left( p_y + \frac{\ell}{2} p_x p_y - \frac{\ell^2}{8} p_y (p_x^2 + p_y^2) \right) \\
- \frac{3}{2} \ell \epsilon_{11} \left( \frac{3}{2} \eta_1 \right) \left( p_x^2 + p_y^2 \mp \frac{\ell^2}{8} p_x^3 + \frac{3}{2} p_x^2 p_y^2 \right) \end{array} \right] \psi_{\vec{p}}$$

$$= v_F \sum_{\vec{p}} \psi_{\vec{p}}^\dagger \left[ \begin{array}{c} \sigma_x \left( p_x - \frac{\ell}{4} (p_x^2 - p_y^2) - \frac{\ell^2}{8} p_x (p_x^2 + p_y^2) \right) \\
\sigma_y \left( p_y + \frac{\ell}{2} p_x p_y - \frac{\ell^2}{8} p_y (p_x^2 + p_y^2) \right) \\
- \frac{3}{2} \ell \epsilon_{11} \left( \frac{3}{2} \eta_1 \right) \left( p_x^2 + p_y^2 \mp \frac{\ell^2}{8} p_x^3 + \frac{3}{2} p_x^2 p_y^2 \right) \end{array} \right] \psi_{\vec{p}}$$

(16)
FIG. 2. In order to see clearly the non-isotropic effect of the transformation, we plot the mapping $P \rightarrow p$ giving in (17) acting on a circle of radius $1.0 \times 10^{-10}$ m$^{-1}$ in the momenta space up to order $O(\ell )$, where $\ell = 1\text{Å}$.

whose structure would hardly induce to think of any Dirac structure, although, as shown in the previous part, in fact it is just a low energy realization of a generalized Dirac structure.

Let us express the expansion of $\vec{P}$ in terms of $\vec{p}$ as follows $\vec{P} = \vec{p} + \Delta \vec{p}$, where

$$
\Delta \vec{p} = \frac{\ell}{4} \left( p_y^2 - p_x^2 - \frac{\ell}{2} p_x (p_x^2 + p_y^2), 2p_x p_y - \frac{\ell}{2} p_y (p_x^2 + p_y^2) \right) = \frac{\ell}{4} p^2 (-\cos 2\theta - \frac{\ell}{2} p \cos \theta, \sin 2\theta - \frac{\ell}{2} p \sin \theta),
$$

(17)

We can visualize this as transformation acting on the whole momenta plane, as plotted in Figure 2 where we show the mapping $\vec{P} \rightarrow \vec{p}$ for a circle of radius $1.0 \times 10^{-10}$ m$^{-1}$ ($\ell = 1\text{Å}$).

Of course, in order to obtain the operator expression for $H$ in (16), one needs to perform the customary substitution $p_i \rightarrow -i\partial / \partial x_i$.

Finally, after the expansion, the commutation relations one has to write are obtained by first noticing that now $[x_i, P_j] \neq i\delta_{ij}$, because the role of the low energy momentum is now played by $\vec{p}$ and not by $\vec{P}$ ($[x_i, p_j] = i\delta_{ij}$). Then, with the help of $[x_i, P_j]$ and using (13), the commutations of the system are $[x_i, Q_j]$ fully expressed in terms of $Q_i$ (see details in Appendix B). The actual structure changes according to the order $O(\ell^n)$. For instance, to
$O(\ell),$ 

$$[x, Q_x] = i \left( 1 - \frac{\ell}{2} Q_x - \frac{\ell \epsilon_1}{\eta_1} \left( |\vec{Q}| + \frac{Q_x^2}{|\vec{Q}|} \right) \right),$$

$$[x, Q_y] = i \left( \frac{\ell}{2} Q_y - \frac{\ell \epsilon_1}{\eta_1} |\vec{Q}| Q_x Q_y \right),$$

$$[y, Q_x] = i \left( \frac{\ell}{2} Q_y - \frac{\ell \epsilon_1}{\eta_1} |\vec{Q}| Q_x Q_y \right),$$

$$[y, Q_y] = \left( 1 + \frac{\ell}{2} Q_x - \frac{\ell \epsilon_1}{\eta_1} \left( |\vec{Q}| + \frac{Q_y^2}{|\vec{Q}|} \right) \right).$$

