Enhanced asymmetric valley scattering by scalar fields in non-uniform out-of-plane deformations in graphene

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We study the electron scattering produced by local out-of-plane strain deformations in the form of Gaussian bumps in graphene. Of special interest is to take into account the scalar field associated with the redistribution of charge due to deformations, and in the same footing as the pseudomagnetic field. Working with the Born approximation approach we show analytically that even when a relatively small scalar field is considered, a rather strong valley asymmetric scattering could arise as a function of the energy and angle of incidence. In addition, we find that the valley polarization can reverse its sign as the incident energy is increased. These behaviors are totally absent if the scalar field is neglected. These results are supported by quantum dynamical simulations of electron wave packets. Results for the average trajectories of wave packets in locally strained graphene clearly show focusing and beam splitting effects enhanced by the presence of the scalar field that can be of interest in the implementation of valleytronic devices.

I. INTRODUCTION

The appearance in graphene of massless Dirac Fermions and constant velocity $v_F$ at low energies, emerges because it encloses two equivalent carbon sublattices of trigonal symmetry.\textsuperscript{2} In the presence of strain, the corresponding graphene Hamiltonian and thereby its linear dispersion laws near the $K(K')$ Dirac points gets modified accordingly. From the theoretical point of view, symmetry considerations allows up to six additional terms in its low energy Hamiltonian.\textsuperscript{2,3} Namely, those terms due to uniform strains which give rise to the pseudomagnetic and scalar fields, a gap opening term due to possible non-uniform strains, a Dirac cone strain-induced tilt term, and those due to the presence of isotropic and anisotropic position dependent Fermi velocities. Among them, the strain-induced pseudomagnetic field effects associated with the shift of the Dirac cones in the momentum space is the one most studied recently. The latter because of its natural interpretation as a sort of magnetic field\textsuperscript{2,4} (pseudomagnetic field) that under appropriate physical conditions generates, by analogy with a real magnetic field, a Landau level spectrum,\textsuperscript{5,6} phenomena that has been beautifully demonstrated in recent experiment.\textsuperscript{7,8} Moreover, in the same manner as the real magnetic field couples with the intrinsic angular momentum of the electron, the pseudomagnetic field can also couple with the pseudospin\textsuperscript{8} generating a Zeeman-like splitting as observed in very recent STM experiments.\textsuperscript{9}

Several experimental setups from different groups have reported to produce strains in graphene membranes.\textsuperscript{3,10} They range from the deposition on substrates\textsuperscript{7,10,11} of strain, the formation of bubbles\textsuperscript{12} or AFM\textsuperscript{13} tips, to the deposition of graphene membranes in nanostructured arrays.\textsuperscript{14} The induced pseudomagnetic field in graphene has several advantages over the real magnetic field, for instance, since graphene is very flexible\textsuperscript{15} the magnitudes of the pseudomagnetic field obtained by strain are many times stronger compared with real magnetic fields\textsuperscript{16,17} ($\sim 300$ T).

On the other hand, due to its mechanical origin, the pseudomagnetic field does not break time-reversal symmetry; so in the effective Hamiltonian it appears only as a reverse sign in the $K(K')$ valley.\textsuperscript{18} This unique physical characteristic have been proposed as a mechanism of control of the valley degree of freedom in various scenarios. For instance, M. Settnes \textit{et al.}\textsuperscript{19} proposed the use of pseudomagnetic profiles of Gaussian shapes in order to generate valley filtering effects. Other proposals include the combination of strain effects with geometrical confinement,\textsuperscript{19,21} inclusion of resonant structures\textsuperscript{20} or even under the presence of real magnetic fields.\textsuperscript{21,22} Due to the addition of an artificial mass\textsuperscript{23} to promote valley polarization and spin-valley polarization. However, strain is not a necessary requirement to produce valley filtering effects, as local electrostatic fields alone can render the same effect as long as it is strong enough and/or has the appropriate geometry.\textsuperscript{24,25}

