Periodic forcing of graphene as geometric ripples on its surface

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We explore the possibility of using modulated high frequency periodic driving of mono-layer graphene to create effects of curved geometry. The low energy continuum limit of graphene is modeled using Dirac equation in (2+1) dimensions. We suggest that the modifications to the Dirac equation written in a curved background space can also be induced by a suitable driving scheme. The time dependent system yields, in the approximate limit of high frequency pulsing, an effective time independent Hamiltonian that governs the time evolution, except for an initial and a final kick. We use a specific form of 4-phase pulsed forcing with suitably tuned choice of modulating operators to mimic the effects of weak metric perturbations and thereby effectively induce mild wrinkles on the surface. The strength of the perturbation is found to be directly related to \(\omega^{-1}\) the time period of the driving field at the leading order. We apply the method to engineer some specific ‘nearly flat’ metrics and we find that the imprint of curvilinear geometry modifies the band structure significantly. The emergence of band gap at the Dirac point is crucial in this regard. We suggest that this method shall be useful in studying the response of various properties of such materials to non-trivial geometry without requiring any actual physical deformations.

I. INTRODUCTION

Quantum systems subjected to high-frequency periodic driving have become a prominent feature of quantum simulation studies. These studies are mostly aimed at modelling various unique condensed-matter systems. Field induced driving, or that generated through mechanical straining, for instance, in graphene have demonstrated their ability to create novel gauge structures and modify the energy spectra. Such driving schemes have hence become increasingly popular in cold atom and ion-trap systems as a means of implementing effective potentials that could simulate magnetic fields or spin-orbit couplings.

The theoretical formalism underlying these driven quantum systems relies on a time dependent forcing of the system that synthesizes an effective approximate time independent Hamiltonian. A recent trend in the investigations has been inclined towards looking at a variety of driving schemes to explore potentially interesting Hamiltonians. These studies, build on previous experimental and theoretical investigations of time-dependent Hamiltonians, especially for high-frequency perturbations. The significant advantage offered over other approaches is the clear decomposition of system dynamics into an effective Hamiltonian governing long-term evolution, the micro-motion and effects of initial modulation phase of the driving signal.

We consider the possibility of choosing a specifically modulated pulse signal to periodically drive planar graphene which would, effectively simulate ripples on the surface of the material. We use the fact that the band structure of graphene resembles the energy spectrum of a Dirac system in the low energy limit.

This motivates us to invoke the continuum limit for graphene for the purpose of our analysis, whereby the electronic behaviour is described by the Dirac equation in (2+1)-dimensions. The introduction of rippled graphene in this approach shall be described by the Dirac equation written in a curved spatial background. Several works have addressed the issues relating to curvature in graphene sheets illustrating the relationship between the geometric curvature of the sheet and an effective curved space-time for the Dirac equation governing its electronic properties. They layout in detail the physical consequences one should look for if the graphene surface possessed defects or wrinkles. These studies focus on the changes to the local density of states and other transport properties arising due to the curvature of the background space-time. In this context it is also worth mentioning the progress in studying the Dirac equation in artificial curved space-times from a cold atom /optical lattice perspective. Our claim is that it is possible to generate similar effects on planar mono-layer graphene through a well defined periodic driving scheme. The Dirac equation in (2+1)-dimensional space-time has also received much attention, apart from graphene, in the contexts of planar Coulomb and magnetic fields, (2+1)-dimensional gravity, minimal length formalism, Aharonov-Bohm solenoids and non-linear scenarios. These varied approaches provide for a solid framework in our analysis.