In the Appendix B we give the result up to order $O(\ell^2).$

IV. CONCLUSIONS

This work proposes graphene as an indirect experimental realization of certain quantum gravity scenarios. In particular those that see emergent continuous fields and continuous spacetimes as stemming from a granular underlying structure. Indeed, we were able to very naturally reproduce the GUP of [11–13], hence the quantum gravity scenario with a fundamental scale [14], including the particle/hole asymmetry corresponding to matter/anti-matter asymmetry and the non-isotropic trigonal warping terms related to Lorentz violation, similar to those of Kostelecky Standard Model Extension (SME) [20–22] (here the fundamental length is the carbon-to-carbon distance $\ell_{\text{Planck}} \rightarrow \ell$). The anisotropy of the continuous field theory for graphene was seen in [7], and anisotropy of the universe has been observed, and called “the axis of evil” [23][24].

It is known that exotic phenomena, like the Klein Paradox [25], the fractional quantum hall effect [26][27], and even Hawking-Unruh phenomena [5][6] may occur in graphene. These studies are based on the low energy Dirac structure. Therefore, it is a natural direction to pursue to analyze the impact of this type of GUP-deformed Dirac structure on the above. Among those, cosmology within the Jacobson thermodynamic formalism, where it is possible to incorporate the effects of GUP [28][29].

Notice that our theoretical considerations do not require potentially difficult dedicated experiments. On the contrary, they simply require that we look at the higher order contributions to the dispersion relations for the simplest graphene setting of all. Indeed, this scenario
is pointing to flat spacetime that, in this respect, is not less interesting and non-trivial than other geometries.

Finally, let us mention that there are other materials that exhibit emergent pseudo-relativistic fermions [30, 31], and it would be interesting to perform a similar study for these materials.

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Appendix A: Structure of the \( m \)-nearest neighbor Hamiltonian

Here we give some more details of the construction leading to the tight binding Hamiltonian in general, focussing on the structure

Let us start by listing the \( \vec{s}_i^{(m)} \) ‘s vectors up to \( m = 6 \). First, the onsite \( \vec{r}' = \vec{r} \) vector is clearly zero, \( \vec{s}^{(0)} = 0 \). Then, the nearest neighbor vectors, \( \vec{s}_i^{(1)} \), \( i = 1, 2, 3 \), are

\[
\vec{s}_1^{(1)} = \ell(0, -1), \quad \vec{s}_2^{(1)} = \frac{\ell}{2}(\sqrt{3}, 1), \quad \vec{s}_3^{(1)} = \frac{\ell}{2}(-\sqrt{3}, 1)
\]

with \( \ell \approx 1.42 \text{Å} \) the carbon-to-carbon distance. The next to nearest neighbor vectors, \( \vec{s}_i^{(2)} \), \( i = 1, \ldots, 6 \), are

\[
\begin{align*}
\vec{s}_1^{(2)} &= \vec{s}_2^{(1)} - \vec{s}_3^{(1)}, & \vec{s}_2^{(2)} &= \vec{s}_2^{(1)} - \vec{s}_1^{(1)}, & \vec{s}_3^{(2)} &= \vec{s}_3^{(1)} - \vec{s}_1^{(1)}, \\
\vec{s}_4^{(2)} &= -\vec{s}_1^{(2)}, & \vec{s}_5^{(2)} &= -\vec{s}_2^{(2)}, & \vec{s}_6^{(2)} &= -\vec{s}_3^{(2)}.
\end{align*}
\]