It is also known that strain produces a scalar field that arises because of the redistribution of charge that occurs as a result of the change in the deformed area within each unit cell of graphene under elastic deformation.\textsuperscript{26,27} To what extent such concomitant scalar field in locally strained graphene could yield to sizable changes on the scattering phenomena is yet a physics to be investigated. The aim of this work is to study the interplay of pseudomagnetic and scalar fields due to out-of-plane mechanical deformations in the form of Gaussian bumps in graphene.
and explore its role in the electron scattering. We focus our study of the electron quantum scattering problem within the Born approximation theory. The approach allow us to derive exact analytical expressions for the differential cross section for each valley $K(K')$, treating both the pseudomagnetic and scalar fields in the same footing. Our findings predicts that even when a relatively small scalar field is considered, a rather strong valley asymmetric scattering could arise as a consequence of its interplay with the pseudomagnetic field. We show that the presence of the scalar field could induce strong valley polarization of the scattering events as a function of the energy and angle of incidence. In addition, the valley polarization can reverse its sign as the incident energy is increased. These behaviors are totally absent if the scalar field is neglected. In order to go beyond the Born approximation we also performed numerical simulations of the dynamics of electron wave packets and study the quantum average trajectories of the scattered wave packets. Our quantum numerical simulations agrees quite well with phenomenology predicted in the Born approximation. We present results of the semi-classical scattering trajectories for different angles and energies of incidence that clearly shows wave packet focusing and beam splitting effects enhanced by the presence of the scalar field.

II. MODEL: GRAPHENE WITH A GAUSSIAN BUMP

The dynamic of the low energy excitations in strained graphene in the absence of interactions is governed by the Dirac-like equation given by[6]

$$i\hbar \frac{\partial}{\partial t} \Psi_{\eta}(r,t) = [v_F \sigma_\eta \cdot (\hat{p} - \eta \mathcal{A}(r)) + V(r)] \Psi_{\eta}(r,t)$$

where the subindex $\eta = \pm$ labels the $K$ and $K'$ Dirac points, $v_F$ is the Fermi velocity, $\hat{p} = (\hat{p}_x, \hat{p}_y)$ is the momentum operator of the charge carriers, and $\sigma_\eta = (\eta \sigma_x, \sigma_y)$ is the vector of the Pauli matrices. The terms $\mathcal{A}$ and $V$ describe the pseudo-vector (gauge field) and the pseudo-scalar potentials, originated by the change of the carbon bonds due to mechanical strain[13]. These potentials have the form

$$V = g (\varepsilon_{xx} + \varepsilon_{yy}),$$

$$\mathcal{A} = (\mathcal{A}_x, \mathcal{A}_y) = \frac{\hbar \beta}{2 a_{cc}} (\varepsilon_{xx} - \varepsilon_{yy}, -2 \varepsilon_{xy}),$$

where $g$ describes the coupling with long-wave acoustical phonons due the screening with the pseudo-scalar potential in graphene, having a wide range of energy values, from 0 to 20 eV[21,15]. The parameter $a_{cc} = 1.42$ Å is the carbon-carbon interatomic distance for the unstrained graphene. The dimensionless constant coefficient $\beta \simeq 3.0$ characterizes and tunes the effect of strain on the hopping parameter, and $\varepsilon_{\mu\nu}$ is the strain tensor, which is defined in terms of the in-plane displacement components $u_\nu$ with $\{\mu, \nu\} = x, y$ and out-of-plane $h$ deformations. The strain tensor is dictated by the following general expression[30],

$$\varepsilon_{\mu\nu} = \frac{1}{2} (\partial_\nu u_\mu + \partial_\mu u_\nu + \partial_\mu h \partial_\nu h).$$

Here we shall consider only out-of-plane deformations to model the nanoscale bump in graphene, thus Eq.(4) reduces to

$$\varepsilon_{\mu\nu} = \frac{1}{2} (\partial_\nu h \partial_\mu h).$$

For the analytical model of the bump itself we consider a centro-symmetrical Gaussian-shaped deformation described by the following expression

$$h(x,y) = h_o \exp \left( -\frac{x^2 + y^2}{b_o^2} \right),$$

where $h_o$ fixes the height of the bump, and $b$ its effective width. The nature of the gauge field $\mathcal{A}$ in Eq.(3) can be interpreted as a pseudo-vector potential[8] such that its corresponding pseudo-magnetic field[5] $B_{ps}$ can be written as

$$B_{ps} = \eta \nabla \times \frac{1}{c} \mathcal{A},$$

where $e$ is the electron charge. Clearly the sign of $B_{ps}$ is valley-dependent and has units of magnetic field. Notice that the Hamiltonian associated to Eq.(1) is symmetric under charge conjugation since the charge $q$ does not appear here explicitly in front of the pseudovector potential $\mathcal{A}$.