In this paper, we consider the Dirac equation in (2+1)-dimensional background described by a metric with a conformally flat spatial part. The Dirac equation in this curved background is cast in a Hamiltonian form to allow easy comparison with the graphene Hamiltonian in the continuum limit. The effect of the background curvature is noted. We outline a scheme for the generation of an approximate Hamiltonian using periodic time dependent forcing on flat graphene such that the resulting static effective system mimics the features of a curved background. We find that if the metric is treated as...
a weak perturbation to flat space then the consequent Dirac Hamiltonian can be effectively simulated by a suitable periodic pulsing of planar graphene with a direct correspondence between the period of driving and the parameter of metric perturbation. The method is applied to surfaces with geometry that is spherical, spheroidal, toroidal and a Beltrami pseudosphere. The modification to the band structure is studied specially in low energy regimes near the Dirac points. Here, the crucial emergence of band gap as a effect of metric perturbations in the background space is noted.

II. FORMALISM

We consider a (2+1) dimensional space-time as the backdrop for our analysis. Noting that the treatment of mono-layer graphene shall essentially be confined to two dimensional space we choose a space-time metric of the form

\[ ds^2 = dt^2 - e^{-2Λ(x,y)}(dx^2 + dy^2). \]  

where \( t \) represents the time coordinate, \( x \) and \( y \) are the spacial isothermal coordinates, and \( e^{-2Λ(x,y)} \) denotes an arbitrary conformal factor. The two dimensional spatial part of this metric is completely general. The metric tensor \( g_{\mu\nu} \) for this space-time is \( \text{diag}(1, e^{-2Λ(x,y)}) \). This metric has been used in the context of studying Dirac equation coupled to curved space-time \[33\] with a distribution of defects, for instance, in the case of corrugated graphene sheets \[6\].

The Dirac equation in curved space-time takes the form

\[ iγ^\mu(x)(\partial_\mu + \Gamma_\mu(x))ψ = 0 \]  

where \( iγ^\mu(x) \) denote the usual vielbeins and their inverses respectively, \( \Gamma_\mu \) are the Christoffel connection coefficients and \( s^\lambda_{\nu\mu} \) are the generators of spinor transformation in curved space-time.

The expression illustrates the indeterminacy of the connection term to within a constant \( a_\mu \) and hence \( \Gamma_\mu \) has arbitrary trace \[33\]. This offers a gauge freedom which can be exploited depending on the nature of the problem. We take the standard choice for \( \Gamma_\mu \) as

\[ \Gamma_\mu(x) = \frac{1}{2}g_{\lambda\alpha}(e^i_{\nu\mu}E^\alpha_i - \Gamma^\alpha_{\nu\mu})s^\lambda_{\nu\mu} \]

(3)

with,

\[ s^\lambda_{\nu\mu}(x) = \frac{1}{2}[γ^\lambda(x), γ^\nu(x)] \]  

(5)

The \( γ \) matrices with space-time indices are related to the usual Dirac matrices in flat space by \( γ^\mu(x) = E^\mu_i(x)γ^i \)

We choose the following representation using the Pauli matrices for the \( γ \)'s

\[ γ^0 = σ_z \quad γ^1 = iσ_y \quad γ^2 = -iσ_x \]  

(6)

In our choice of representation \( σ_z \) is diagonal and \( σ_y \) is complex.

The spin connection components, for our metric [see Eq. (1)] are

\[ Γ_1(x) = \frac{i}{2} \frac{∂Λ(x,y)}{∂y}σ_z, \quad Γ_2(x) = \frac{-i}{2} \frac{∂Λ(x,y)}{∂x}σ_z \]  

(7)

The mass-less Dirac equation in curved (2+1) space-time, can hence be written as

\[ \left[ iσ_3 \frac{∂}{∂t} - e^{Λ(x,y)}\left( σ_y \frac{∂}{∂x} - σ_x \frac{∂}{∂y} \right) + \frac{e^{Λ(x,y)}}{4} \left( \frac{∂Λ(x,y)}{∂y}σ_z - \frac{∂Λ(x,y)}{∂x}σ_y \right) \right] ψ = 0, \]  