The 3\textsuperscript{rd}-nearest neighbor vectors, \( \vec{s}_i^{(3)} \), \( i = 1, 2, 3 \), are

\[
\begin{align*}
\vec{s}_1^{(3)} &= \vec{s}_1^{(2)} + \vec{s}_1^{(1)}, & \vec{s}_2^{(3)} &= -\vec{s}_2^{(2)} + \vec{s}_3^{(1)}, & \vec{s}_3^{(3)} &= \vec{s}_3^{(2)} - \vec{s}_1^{(1)}.
\end{align*}
\]

The 4\textsuperscript{th}-nearest neighbor vectors, \( \vec{s}_i^{(4)} \), \( i = 1, \ldots, 6 \), are

\[
\begin{align*}
\vec{s}_1^{(4)} &= \vec{s}_1^{(2)} + \vec{s}_2^{(1)}, & \vec{s}_2^{(4)} &= \vec{s}_2^{(2)} + \vec{s}_3^{(1)}, & \vec{s}_3^{(4)} &= \vec{s}_3^{(2)} + \vec{s}_3^{(1)}, \\
\vec{s}_4^{(4)} &= -\vec{s}_1^{(2)} + \vec{s}_3^{(1)}, & \vec{s}_5^{(4)} &= -\vec{s}_2^{(2)} + \vec{s}_1^{(1)}, & \vec{s}_6^{(4)} &= -\vec{s}_3^{(2)} + \vec{s}_1^{(1)}.
\end{align*}
\]
The 5\textsuperscript{th}-nearest neighbor vectors, \( \vec{s}_i^{(5)} \), \( i = 1, \ldots, 6 \), are

\[
\begin{align*}
\vec{s}_1^{(5)} &= s_1^{(2)} + s_2^{(2)}, \\
\vec{s}_2^{(5)} &= s_2^{(2)} + s_3^{(2)}, \\
\vec{s}_3^{(5)} &= -s_1^{(2)} + s_3^{(2)}, \\
\vec{s}_4^{(5)} &= -s_1^{(5)}, \\
\vec{s}_5^{(5)} &= -s_2^{(5)}, \\
\vec{s}_6^{(5)} &= -s_3^{(5)}.
\end{align*}
\] (A5)

The 6\textsuperscript{th}-nearest neighbor vectors, \( \vec{s}_i^{(6)} \), \( i = 1, \ldots, 6 \), are

\[
\begin{align*}
\vec{s}_1^{(6)} &= 2s_1^{(2)} + s_2^{(2)} = 2s_2^{(2)}, \\
\vec{s}_2^{(6)} &= 2s_3^{(2)}, \\
\vec{s}_3^{(6)} &= s_1^{(6)}, \\
\vec{s}_4^{(6)} &= -s_2^{(6)}, \\
\vec{s}_5^{(6)} &= -s_3^{(6)}, \\
\vec{s}_6^{(6)} &= -s_3^{(6)}.
\end{align*}
\] (A6)

Notice that the number of vectors necessary to reach all the \( m \)-th nearest neighbors varies, \( i = 1, \ldots, n_m \), but it is always a multiple of 3 (3, 6, 12 for \( n_{10} \) etc). A rule is that: When the \( \vec{s}_i^{(m)} \) vectors connect atoms of the same sublattice (hence contribute to the diagonal terms in the Hamiltonian, see the paper), then \( n_m \) is always a multiple of 6, and there is a reflection symmetry between the vectors (e.g., for \( m = 6, \vec{s}_4^{(6)} = -\vec{s}_1^{(6)}, \vec{s}_5^{(6)} = -\vec{s}_2^{(6)}, \vec{s}_6^{(6)} = -\vec{s}_3^{(6)} \)); on the other hand, when the \( \vec{s}_i^{(m)} \) vectors connect atoms of a different sublattices (hence contribute to the off-diagonal terms in the Hamiltonian, see the paper) then \( n_m \) is a multiple of 3, and there is no reflection symmetry.

Therefore, \( V_k^{(m)} \) is the potential between atoms located at distance \(|\vec{s}_i^{(m)}| \equiv |\vec{s}^{(m)}|\), \( \forall i = 1, \ldots, n_m \) (in the ideal case of a perfect lattice), while \( H_k^{(o)} \) is the Hamiltonian whose eigenfunctions are the orbitals \( \varphi^I(\vec{r}) \) with corresponding eigenvalues \( e^{(0)} \) that is the onsite energy.