However it does appears with opposite signs for different valleys, preserving the global time-reversal symmetry[8]. It is has been already discussed that the conjugation of such symmetries can generate pseudo-spin polarization[5,13,15], valley splitting[10,39] and valley filtering[20,22] in strained graphene.

In this work we have considered a local Gaussian-shaped mechanical deformation in a graphene sheet with a height $h_o = 10$ nm and width $b = 50$ nm. We then proceed to study the electron scattering and wave packet dynamics with ($g \neq 0$) and without the presence of the scalar field ($g = 0$). For illustration, plots of the pseudomagnetic and scalar fields are shown in Fig.[1] for $g = 3$ eV. Notice that taking such value does not imply that the scalar field will go as high in energy, actually, for such relatively large $g$-value of the deformation, the maximum value for the scalar field achieved is just $V_{max} = 0.0441$ eV. In both, scattering and wave packet dynamics, we fix the incident energy at $E = 0.11$ eV, and thus the corresponding incident wave number shall be given by $k_o = E/(\hbar v_F) = 0.167$nm$^{-1}$. 
states are given by

\[ \mathbf{U}(r) = -\eta v_F \mathbf{\sigma} \cdot \mathbf{A} + V(r). \] (8)

Due the rotational symmetry of the deformation perpendicular to the graphene sheet considered, Eq. (8) can be rewritten in polar coordinates as

\[ U_\eta = \frac{1}{2} \left( \frac{\partial h}{\partial r} \right)^2 \begin{bmatrix} g & -e^{2i\eta\phi}\Gamma \\ -e^{-2i\eta\phi}\Gamma & g \end{bmatrix} \] (9)

with \( r = \sqrt{x^2 + y^2} \), \( \phi = \text{atan}(y/x) \), and

\[ \Gamma = \frac{\hbar \beta}{2\alpha_{cc}} v_F. \] (10)

Up to first order in the Born approximation, the scattering probability is determined by the matrix element

\[ U_{k_2,k_1}^{(0)}(\eta) = \langle k_2, \eta | U_\eta | k_1, \eta \rangle, \]

where the normalized eigenstates are given by

\[ |k, \eta\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i\eta^2} \\ \pm \eta e^{i\eta^2} \end{bmatrix} e^{ik \cdot r}, \] (11)

with \(|k_1| = |k_2| = k\) to ensure energy conservation during the scattering process. Thus the differential cross section per Dirac point \( \eta \) in terms of the scattering probability is determinate by

\[ \sigma_D^{\eta} = \frac{k}{2\pi\hbar^2 v_F} |U_{k_2,k_1}^{(0)}(\eta)|^2. \] (12)

Similarly as done for the case without scalar fields[40], we can write the differential cross sections as follows,

\[ \sigma_D^{\eta} = \frac{k}{2\pi\hbar^2 v_F} \left| g \cos (\theta_m) F_{k_0}(\theta_m) + \eta \Gamma \cos (3\theta_p) F_{k_2}(\theta_m) \right|^2. \] (13)

where we have defined the function

\[ F_{kn}(\theta_m) = \pi \int_0^\infty J_n[2kr \sin \theta_m] \left( \frac{\partial h}{\partial r} \right)^2 r dr, \] (14)

here \( J_n(z) \) is the Bessel function of order \( n = 0, 2 \), with \( \theta_{m/p} = (\theta_2 \mp \theta_1)/2 \), being \( \theta_2 \) the angle of incidence, \( \theta_1 \) the scattered angle, with a deformation out-of-plane characterized by Eq. (6) as,

\[ \frac{\partial h}{\partial r} = -\frac{\hbar_o r}{b_o^2} \exp \left[ -\frac{r^2}{b_o^2} \right]. \] (15)

