Dirac electrons in a Kronig-Penney potential: Dispersion relation and transmission periodic in the strength of the barriers

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The transmission T and conductance G through one or multiple one-dimensional, δ-function barriers of two-dimensional fermions with a linear energy spectrum are studied. T and G are periodic functions of the strength P of the δ-function barrier V(x,y)/ℏcP=Pδ(x). The dispersion relation of a Kronig-Penney (KP) model of a superlattice is also a periodic function of P and causes collimation of an incident electron beam for P=2m and n integer. For a KP superlattice with alternating sign of the height of the barriers the Dirac point becomes a Dirac line for P=(n+1/2)π.

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I. INTRODUCTION

The study of particle motion in periodic potentials is at the heart of condensed-matter physics and it is usually assumed that the energy spectrum is parabolic. One of the earliest examples is the well-known, one-dimensional (1D) Kronig-Penney (KP) model1 that consists of an infinite succession of very thin (W→0) and very high (V₀→∞) barriers, referred to as δ-function barriers but such that their product P=V₀ remains constant. This results in minibands in the electron spectrum.

One may wonder how such results are modified if the energy is linear-in-wave vector. Such a spectrum occurs for relativistic electrons with energy E=ℏcP≫E₀=mc², where c is the speed of light and m₀ the bare electron rest mass. Even without neglecting E₀ a strict 1D Dirac KP model was considered for relativistic quarks.2 It is also known that electrons can transmit perfectly, upon normal incidence, through arbitrarily wide and high barriers, referred to as Klein paradox or Klein tunneling.3 With the discovery of graphene,4 a one-atom-thick layer of carbon atoms, another system became available in which particles (electrons) moving in two dimensions, have a linear spectrum, E=ℏνk, with k=(kₓ,kᵧ) the wave vector. Importantly, carriers in graphene behave as chiral, massless fermions described by Dirac’s equation without the mass term and move with the Fermi velocity v_F=c/300. There is a wealth of exceptional properties of graphene; see, e.g., Ref. 5.

Because the carriers in graphene move in two dimensions, tunneling through barriers is inherently two dimensional (2D) and depends on the direction of the incident electron beam even in the absence of a magnetic field. Many authors, including ourselves, have studied this tunneling, through single, multiple barriers, and superlattices.6,7 Surprisingly, tunneling through δ-function barriers has received very little attention8 and we are not aware of any Dirac KP model for a superlattice in graphene. An interesting development was the application of periodic potentials to graphene that turned it into a self-collimating material despite the rather unusually high potentials used.9

Motivated by all these results and the absence of a systematic treatment of KP barriers or superlattices, we study in this work the transmission through such structures as well as the dispersion relation of a KP superlattice. Although the model may appear a bit unrealistic since a relatively smooth potential is needed to describe the carrier dynamics by the Dirac equation,10 its simplicity is attractive and elucidates certain symmetry properties of the spectrum. Furthermore one can realize the model by using a potential which is smooth on the scale of the atomic distance while the barrier width should remain small compared to the typical electron wavelength. The unexpected results mentioned in the abstract are in sharp contrast with those for carriers with a parabolic energy spectrum described by the Schrödinger equation. We will use graphene as an example but the results apply to any 2D system with a linear-in-wave-vector spectrum and a two-component spinor.

II. TRANSMISSION THROUGH A δ-FUNCTION BARRIER

We describe the electronic structure of an infinitely large flat graphene flake in single valley approximation by the zero-mass Dirac equation and consider solutions with energy and wave vector near the K point. The Hamiltonian is $\mathcal{H} = \nu_F \sigma \cdot \vec{p} + iV$ with $\vec{p}$ the momentum operator and 1 the 2×2 unit matrix. In the presence of a 1D potential V(x) the equation $(\mathcal{H}−E)\psi=0$ admits solutions of the form $\psi(x)e^{i\phi_0}$, where

$$\psi(x) = \begin{cases} 1 & e^{i\lambda x}, \\ 1 & e^{-i\lambda x} \end{cases}$$

