



Low-energy quantum scattering induced by graphene ripples



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ABSTRACT

We report a quantum study of the carrier scattering induced by graphene ripples. Crucial differences between the scattering induced by the ripple and ordinary scattering were found. In contrast to the latter, in which the Born approximation is valid for high-energy process, the former is valid for the low-energy process with a quite broad energy range. Furthermore, in polar symmetry ripples, the scattering amplitude exhibits a pseudo-spin structure, an additional factor $\cos\theta/2$, which leads to an absence of backward scattering. We also elucidate that the scattering cross sections are proportional to the energy cubed of the incident carrier.

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1. Introduction

Graphene [1,2], which is a single atomic layer of carbon, is a two-dimensional crystal that can be embedded into a three-dimensional space. In the past decade, its isolation has attracted a substantial amount of theoretical and experimental research, most of which stemmed from the peculiar behavior of graphene carriers. Many applications focus on the flat graphene, in which the movement of carriers was represented by the Dirac Hamiltonian with massless fermion in $2 + 1$ dimensional space–time [3–5].

Iorio et al. [6–10] studied the Weyl-gauge symmetry of graphene Hamiltonian and its application to gravity research. Their results revealed that if one accepts the flat space–time description of conduct electron, one must also accept a curved space–time description because through a Weyl redefinition of the fields, actions are the same.

However, the Dirac description of graphene is only valid for low energies and small momentum around the Dirac points $ka_l \ll 1$, where $a_l \sim 10^{-10}$ m is the nearest carbon-to-carbon distance. In other words, the Dirac description of graphene is valid for carrier energies satisfying $E = \hbar v_F k \ll E_l = \hbar v_F / a_l \simeq 3$ eV. Then, in the following, we restrict all the discussions in the constraints $|E| \ll 3$ eV around the Dirac points.

It is well known that both experimental and theoretical studies have revealed that graphene is always corrugated and covered by ripples, which can be either intrinsic [11,12] or induced by roughness of substrate [13,14]. Although graphene ripples complicate the system, they also extend their application because additional adjustable parameters are associated with the ripples [2,15].

For instance, incident carriers are scattered or deflected by the nonzero curvature induced by graphene ripples. However, in such process the quantum behaviors of the carriers should be considered. In fact, many questions remain, such as the role of the pseudospin in the scattering process.

Katsnelson and Geim [16] have studied the influence on the electronic quality by the corrugation scattering effect using a fractal dimension theory. They showed that when the corrugation graphene can be depicted by a fractal dimensional surface, i.e. the height-correlation function behaviors as $\langle [h(\mathbf{r}) - h(0)]^2 \rangle \propto r^{2H}$, the effective potential is a long-range one, such as Eq. (15) in Ref. [16]. However, when graphene ripples cannot be depicted by fractal dimension theory, the detailed study on the quantum scattering induced by, for instance, isolated ripple, is needed.

In this manuscript we report a quantum study on the carrier scattering induced by graphene ripples. Surprisingly, our study showed a crucial difference between the scattering induced by the graphene ripple and ordinary scattering. In the latter, the Born approximation was valid in the high-energy process, whereas in the scattering by typical graphene ripples, the Born approximation showed an opposite validity but with a quite broad energy range provided the Dirac description of graphene is valid. We furthermore showed that, in a polar symmetry ripple, the scattering process emerged an explicit pseudospin structure, in which an

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additional factor $\cos \theta/2$ was exhibited in the expression of scattering amplitude, which leads to the absence of backward scattering. Compared to ordinary quantum scattering, the scattering cross sections were proportional to the energy cubed of the incident carrier. Furthermore, the Hamiltonian also showed that if the graphene was bent in only one direction, its properties did not change if there is no phase transition because suitable parameters could be rearranged.

2. Hamiltonian in the ripple graphene

In this study, we assume that the graphene is not consistently flat, that is, the curvature of graphene is not zero. To depict the curvature, we first formulate graphene metric.