The terms out-of-diagonal in Eq. (9) generate a non-uniform pseudo-magnetic field with a three-fold symmetry per valley given by

\[ B_{ps} = \eta \frac{2h_o^2 B_o}{b_o^2} \left( \frac{r}{b_o} \right)^3 e^{-2(r/b_o)^2} \sin(3\phi) \hat{z}, \] (16)

with \( B_o = 4\Gamma/(ev_F b_o) \), whereas the diagonal terms act as the scalar field

\[ V = 2g \left( \frac{r}{b_o} \right)^2 e^{2(r/b_o)^2}. \] (17)

The radial integrals defined in Eq. (14) can be obtained analytically, having the following closed form (see Appendix, section A),

\[ F_{k_0}(\theta_m) = \frac{\pi h_o^2}{2} \left[ 1 - \lambda_k^2 \right] e^{-\lambda_k^2}, \] (18)

\[ F_{k_2}(\theta_m) = \frac{\pi h_o^2}{2} \lambda_k^2 e^{-\lambda_k^2}, \] (19)

with \( \lambda_k^2 = k^2 b_o^2 \sin^2(\theta_m)/2 \). Although previous scattering studies[40-42] have considered similar effects of the pseudo-magnetic field as studied here, however, the effect of the concomitant scalar field itself was ignored in these works. Moreover, while in Ref. [40] only provide of approximate expressions for the radial integral involved in the calculation of the differential cross section, here in contrast, we were able to provide exact analytical formulas for these integrals even for the case of the presence of the scalar field effect. After evaluating the integrals, we can write the exact differential cross section as,

\[ \sigma_D^{\eta} = \frac{\pi h_o^4}{8\hbar^2 v_F} \left| g \cos (\theta_m)(1 - \lambda_k^2) \mp \eta \Gamma \cos (3\theta_p) \lambda_k^2 \right|^2 e^{-2\lambda_k^2}. \] (20)

This is one of the main results of this work. Clearly in the absence of the scalar field \( g = 0 \), there is no difference between the contribution to the quantum scattering of the \( K \) and \( K' \) Dirac points to the total differential cross section \( \sigma_D^{\eta} + \sigma_D^{\eta} \). However, for \( g \neq 0 \) we have that the differential scattering cross sections \( \sigma_D^{\eta} \neq \sigma_D^{\eta} \) in general, which points out the importance of considering on the
same footing the interaction of both fields, as we shall discuss in more detail below for specific cases.

In Fig. 2 we depict in polar plots the differential scattering cross section $\sigma^D_\theta$ as a function of the angle $\theta_2$ of the out-going (scatter) wave for horizontal and vertical incidence, respectively. The incident direction is shown by a dark blue arrow with an incident effective momentum of $k = 0.167 \text{ nm}^{-1}$. Blue curves represent the contribution for $K$-point (valley) to the differential scattering cross section, while orange curves are from $K'$-point (valley) contribution. In the left panels (a and c), the scalar field is set to zero, $(g = 0)$, therefore the curves for each $\eta = \pm$ overlaps as expected from Eq. (20). On the other hand, in the right panels (b and d) we are taking $g = 3 \text{ eV}$. Notice that for horizontal incidence, the interplay of the scalar and pseudomagnetic fields promotes the appearance of a narrow angular region with rather different angular distribution of the scattering cross section of the $K, K'$ valleys (see e.g. Fig. 2). In fact, such horizontal incidence configuration has been proposed earlier in the literature as a possible valley splitter for vanishing $g$. Here we find that vertical incidence can also generate narrow angular distribution of the scattering cross section that can give rise to sizable valley polarization at $g = 3 \text{ eV}$, as shown in Fig. 2.

The total scattering cross section per valley $\eta$ is given by

$$\sigma^T_\eta = \int_0^{2\pi} \sigma^D_\theta d\theta_2.$$  \hfill (21)

Plots of the total scattering cross section as a function of the incident angle $\theta_1$ for different energies from 60 to 140 meV are shown in Fig. 3. In panel (a), we are ignoring the scalar field $(g = 0)$, and therefore the results are identical for both $K, K'$ valleys. The behavior $\sigma^D_T$ with energy is non monotonic, instead it oscillates with the incident energy (below we discuss this dependence), and for certain values of energy it shows an uniform angular distribution. In panels (b) and (c), we present $\sigma^T_\eta$ as a function of the incident angle, for $g = 3 \text{ eV}$. Though there is an oscillating behavior, the plots clearly shows that for certain angles the scattering for one valley is maximum, while for the other valley is minimum. For example at $60^\circ$ angle, the $\sigma^T_\eta$ is a maximum for valley $K$ and a minimum for valley $K'$, and the situation reverses at the angle of $120^\circ$. Thus a valley splitting effect is expected at these particular angles of dispersion. The situation will be the same for horizontal incidence and it will repeat each $60^\circ$ angle because of the six-fold symmetry of the pseudomagnetic field. Notice that for vertical incidence, i.e. $\theta_1 = 270^\circ$, yields $\sigma^T_\eta$ identical for both valleys (Fig. 3 and Fig. 5).