Putting together all this, the field Hamiltonian (2) of main the manuscript becomes

\[
\mathcal{H}_k = \sum_m \sum_{i=1}^{n_m} \int d^2\vec{r} |a_k^* \phi^A(\vec{r}) (H_k^{(o)} + V_k^{(m)}) a_k \phi^A(\vec{r} + \vec{s}_i^{(m)}) + b_k^* \phi^B(\vec{r})(H_k^{(o)} + V_k^{(m)}) b_k \phi^B(\vec{r} + \vec{s}_i^{(m)}) + h.c.\] (A7)

By using that \( \phi^I(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} \varphi^I(\vec{r}) \) are Block functions, hence that \( \varphi^I(\vec{r}) \) are periodic, the products in (A7) all produce phase factors \( \phi^A(\vec{r}) \phi^B(\vec{r} + \vec{s}_i^{(m)}) = e^{-i\vec{k} \cdot \vec{r}} \phi^A(\vec{r}) e^{i\vec{k} \cdot (\vec{r} + \vec{s}_i^{(m)})} \psi^I(\vec{r} + \vec{s}_i^{(m)}) = e^{i\vec{k} \cdot \vec{s}_i^{(m)}} \varphi^I(\vec{r}) \varphi^J(\vec{r} + \vec{s}_i^{(m)}) \). Therefore

\[
\mathcal{H}_k = \sum_{m \in \text{diag}} (e^{(0)} \zeta_m + \eta_m) \mathcal{F}_m(k) (a_k^* a_k + b_k^* b_k) + \left( \sum_{m \in \text{off}} (e^{(0)} \zeta_m + \eta_m) \mathcal{F}_m^*(k) a_k^* b_k + h.c. \right)
\] (A8)
where

$$\varsigma_m = \int d^2 \vec{r} \varphi^I(\vec{r}) \varphi^J (\vec{r} + \vec{s}_i^{(m)}), \quad (A9)$$

$$\eta_m = \int d^2 \vec{r} \varphi^I(\vec{r}) V^{(m)}(\vec{r}) \varphi^J (\vec{r} + \vec{s}_i^{(m)}) \quad (A10)$$

and $\mathcal{F}_m(\vec{k}) = \sum_{i=1}^{n_m} \epsilon^{i \vec{k} \cdot \vec{s}_i^{(m)}}$, with the $m$s contributing to the diagonal terms when $I = J$, and to the off-diagonal terms when $I \neq J$.

Let us write down here the first six $\mathcal{F}_m$s

$$\mathcal{F}_1 = \sum_{i=1}^{3} e^{i \vec{k} \cdot \vec{s}_i^{(1)}} = e^{-i \ell k_y}[1 + 2e^{i \frac{2 \ell}{2} k_y} \cos(\frac{\sqrt{3} \ell k_x})] \quad (A11)$$

and $|\mathcal{F}_1|^2 = 3 + 2 \sum_{i=1}^{3} \cos(\vec{k} \cdot \vec{s}_i^{(2)})$.

Then, $\mathcal{F}_3 = \sum_{i=1}^{3} e^{i \vec{k} \cdot \vec{s}_i^{(3)}}$, that gives $|\mathcal{F}_3|^2 = 3 + 2 \sum_{i=1}^{3} \cos(2 \vec{k} \cdot \vec{s}_i^{(2)})$.