(8)

where we have used Eqs. (2) and (4). This equation can be recast in an explicitly Hamiltonian form by breaking the manifestly covariant form as

\[ \frac{dψ}{dt} = e^{Λ(x,y)} \left[ σ \cdot p - \frac{i}{2} \left( \frac{∂Λ(x,y)}{∂y}σ_y + \frac{∂Λ(x,y)}{∂x}σ_x \right) \right] ψ, \]

(9)

with \( σ = (σ_x, σ_y) \) and \( p = (p_x, p_y) \). The equation can be expressed in a more manifestly Hermitian form as

\[ \frac{dψ}{dt} = \frac{1}{2} e^{Λ(x,y)} \left[ σ \cdot p + σ \cdot p \right] ψ = Hψ. \]  

(10)

We shall henceforth refer to the operator \( H \) appearing in the right hand side of this equation as the Dirac Hamiltonian in curved space. We note that the low energy limit of a continuum approximation of graphene has the Hamiltonian of the form 20

\[ H_G = v_Fσ \cdot p \]  

(11)

where \( v_F \) is the Fermi velocity. We shall subsequently work in units where \( v_F = 1 \). This Hamiltonian \( H_G \) shall be generalised to \( H \) in curved space [see Eq. (10)].

We shall now consider the possibility of constructing an effective Hamiltonian of the form \( H \), starting from its flat space counterpart by considering a high frequency periodic forcing. In the study of quantum systems having periodic time dependent Hamiltonians \[21, 22\], a special category is devoted to the class of systems subject to high frequency periodic perturbations \[19\]. The theoretical treatment of such systems has its roots in the study of similar classical systems \[40, 41\]. The literature suggests various routes to arrive at such an effective time-independent Hamiltonian \[20, 22, 23\]. A recent approach \[18\], inspired by \[23\], forms the basis of our formalism. It uses the idea of engineering effective Hamiltonians by
applying carefully selected periodic driving schemes to quantum systems, geared towards generating desired effective static systems.

The technique may be outlined as follows. One considers a time-periodic Hamiltonian \( H(t) \) that can be written as

\[
H(t) = H_0 + V(t) \tag{12}
\]

where \( H_0 \) is time independent and \( V(t) \) is the periodic time dependent part such that \( V(t + T) = V(t) \). The idea is to decompose the dynamical evolution of the system between time slices \( t_i \) and \( t_f \) governed by a unitary evolution operator \( U(t_i, t_f) \) of the form

\[
U(t_i, t_f) = e^{-iF(t_f)}e^{-iH_{\text{eff}}(t_f-t_i)}e^{iF(t_i)} \tag{13}
\]

where, \( H_{\text{eff}} \) is a time-independent effective Hamiltonian and \( F(t) \) is a Hermitian, time dependent operator with \( F(t + T) = F(t) \). It is important to note here that \( H_{\text{eff}} \) is independent of both \( t_i \) and \( t_f \), which, have been transferred into the “Kick” terms \( e^{iF(t_i)} \) and \( e^{-iF(t_f)} \) respectively. It is generally not possible to extract the operators \( F(t) \) and \( H_{\text{eff}} \) in closed analytic form except for some special cases. However, if the driving frequency \( \omega = 2\pi/T \) is high, one can consider a perturbative expansion using the small parameter \( 1/\omega \). The expansions for \( H_{\text{eff}} \) and \( F \) are

\[
H_{\text{eff}} = \sum_{0 \leq n < \infty} \frac{1}{\omega^n} H^{(n)} \quad F = \sum_{1 \leq n < \infty} \frac{1}{\omega^n} F^{(n)}. \tag{14}
\]

The time evolution equation for \( U(t_i, t_f) \) given by \( i\partial_t U(t) = HU(t) \) yields

\[
H_{\text{eff}} = e^{iF(t)}H e^{-iF(t)} + \frac{\partial}{\partial t} \left( e^{iF(t)} \right) e^{-iF(t)}. \tag{15}
\]