A curve graphene can be considered a two-dimensional surface embedded in a three-dimensional space. The surface is defined by the function $z(\mathbf{r})$, which is the height with respect to the $z = 0$ plane and $\mathbf{r} = (x, y)$ is the coordination in $z = 0$ plane, as shown in Eq. (1):

$$dz^2 = z_x^2 dx^2 + z_y^2 dy^2 + 2z_x z_y dx dy, \quad (1)$$

where $z_x = \frac{\partial z}{\partial x}$, $z_y = \frac{\partial z}{\partial y}$, $z_{xy} = \frac{\partial^2 z}{\partial x \partial y}$ etc.

The space-time metric is (in this study we set $\hbar = v_F \equiv 1$)

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -(z_x(x, y)^2 + 1) & -z_x(x, y)z_y(x, y) \\ 0 & -z_x(x, y)z_y(x, y) & -(z_y(x, y)^2 + 1) \end{pmatrix}, \quad (2)$$

where the zeroth component on 2 + 1 dimensional space-time, t , does not mix with space components. Thus, in the following, the zeroth component is ignored if there is no confusion.

The vielbein fields $e^a_{\mu}(x, y)$, which satisfy $e^a_{\mu} e^b_{\nu} \eta_{ab} = g_{\mu\nu}$ with the constant metric $\eta_{a,b} = \text{diag}\{-1, -1\}$ is chosen as $e^1_2 = e^2_1$,

$$e^a_{\mu} = \begin{pmatrix} \frac{z_x^2 \sqrt{z_x^2 + z_y^2 + 1} + z_y^2}{z_x^2 + z_y^2} & \frac{z_x z_y (\sqrt{z_x^2 + z_y^2 + 1} - 1)}{z_x^2 + z_y^2} \\ \frac{z_x z_y (\sqrt{z_x^2 + z_y^2 + 1} - 1)}{z_x^2 + z_y^2} & \frac{z_y^2 \sqrt{z_x^2 + z_y^2 + 1} + z_x^2}{z_x^2 + z_y^2} \end{pmatrix}. \quad (3)$$

This choice guarantees that when graphene is flat, vielbein matrices are consistently unitary transformations.

Because the affine connection are defined by $\Gamma^{\mu}_{\nu\lambda} = \frac{1}{2} g^{\rho\mu} (g_{\rho\nu, \lambda} + g_{\rho\lambda, \nu} - g_{\nu\lambda, \rho})$, the affine connections are read as

$$\Gamma_1 = \Gamma_{1\nu}^{\mu} = \begin{pmatrix} \frac{z_x z_{xx}}{1+z_x^2+z_y^2} & \frac{z_x z_{xy}}{1+z_x^2+z_y^2} \\ \frac{z_y z_{xx}}{1+z_x^2+z_y^2} & \frac{z_y z_{xy}}{1+z_x^2+z_y^2} \end{pmatrix},$$

$$\Gamma_2 = \Gamma_{2\nu}^{\mu} = \begin{pmatrix} \frac{z_x z_{xy}}{1+z_x^2+z_y^2} & \frac{z_x z_{yy}}{1+z_x^2+z_y^2} \\ \frac{z_y z_{xy}}{1+z_x^2+z_y^2} & \frac{z_y z_{yy}}{1+z_x^2+z_y^2} \end{pmatrix}. \quad (4)$$

In flat space, the gamma matrices are

$$\gamma^i = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \gamma^j = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix},$$

$$\gamma^0 = \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (5)$$

Whereas in ripple graphene they are defined as $\gamma^{\mu} = e^{\mu}_a \gamma^a$,

$$\gamma^1 = \begin{pmatrix} 0 & \frac{z_x}{\sqrt{1+z_x^2+z_y^2}} + iz_y \\ iz_y - \frac{z_x}{\sqrt{1+z_x^2+z_y^2}} & 0 \end{pmatrix},$$

$$\gamma^2 = \begin{pmatrix} 0 & \frac{z_y}{\sqrt{1+z_x^2+z_y^2}} - iz_x \\ -iz_x - \frac{z_y}{\sqrt{1+z_x^2+z_y^2}} & 0 \end{pmatrix}. \quad (6)$$