![FIG. 2. (Color online) Differential scattering cross section $\sigma^D_\theta$ for valley K (blue) and (K') (orange) as function of the outgoing angle $\theta_2$ for horizontal incidence (first row) and vertical incidence (second row); in the left column $g = 0$ and for the right column $g = 3 \text{ eV}$.

![FIG. 3. (Color online) Total scattering cross section $\sigma_T$ as function of the incident angle $\theta_1$ for (a) $g = 0$, and $g = 3 \text{ eV}$ for valley K (b) and K' (c).]
Nevertheless as we discuss above, the direction of scattering will differ for each valley (see Fig. 2). To characterize further the valley polarization, we define a valley polarization efficiency $\mathcal{P}$, as

$$\mathcal{P} = \frac{\sigma_T^- - \sigma_T^+}{\sigma_T^- + \sigma_T^+},$$

which is positive for the $K$ valley polarization and negative for $K'$. We show several plots for relevant cases in Fig. 4. In panel a) we fix the incident energy to $E = 15$ meV and plot $\mathcal{P}$ as function of the incident angle $\theta_1$. Panel b) Fig. 4 shows the corresponding results for $E = 60$ meV. Both plots show a six-folded (three-fold per valley) structure similar to the one of the pseudomagnetic field, but with a $30^\circ$ rotation. These results support the proposal of three-terminal structures like the one in Ref. [43]. Interestingly the sign of the polarization is inverted between these two plots. The reason behind this fact is that for low energy, the back-scattering becomes dominant and become strongly K-valley dependent. The later effect can be seeing in panel c), where we plot the dependence of $\mathcal{P}$ with the incident energy. The dashed line correspond to the zero polarization output for the absence of scalar field, and the continuous curves show results for different incident angle $\theta_1$ with $g = 3$ eV. In particular, the blue curve shows the valley polarization efficiency $\mathcal{P}$, for horizontal incidence ($\theta_1 = 0^\circ$). It increases with energy, presenting a maximum around 18 meV, then it decreases uniformly till it change sign with a minimum at 60 meV. A similar behavior is shown by the red curve, at $\theta_1 = 15^\circ$ while the sign is inverted for the purple and green curves at $\theta_1 = 60^\circ$ and $\theta_1 = 45^\circ$, respectively. For $\theta_1 = 30^\circ$ the polarization is zero for all energies. All the curves shows an approximated constant behavior for energies greater than 150 meV and with exception of the yellow one they present values of polarization close to 20%. We attribute the oscillatory behavior with energy to the quantum backscattering effect that becomes relevant for small energies (i.e. $\lambda_o \sim b_o$).

It has been shown using Boltzmann transport equation that the electronic transport in graphene under strains is mainly governed by the acoustic gauge field, while the contribution due to the deformation potential may be negligible and strongly screened[23]. Clearly in such cases the valley-asymmetric scattering showed in Eq. (20) will not be present. However it is very important to remark that a similar valley-asymmetric scattering behavior is expected in presence of any other scalar potential even if they are not produced by strain. Consider for example a scalar potential proportional to the height of the membrane $h(x,y)$, namely

$$V_{ext} = \epsilon A \exp \left(-\frac{x^2+y^2}{b_0^2}\right) = \epsilon h(x,y).$$

being $\epsilon$ some constant. Such a field will appear for instance if there is a nonuniform electric field pointing to the $z$-direction perpendicular to the membrane, as the case of AFM-tip[50] and/or a gate[51] pulling the membrane. Taking $g = 0$ (ignoring the scalar field associated with strain) the corresponding differential cross section is instead,

$$\sigma_D^\eta = \frac{\pi k \hbar^2}{8 \epsilon^2 v_F^2} \left| 2 \epsilon \cos (\theta_m) e^{-\lambda_k^2} + 2 \tilde{\eta} \cos (3\theta_p) \lambda_k^2 \right|^2 e^{-2\lambda_k^2}.$$  

Hence, a non-uniform electric field will also generate valley polarization and similar angular dependence as in Eq. (20) even in the absence of the scalar field produced by the strain.