This may be expanded as a perturbation series in \( 1/\omega \) using Eq. (14). At a given order of perturbation in \( 1/\omega \), one retains the time independent average in \( H_{\text{eff}} \) and adjust \( F(t) \) to annihilate any time dependence. The procedure is repeated at each order and results obtained at the previous order is incorporated in the subsequent orders. This allows us to determine \( H^{(n)} \) and \( F^{(n)} \) up to the desired accuracy. We note that the operators \( F^{(n)} \) are all periodic with zero mean

\[
\langle F^{(n)} \rangle = 0, \quad F^{(n)}(t + T) = F^{(n)}(t). \tag{16}
\]

The driving potential \( V(t) \) is usually considered to be a sequence of pulses that repeat periodically. Increasing the number of phases in the pulse sequence offers a wide variety of possibilities. Let us consider a general N-phase pulse sequence of the type

\[
V(t) = \sum_{r=1}^{N} f_r(t) \tilde{V}_r \tag{17}
\]

where \( f_r \) denotes a square profile such that \( f_r(t) = 1 \) during \( (r-1)T/N \leq t \leq rT/N \), else \( f_r(t) = 0 \).

Among the wide range of choices that do exist, our problem lends itself rather neatly to a 4-phase pulse sequence with modulation of the Hamiltonian given by

\[
\mathcal{P}_4 = \{ H_0 + A, H_0 + B, H_0 - A, H_0 - B \} \tag{18}
\]

This compares to (17) for \( N = 4 \) with \( V_1 = -V_4 = A \) and \( V_2 = -V_3 = B \), where \( A \) and \( B \) are suitable operators.

Instead of using square pulses, a smooth driving scheme equivalent to this pulsing scheme, of the kind \( V(t) = A \cos(\omega t) + B \sin(\omega t) \) may be used.

This choice of the time dependent potential yields

\[
H_{\text{eff}} = H_0 + \frac{i}{2\omega} [A, B] + \frac{1}{4\omega^2} ([A, H_0], A) + ([B, H_0], B)) + \mathcal{O}(1/\omega^3) \tag{19}
\]

It is significant in our context that the expression for \( H_{\text{eff}} \) has both first order and second order terms in \( \omega \) with the appropriate commutator brackets. The freedom in the choice of \( A \) and \( B \) allows us to engineer the desired Hamiltonian in curved space.

The conformal factor \( e^{\Lambda(x,y)} \) in the metric, encapsulates the curved nature of the space. For a space that differs slightly from the flat, the metric is expected to be expressible as a small perturbation around the flat metric. In terms of the conformal factor we may hence write

\[
e^{\Lambda(x,y)} \approx 1 + \epsilon f(x, y) + \mathcal{O}(\epsilon^2) \tag{20}
\]

where, \( \epsilon \) is a perturbation parameter. The Dirac Hamiltonian for such a weakly perturbed space can be obtained by substituting the above approximate form of the conformal factor in the Eq. (10).

The periodic driving scheme has a small parameter \( 1/\omega \), the time-period of forcing. We would like to map this parameter to the small parameter in metric perturbation. It is our contention that it is possible to use the formalism of generating effective approximate Hamiltonians, through a choice of suitable operators \( A \) and \( B \) as mentioned in Eq. (13), to reproduce a conformally flat metric on graphene with weak perturbation limit. This would involve impinging graphene with the appropriate pulsing scheme. This method, hence attempts to simulate a weakly perturbed space for the conducting electrons on an otherwise planar surface. In terms of our adopted formalism this essentially implies generating an effective Hamiltonian such that it matches the Dirac Hamiltonian in curved space with weakly perturbed metric having \( \epsilon \sim (1/\omega) \).