$$\mathcal{F}_4 = \sum_{i=1}^{6} e^{i \vec{k} \cdot \vec{s}_i^{(4)}} = e^{i \vec{k} \cdot \vec{s}_1^{(1)}} \left( e^{-i \vec{k} \cdot \vec{s}_2^{(2)}} + e^{-i \vec{k} \cdot \vec{s}_3^{(2)}} \right) + e^{i \vec{k} \cdot \vec{s}_2^{(1)}} \left( e^{-i \vec{k} \cdot \vec{s}_2^{(2)}} + e^{-i \vec{k} \cdot \vec{s}_1^{(2)}} \right) + e^{i \vec{k} \cdot \vec{s}_3^{(1)}} \left( e^{i \vec{k} \cdot \vec{s}_3^{(2)}} + e^{-i \vec{k} \cdot \vec{s}_1^{(2)}} \right) \quad (A13)$$

$$\mathcal{F}_5 = \sum_{i=1}^{6} e^{i \vec{k} \cdot \vec{s}_i^{(5)}}$$

$$= 2(\cos[\vec{k} \cdot (\vec{s}_1^{(2)} + \vec{s}_2^{(2)})]$$

$$+ \cos[\vec{k} \cdot (\vec{s}_1^{(2)} + \vec{s}_3^{(2)})]$$

$$+ \cos[\vec{k} \cdot (\vec{s}_3^{(2)} - \vec{s}_1^{(2)})]) \quad (A14)$$

$$\mathcal{F}_6 = \sum_{i=1}^{6} e^{i \vec{k} \cdot \vec{s}_i^{(6)}} = 2 \sum_{i=1}^{3} \cos(2 \vec{k} \cdot \vec{s}_i^{(2)}) = |\mathcal{F}_3|^2 - 3 \quad (A15)$$

Clearly there is a regularity (pattern) linking the various functions. We shall not investigate this here because it is out of our scope.

Let us now explain our choice of the zero of the energy, and explain, along the way, some more details of the structure of the diagonal and off-diagonal terms.

Define $\hat{H}_k \equiv \tilde{\hat{H}}_k + \epsilon^{(0)} \tilde{\hat{S}}_k$, where

$$\tilde{\hat{S}}_k = \begin{pmatrix} \hat{S}^{\text{diag}}_k & \hat{S}^{\text{off}}_k \\ \hat{S}^{\text{off}}_k & \hat{S}^{\text{diag}}_k \end{pmatrix} \quad (A16)$$
is the overlapping matrix, with

$$S^\text{diag}_k = \sum_{m \in \text{diag}} \varsigma_m F_m(\vec{k}) = 1 + \varsigma_2 F_2(\vec{k}) + \varsigma_5 F_5(\vec{k}) + \varsigma_6 F_6(\vec{k}) + \cdots \quad (A17)$$

and

$$S^\text{off}_k = \sum_{m \in \text{off}} \varsigma_m F_m(\vec{k}) = \varsigma_1 F_1(\vec{k}) + \varsigma_3 F_3(\vec{k}) + \varsigma_4 F_4(\vec{k}) + \cdots \quad (A18)$$

With these, the Schrödinger equation becomes

$$\psi^\dagger_k \hat{\mathcal{H}}_k \psi_k = (E(\vec{k}) - \epsilon^{(0)}) \psi^\dagger_k \hat{S}_k \psi_k \quad (A19)$$

where, as usual, $\psi^\dagger_k \equiv (a^*_k, b^*_k)$. The energy $\epsilon^{(0)}$ merely shifts the zero of the energy bands, hence we are free to reset the zero of the scale ignoring that term. On the other hand, that zero can still be fixed with the on-site energy included in the Hamiltonian (see later (A22)). Thus, by renaming the Hamiltonian as $\hat{\mathcal{H}}_k \equiv \hat{\mathcal{H}}_k$, we eventually have

$$\psi^\dagger_k \hat{\mathcal{H}}_k \psi_k = E(\vec{k}) \psi^\dagger_k \hat{S}_k \psi_k \quad (A20)$$

where

$$\hat{\mathcal{H}}_k = \begin{pmatrix} h^\text{diag}_k & h^\text{off}_k \\ h^\text{off}_k & h^\text{diag}_k \end{pmatrix} \quad (A21)$$

with

$$h^\text{diag}_k = \sum_{m \in \text{diag}} \eta_m F_m(\vec{k}) = \eta_0 + \eta_2 F_2(\vec{k}) + \eta_5 F_5(\vec{k}) + \eta_6 F_6(\vec{k}) + \cdots \quad (A22)$$

$$h^\text{off}_k = \sum_{m \in \text{off}} \eta_m F_m(\vec{k}) = \eta_1 F_1(\vec{k}) + \eta_3 F_3(\vec{k}) + \eta_4 F_4 + \cdots \quad (A23)$$