IV. WAVE PACKET PROPAGATION

The Born approximation describes correctly the scattering in the limits of low and high energies. In order to go beyond the Born approximation and explore the intermediate energy regime, we study the dynamics of the scattering process of electron wave packets in strained graphene by numerically solving Eq. (1) in finite differences in real space. The scheme employs a suitable splitting of the time evolution operator. The resulting differential equations are solved in a recursive approach for any given time step provided the initial and boundary conditions of the strained graphene sheet (for details see Appendix, section B).

As for the initial condition, we take an incident Gaussian wave packet of standard deviation, $w$, mean posi-
tion, \( r_0 = (x_0, y_0) \), moving with an average momentum, \( p_o = i k_o \), given by,

\[
\Psi_{k_o}^0(r, 0) = \frac{1}{\sqrt{4\pi w^2}} \exp \left[ \frac{(r - r_0)^2}{2w^2} + i k_o \cdot r \right] \left[ e^{-i\eta e^{i\eta e}} \right].
\]

(25)

where \( \frac{1}{\sqrt{2}}(e^{-i\eta e} - e^{i\eta e}) \) is the initial pseudospin polarization, aligned with the direction of average momentum, \( p_o \). In particular, for all our numerical simulations we use a wave packet with \( w = 30 \) nm and total momentum \( k = 0.167 \) nm\(^{-1} \), corresponding to an incident energy \( E = 0.11 \) eV. We considered two limiting cases for the incidence angle: (1) horizontal incidence where the wavepacket is originally centered at \( (x_0, y_0) = (-150, 0) \) nm with \( E = 110 \) meV at time, \( t = 350 \) fs with \( g = 0 \) (first row) and \( g = 3 \) eV (second row). Different columns correspond to different valleys: (a) and (c) to valley \( K \), and (b)-(d) to valley \( K' \).

![Graphs showing probability density for different valleys](attachment:image.png)

FIG. 5. (Color online) Probability density \(|\Psi(x, y)|^2\) of an incident wave packet coming from the left \([x_0, y_0] = (-150, 0)\) nm] with \( E = 110 \) meV for different impact parameters plotted on top of the pseudomagnetic field profile for valleys \( K \) (left column) and \( K' \) (right column) with \( g = 0 \) (a-b) and \( g = 3 \) eV (c-d).

When the scalar field is present, Fig. 5(c) and Fig. 5(d), the valley asymmetric scattering persist but the wavepacket profiles for each valley changes. Particularly, for the valley \( K \) we can see a strong backscattering making

![Graphs showing trajectories for different valleys](attachment:image.png)

FIG. 6. (Color online) Trajectories of \((r)\) (black) of an incident wave packet coming from the left with \( E = 110 \) meV for different impact parameters plotted on top of the pseudomagnetic field profile for valleys \( K \) (left column) and \( K' \) (right column) with \( g = 0 \) (a-b) and \( g = 3 \) eV (c-d).

...
the Gaussian deformation basically transparent for valley
\( K \) and reflective for \( K' \) for normal incidence. Compar-
ison of Fig. 2a with Fig. 3a and Fig. 3b shows qualita-

tively agreement between the results of Born approximation

tive agreement between the results of Born approximation

and wave packet dynamics approach.

Classical studies of scattering usually include the cal-
culation deflection angle as a function of the impact pa-
ter. In our case, we define the deflection angle

as the angle between the incoming and outgoing direc-
tion, using the trajectory on the expected value of the
position operator \( \langle \vec{r} \rangle \). Classical trajectories of the

wave packet for horizontal incidence (from the left) to
the pseudomagnetic field region produced by the bump
for both valleys, are shown in Fig. 6 (panels a,b with
the presence of the scalar field, and c, d without it).