Let us consider a driving scheme with \( H_0 = \sigma \cdot p \), the Dirac Hamiltonian in flat space and choose the operators \( A \) and \( B \) of the form

\[
A = \sigma \cdot \alpha \quad B = \sigma \cdot \beta \tag{21}
\]

where, \( \alpha = (-p_y, p_z, 0) \) and \( \beta = (0, 0, -f) \). With this choice, Eq. (19) gives the Dirac Hamiltonian in a weakly
curved space up to order $1/\omega$. For large $\omega$ this is a good approximation whereby the leading correction term in equation (19) mimics curved space. The term of $\mathcal{O}(1/\omega^2)$ is significantly suppressed and manifests as non-trivial spin-orbit couplings and maybe ignored for our present analysis.

We then have an approximate effective Hamiltonian $H_{\text{eff}}$ given by

$$H_{\text{eff}} = \frac{1}{2} \left[ \left( 1 + \frac{f(x,y)}{\omega} \right) \sigma \cdot p + \sigma \cdot p \left( 1 + \frac{f(x,y)}{\omega} \right) \right]$$

which on comparison with Eqs. (10) and (11) clearly describes graphene on a weakly rippled surface. The form of the function $f(x,y)$ shall decide the nature of curvature as we shall see in the next section.

### III. RESULTS AND DISCUSSION

![FIG. 1. (Color online)Variation of ground state energy with wavevector $k_x$: (a) Shows the variation for spherical perturbations with $\omega^{-1} = 0, 0.1, 0.3$ and 0.5, color coded as black, red, green and blue respectively. (b) Shows the variation for oblate spheroidal perturbations with $(\omega^{-1}, \delta)$ values as $(0, 0)$ black, $(0.5, 0.3)$ red, $(0.5, 0.5)$ green and $(0.5, 0.8)$ blue. The insets in (a) and (b) magnify the region in the close vicinity of the Dirac points for better illustration. (c) Shows the variation for Rindler like perturbations in the same scheme as (a) above. (d) Shows the variation for toroidal perturbations with $\omega^{-1}$ values $0, 10^{-4}, 2 \times 10^{-4}$ and $3 \times 10^{-4}$ represented by the black, red, green and blue lines respectively.](https://example.com/figure1)

To illustrate the prescription outlined in the last section for generating weak ripples on graphene, we consider ‘nearly flat’ metrics in the form of small perturbations about the flat metric. We consider the following cases: spherical, oblate spheroidal, Rindler and toroidal perturbations. We also investigate the changes to the ground state band structure brought about by these metrics, especially around the Dirac points.

The behavior of the ground state energy at and around the Dirac points for graphene under strain, deformation and in the presence of substrate interaction has been studied \[5, 42, 43\]. These works discuss the possibility of opening a band gap in graphene at the Dirac point, which is known to be topologically protected by inversion and time reversal symmetries. The techniques employed to generate the band gap usually attempt to break the time reversal symmetry in some fashion \[44\], such as through the appearance of pseudo-magnetic fields \[45, 46\]. Cutting of graphene into nano-ribbons of various widths offers a means of engineering desired band gaps \[47\]. The gap introduced marks a phase transition from massless to massive Dirac fermions in graphene \[48, 49\]. Recent studies treat the emergence of the gap in the continuum limit by applying periodic magnetic and electric fields \[50\]. There is also an attempt to tune this gap by use of potentials or doping \[51, 52\], a feature of interest in transistor like applications of graphene \[53\].

Our treatment of periodically driven graphene as curved monolayer graphene leads us to expect the band gap characteristic of strained graphene geometries in our system. The results obtained through our computations reflect this. As illustrated in Fig. (1) all our weak metric perturbation choices introduce a band gap to varying extents as compared to planar graphene. Therefore, our technique offers an alternative way of engineering a band gap in graphene and also tuning it by use of suitable driving schemes. In the following paragraphs we proceed to discuss the details of the effects on the ground state as observed for our choices of metric perturbations.