**Appendix B: Modified commutation relations**

We defined the modified momentum as $\vec{p} = \vec{p} + \Delta \vec{p}$ (see conventions in the main manuscript) where

$$\Delta \vec{p} = \frac{\ell}{4} \left( p_y^2 - p_x^2 - \frac{\ell}{2} p_x(p_x^2 + p_y^2), 2 p_x p_y - \frac{\ell}{2} p_y(p_x^2 + p_y^2) \right) \quad (B1)$$

$$= \frac{\ell}{4} \left( -\cos 2\theta - \frac{\ell}{2} p \cos \theta, \sin 2\theta - \frac{\ell}{2} p \sin \theta \right),$$

where the low energy momentum $\vec{p}$ fulfills the standard commutation relation

$$[x_i, p_j] = i\hbar \delta_{ij}. \quad (B2)$$
In order to get the commutation relation with the modified momentum, we use the standard commutators (B2) and (B1) to compute \([x_i, P_j]\), leading to
\[
[x, P_x] = i \left( 1 - \frac{\ell}{2} P_x - \frac{\ell^2}{8} (P_x^2 - P_y^2) \right),
\]
\[
[x, P_y] = i \left( \frac{\ell}{2} P_y - \frac{\ell^2}{4} P_x P_y \right),
\]
\[
[y, P_x] = i \left( \frac{\ell}{2} P_y - \frac{\ell^2}{4} P_x P_y \right),
\]
\[
[y, P_y] = i \left( 1 + \frac{\ell}{2} P_x + \frac{\ell^2}{8} (P_x^2 - P_y^2) \right).
\]
By inverting (13) in the main paper, we get
\[
\vec{P} \equiv \vec{Q}(1 + A|\vec{Q}|), \tag{B3}
\]
from which
\[
[x, Q_x] = i \left( 1 - \frac{\ell}{2} Q_x - A \left( |\vec{Q}| + \frac{Q_x^2}{|\vec{Q}|} \right) - \frac{\ell^2}{8} (Q_x^2 - Q_y^2) - \frac{\ell}{2} A Q_x |\vec{Q}| - A^2 \left( |\vec{Q}|^2 + Q_x^2 \right) \right),
\]
\[
[x, Q_y] = i \left( \frac{\ell}{2} Q_y - \frac{A}{|\vec{Q}|} Q_x Q_y - \frac{\ell^2}{4} Q_x Q_y - \frac{\ell}{2} A Q_x |\vec{Q}| + \frac{\ell}{2 |\vec{Q}|} A Q_y (Q_x^2 - Q_y^2) - \frac{\ell}{2} A |\vec{Q}| Q_y \right),
\]
\[
[y, Q_x] = i \left( \frac{\ell}{2} Q_y - \frac{A}{|\vec{Q}|} Q_x Q_y - \frac{\ell^2}{4} Q_x Q_y - \frac{\ell}{2} A Q_x |\vec{Q}| - \frac{\ell}{2 |\vec{Q}|} A Q_y Q_x^2 - \frac{\ell}{2} A |\vec{Q}| Q_y \right),
\]
\[
[y, Q_y] = \left( 1 + \frac{\ell}{2} Q_x - A \left( |\vec{Q}| + \frac{Q_y^2}{|\vec{Q}|} \right) + \frac{\ell^2}{8} (Q_x^2 - Q_y^2) - \frac{\ell A}{|\vec{Q}|} Q_x Q_y - A^2 \left( |\vec{Q}|^2 + Q_y^2 \right) \right),
\]
where \(A \equiv \ell \epsilon_1 / \eta_1\).

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