Explicitly we take a Gaussian wave packet initially cen-
tered at \((-150, y_0)\) nm moving (with average wave num-
ber \( k_0 = k_{ax} \hat{x} \)) towards the locally strained region. For
this setup, \( y_0 \) defines the impact parameter. Black curves

correspond to the average trajectories with different val-
nues of the impact parameter \( y_0 = \{-75, 70, 65..., 75\} \) nm.

We observe an opposite behavior of the classical trajec-
tories when comparing the cases for the \( K \) and \( K' \) valleys.

While for valley \( K \) the bump acts -in terms of geomet-
trical optics arguments- as a divergent pseudomagnetic

lens, for valley \( K' \) it behaves as a convergent lens. For
instance, the case for \( g = 0 \) shows a focusing of the stream
of electrons to a narrow region (Fig. 4a) for valley \( K \),
whereas it shows deflecting trajectories in a bifurcated

pattern at \( \pm y \) direction for valley \( K' \) (Fig. 4b). Notice

that in the first scenario the classical trajectories pen-

e-trates the whole distorted region whiles in the second
case experiences a deflection, avoiding the bump region.

Therefore the locally strain region will yield preferential
directions of valley polarization, as being discussed in the
literature. The overall behavior of the classi-
cal trajectories remains unchanged in the presence of the
scalar field, as shown in Fig. 6d-f. However, in this case
the deflection angles for valley \( K \) are greater, with well
defined directions of valley polarization as well. Other

incident directions may also offer valley splitting prop-
erties, in particular when the incidence is directed to-
wards one of the lobules of pseudomagnetic field, (see
Fig. 7). This is also consistent with the results within

FIG. 7. (Color online) Trajectories of \( \langle \vec{r} \rangle \) (black) of an inci-
dent wave packet coming from the bottom with \( E = 110 \) meV
for different impact parameters plotted on top of the pseudo-
magnetic field profile for valleys \( K \) (left column) and \( K' \)
(right column) with \( g = 0 \) (a-b) and \( g = 3 \) eV (c-d).

the Born approximation when the scalar field is present

(see Fig 2d); vertical incidence produce directions around

60° and 120° degrees with high valley polarization.

Finally we explore the relation between the deflection

angle \( \theta \) and the impact parameter for horizontal (Fig. 6)
and vertical (Fig. 7) incidences and are depicted in Fig. 8.

In the case of horizontal incidence, we call the attention
to the fact that there is a small range of values for the

impact parameter (b/10) where one valley component

(\( K \)) is almost not deflected, while the other valley

(\( K' \)) presents two maximal values of deflection around zero,
the latter occurs in both situations with (Fig. 8a) and
without (Fig. 8b) scalar field. This valley asymmetric

behavior of the deflection angle is more pronounced in the
case of vertical incidence (Fig. 7c-d), where for small im-

pact parameters (b/10) each valley component is directed
towards opposite directions. More interesting is the fact

FIG. 8. (Color online) Trajectories of \( \langle \vec{r} \rangle \) (black) of an inci-
dent wave packet coming from the left with \( E = 110 \) meV
for different impact parameters plotted on top of the pseudo-
magnetic field profile for valleys \( K \) (left column) and \( K' \)
(right column) with \( g = 0 \) (a-b) and \( g = 3 \) eV (c-d).
that for bigger impact parameters \((b/10 < x_0 < b)\) the valley changes when the scalar field is present, making possible to control this degree of freedom.

V. CONCLUSIONS

Using the low energy approximation to describe the interaction between deformations and electrons moving in a graphene membrane, we have described the role of the scalar field in the ability of Gaussian bumps to generate valley polarization and valley splitting/polarization in graphene systems. Our results were obtained using an analytical approach based on the Born approximation. In addition, we characterize the valley asymmetric scattering by introducing a valley polarization efficiency, \(\mathcal{P}\), that clearly shows the polarization effects. We also use a dynamical approach and studied the wave-packet dynamics of an encounter with the pseudomagnetic profile caused by a Gaussian bump. We present results for the average trajectories of wave packets in locally strained graphene that clearly shows the enhancement of the wave packet focusing and beam splitting effects when the scalar field is present. We believe that these results can be exploited in the implementation of valleytronic devices.