The choice $f(x,y) = \text{sech}^2(x)$, implying $\Lambda(x,y) = \omega^{-1}\text{sech}^2(x)$, for the modulating operators given in (21) yields a weak spherical perturbation to the metric on planar graphene. The $\omega^{-1} = \epsilon$ correspondence is utilized here. In Fig. (1a), for the spherical ripples case, we illustrate the variation of band energy with $k_x$ for the ground state. This is a band structure cross-section plot obtained around a Dirac point. The three curves in the plot correspond to $\omega^{-1} = 0, 0.1, 0.3$ and 0.5 respectively. We note that $\omega^{-1} = 0$ corresponds to the “flat” case. The point of coincidence of the band lines (black) at the centre of the plot represents the Dirac point. Choosing $\omega^{-1} \neq 0$ creates a band gap at the Dirac point, as is clearly visible in the inset. The slope of the $E(k) - vs k$ linear relationship increases as one changes the frequency of driving. This maybe attributed to the changed position dependence of the Fermi velocity in curved space. Thus strengthening the curvature (slower driving) in general has an amplifying impact on the energy levels.

In Fig. (1b), the ground state band structure is plotted for a weakly oblate spheroidal metric. The choice of modulating operator that helps induce this metric on planar graphene is

$$f(x,y) = \text{sech}^2(x) + \delta \tanh^2(x) \text{sech}^2(x),$$
which implies $\Lambda(x, y) = \omega^{-1}f(x, y)$. Here, the parameter $\delta$ is a measure of the deviation of the metric from perfectly spherical form thereby giving it an oblate character. We draw attention to the splitting of the band structure at the Dirac point for $\omega^{-1} \neq 0.0$ owing to weak curvature in the background. The inset depicts this gap which is visibly greater as compared to the case of spherical metric perturbations. The energy values here too appear to undergo an amplification with increasing curvature with the overall increase being greater than in Fig. 1(a). The apparent bunching together of the curves for the $\omega^{-1} \neq 0.0$ cases is due to the nearly vanishing contribution from the term of the order $\omega^{-1} \times \delta$ in $\Lambda(x, y)$.

Fig. 1(c) illustrates the ground state energy for an effective weakly Rindler metric in graphene which is a consequence of a weak Beltrami pseudosphere geometry of the graphene sheet. Such a geometry can be effectively simulated on a planar graphene sheet by making the choice $f(x, y) = x^2$ in the modulation scheme. This entails $\Lambda(x, y) = \omega^{-1}x^2$. The band gap appearing here is directly visible without the aid of any magnification. The gap here is larger than both the previous cases of spherical and oblate spheroidal perturbations. Another distinguishing feature here is that deviations from flatness do not show similar behavior as $\omega^{-1} = 0.1$ shows an increase in energy whereas $\omega^{-1} = 0.3$ and 0.5 show a decrease. This indicates an asymmetry in the dependence of ground state energy on curvature unique to this metric choice.

Fig. 1(d) depicts ground state energy variation for weak toroidal perturbations to the metric of planar graphene. These perturbations are brought about effectively on a flat surface by choosing

$$f(x, y) = \frac{16 \sec^2(\sqrt{2}x)}{[1 + 2 \tan^2(\sqrt{2}x)]^2},$$

which implies $\Lambda(x, y) = \omega^{-1}f(x, y)$. The appearance of band-gap is extremely sensitive to the perturbation parameter. Even though the parameter $\omega^{-1}$ is of the order of $10^{-4}$, the amount of band gap appearing here is the maximum of all the cases. We find that though the qualitative features of the band structure match those of the other cases near the Dirac point, the spectrum is quite different when one moves away along the $k_-$ axis. The specific form of the metric manifests drastically in the behavior of the band structure far away from the Dirac points. Near these points all the weak metric perturbations show the same features with a varying degree of split.

We conclude by noting that the possibility of using periodic forcing to generate the effects of curved space on 2D electron systems has a far reaching influence in theoretical studies and technological applications. The effects of the metric deformation induced by such forcing shall affect the band structure and transport properties of the material. This opens up the possibility of synthesis of new materials finding applications in the technology of tunable transistors.

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