When the spin connection coefficient is defined as $\omega_{\lambda}^{ab} = e^{a\sigma} (e^b_{\sigma, \mu} - \Gamma^{\lambda}_{\mu\sigma} e^b_{\lambda})$, and the spin connection is defined as $\Omega_{\mu} = \frac{1}{8} \omega_{\mu}^{ab} [\gamma_a, \gamma_b]$, we find

$$\Omega_1 = \Omega \begin{pmatrix} \frac{z_x z_{xy} - z_y z_{xx}}{z_x^2 + z_y^2} & 0 \\ 0 & \frac{z_y z_{xx} - z_x z_{xy}}{z_x^2 + z_y^2} \end{pmatrix},$$

$$\Omega_2 = \Omega \begin{pmatrix} \frac{z_x z_{yy} - z_y z_{xy}}{z_x^2 + z_y^2} & 0 \\ 0 & \frac{z_y z_{xy} - z_x z_{yy}}{z_x^2 + z_y^2} \end{pmatrix}, \quad (7)$$

with $\Omega = \frac{i(\sqrt{1+z_x^2+z_y^2}-1)}{2\sqrt{1+z_x^2+z_y^2}}$.

The Hamiltonian is a very complex 2×2 matrix, as shown in Eq. (8),

$$H_{11} = H_{22} = 0,$$

$$H_{12} = -\frac{i}{z_x + iz_y} \left\{ (-iz_x + \frac{z_y}{\sqrt{1+z_x^2+z_y^2}}) (\partial_y - \frac{i(\sqrt{1+z_x^2+z_y^2}-1)(z_x z_{yy} - z_{xy} z_y)}{2(z_x^2+z_y^2)\sqrt{1+z_x^2+z_y^2}}) + (iz_y + \frac{z_x}{\sqrt{1+z_x^2+z_y^2}}) (\partial_x - \frac{i(z_x z_{xy} - z_{xx} z_y)(\sqrt{1+z_x^2+z_y^2}-1)}{2(z_x^2+z_y^2)\sqrt{1+z_x^2+z_y^2}}) \right\},$$

$$H_{21} = -\frac{i}{z_x - iz_y} \left\{ (iz_x + \frac{z_y}{\sqrt{1+z_x^2+z_y^2}}) (\partial_y + \frac{i(\sqrt{1+z_x^2+z_y^2}-1)(z_x z_{yy} - z_{xy} z_y)}{2(z_x^2+z_y^2)\sqrt{1+z_x^2+z_y^2}}) - (iz_y - \frac{z_x}{\sqrt{1+z_x^2+z_y^2}}) (\partial_x + \frac{i(z_x z_{xy} - z_{xx} z_y)(\sqrt{1+z_x^2+z_y^2}-1)}{2(z_x^2+z_y^2)\sqrt{1+z_x^2+z_y^2}}) \right\}. \quad (8)$$

However, the complexity of the Hamiltonian should not be intimidating. If graphene is only bent in x-direction, that is, $z_y = z_{xy} = 0$, the Hamiltonian becomes

$$H' = \begin{pmatrix} 0 & -\partial_y - \frac{i\partial_x}{\sqrt{1+z_x^2}} \\ \partial_y - \frac{i\partial_x}{\sqrt{1+z_x^2}} & 0 \end{pmatrix}.$$

In the above expression, if we make a substitution $x \rightarrow x'$ and $y \rightarrow y'$, where $y' = y$ and $x' = \int_0^x \sqrt{1+z_x^2} dx$, the Hamiltonian is the same as the one in flat graphene. The physics effect is a Fermi velocity renormalization in x-direction, $v_F \rightarrow \frac{v_F}{\sqrt{1+z_x^2}}$.

Such bend leads to an effective potential. To illustrate this point

we consider a bent graphene depicted by $z(x) = \begin{cases} 0, & \text{I: } x \leq 0 \\ cx, & \text{II: } 0 < x < d \\ cd, & \text{III: } x \geq d \end{cases}$ and normal incident conduction electrons (with energy $k > 0$) in the left side. In this case $z_x = c$ at region II and $z_x = 0$ at regions I and III. Wave functions in three regions are

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