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Appendix A: Evaluation of integrals in Eq.\(^\text{[A4]}\)

We depart from the integral formula\(^\text{[B7]}\),

\[
\int_0^\infty e^{-a^2t^2} t^{\nu+1} J_{\nu}(bt) dt = \frac{b^\nu}{(2a^2)^{\nu+1}} e^{-\frac{b^2}{4a^2}} \quad (A1)
\]

where \(J_{\nu}\) is the Bessel function of order \(\nu\). With this formula we can evaluate Eq.\(^\text{[A4]}\) for \(n = 2\). In order to evaluate the integral when \(n = 0\) we can derivate both sides of Eq.\(^\text{[A1]}\) with respect of \(a\), to obtain

\[
\int_0^\infty e^{-a^2t^2} t^{\nu+3} J_{\nu}(bt) dt = \frac{2b^\nu}{(2a^2)^{\nu+2}} \left[ \nu + 1 - \frac{b^2}{4a^2} \right] e^{-\frac{b^2}{4a^2}} \quad (A2)
\]

Appendix B: Numerical Methodology

We start by writing the Dirac Hamiltonian for each valley in the following way,

\[
H_\eta = v_F \sigma_\eta \cdot (\vec{p} - \eta \vec{A}(r)) + V(r) = H^o_\eta + U_\eta(r), \quad (B1)
\]

where the term

\[
H^o_\eta = v_F \sigma_\eta \cdot \vec{p} \quad (B2)
\]

is the bare Hamiltonian for graphene (without strains), at the valley \(K (\eta = 1)\) or \(K' (\eta = -1)\), and depends only on the momentum operator, whereas the strain and scalar potential part is carried by \(U_\eta(r)\), given by Eq.\(^\text{[A9]}\). Note that \([H^o_\eta, U_\eta(r)] \neq 0\), nevertheless, the corresponding time evolution operator \(U_\eta(t) = \exp(-iH_\eta t - t_o)/\hbar\) can be approximated using the standard time-splitting spectral method that consists in a second order Trotter decomposition of the evolution operator at any given time step \(\Delta t\).

\[
U_\eta(t) \approx e^{-iU_\eta \Delta t/2\hbar} e^{-iH^o_\eta \Delta t/\hbar} e^{-iU_\eta \Delta t/2\hbar} + O(\Delta t^3), \quad (B3)
\]

which conveniently decomposes the application of the time-evolution operator in kinetic and potential terms. Then the wave function \(\psi_\eta(t + \Delta t)\) can be obtained in terms of \(\psi_\eta(t)\) by the application of the time evolution operator as follows,

\[
\Psi_\eta(t + \Delta t) \simeq e^{-iU_\eta \Delta t/2\hbar} e^{-iH^o_\eta \Delta t/\hbar} e^{-iU_\eta \Delta t/2\hbar} \Psi_\eta(t), \quad (B4)
\]

which is correct up to second order in \(\Delta t\). Note that the terms within \(H^o_\eta\) do not commute with each other, and neither the terms within \(U_\eta\) as \([\sigma_x, \sigma_y] = 2i\sigma_z\). Thus to avoid diagonalization at each time step, it is convenient to split Eq.\(^\text{[B4]}\) even further. In order to do this we employ the Zassenhaus formula instead, which establish that for any two linear noncommutative \(X\) and \(Y\) operators in the Lie algebra

\[
e^{i(X+Y)} = e^{iX} e^{iY} e^{-\frac{\sigma_y}{2}[X,Y]} e^{\sigma_y^0} (2[Y,[X,Y]]+[X,[X,Y]])... \quad (B5)
\]

in which the exponents of higher order in \(t\) are likewise homogeneous Lie polynomials (nested commutators). Thus we can approximate the time evolution operator as a sequential product of exponential terms of the form \(e^{iA_\sigma}\), where \(\hat{A}\) is an operator that depends either on momentum or the position and the \(\sigma_\mu = \{\sigma_0, \sigma_x, \sigma_y, \sigma_z\}\).

When \(\hat{A}\) is position dependent only its application is straightforward, but when it depends on momentum we use the Cayley’s expansion

\[
e^{iA_\sigma_\mu} \simeq \left(1 + \frac{i}{2} \hat{A}_\sigma_\mu \right) (1 - \frac{i}{2} \hat{A}_\sigma_\mu^{-1}) + O(\hat{A}^2) \quad (B6)
\]

for the exponentials to ensure unitarity and particle conservation at each time step.