with tan $\phi = k_y/\lambda$, $s =$ sign[$\epsilon−u(x)$], $\lambda = [(\epsilon−u(x))^2−k_y^2]^{1/2}$, $\epsilon = E/\nu_F\hbar$, and $u(x)=V(x)/\nu_F\hbar$; $\epsilon$ and $u(x)$ are in units of inverse length. As usual, we approximate a δ-function barrier with a very thin and very high barrier, of width W(−0) and height V₀(−→∞) but keep constant the dimensionless product $P=\hbar v_F/W$ which we call its strength. Referring to Eq. (1) and Fig. 1, the wave function in each of the regions (1)−(3) can be written as a superposition of the eigenstates of Eq. (1) $\psi_n(x)=\sum_{\alpha} A_{\alpha n} \phi_n(x)$, with coefficients $A=(A,B)^T$ and...
The two-terminal conductance is $G = G_0 \int_{-\pi/2}^{\pi/2} T(P, \phi) \cos \phi d\phi$, with $G_0 = 2E_F L_{12} e^2 / (\hbar^2)$ and $L_{12}$.

**Conductance**

The two-terminal conductance is $G = G_0 \int_{-\pi/2}^{\pi/2} T(P, \phi) \cos \phi d\phi$, with $G_0 = 2E_F L_{12} e^2 / (\hbar^2)$ and $L_{12}$.
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Equations with barriers, characterized by the KP model we replace the square barriers by transfer matrix for a conditions we can extract the relation with fermions and gives the spectrum. The solution of Eq. shows the transmission through two parallel barriers. The periodicity in the transmission is also present in the conductance G. We show G in Fig. 4(a) for parallel and in Fig. 4(b) for antiparallel δ-function barriers.

IV. KRONIG-PENNEY MODEL

For an infinite number of periodic square barriers, one can tune the system into a self-collimating material. For special values of W, L and k it was found in Ref. 9 that the dispersion relation near the K point is almost linear in k and constant along k. The system thus behaves as a 1D metal. We look for similar results using δ-function barriers. Within the KP model we replace the square barriers by δ-function barriers, characterized by V(x, y) = ∑ n=−∞ ϕ(0) and A 2 = A 1, with k the Bloch wave vector. From these conditions we can extract the relation e−ikx A 1 (1) A 2 = and M(x) given by Eq. (2). Then setting the determinant of the matrix for a δ-function barrier leads to (λ = sin 4 P 2) = 0, directly onto that for strictly 1D fermions 2 and gives the spectrum

with n an integer.

Equation (9) contrasts very sharply with that for 2D electrons with a parabolic spectrum in a 1D KP potential which, with λ = [2 μP λ 2 P 2], and μ = mv L/ℏs, reads

the resulting dispersion relation is not periodic in P.

Properties of the spectrum

Since the dispersion relation is periodic in P, with period 2π, it is sufficient to study it only for 0 = P = 2π. For particular values of P we find

(1) P = 2π → ε = ± [k 2 + k 2 2π 2] 1/2,

(2) P = π → ε = ± [k 2 + k 2 2n + 1] 1/2,

(3) P = π/2 → cos k = ± (−)ε sin λ/λ.

In limiting cases we are able to obtain explicit expressions for E = E(k, k). We expand the dispersion relation for small k, and ε = P. The resulting quadratic equation for ε is solved by

For small k, we can replace the term 4 sin 2(k L/2) by k 2. Notice that for k = 0 we find ε = P ± k sin P/P which is a linear spectrum with a reduced velocity. For k = 0, we have ε = P ± 2 sin(k L/2), which is linear for small k, but possesses a typical band shape for large k = π. For small k > k, sin P/P we have

For P ≫ 1, ε is highly anisotropic and nearly flat vs k.

Relation to the spectrum of a square superlattice. We now look whether we can find an energy spectrum similar to that of Ref. 9 pertinent to square barriers, with height V 0 = 720 meV, width W = 5 nm, and unit-cell length L = 10 nm. In our units these values correspond to P.
In Fig. 6 the Fermi level in these units is $e_F=2\pi$ and lead to $e=\pm[k_x^2+(k_y+2n\pi)^2]^{1/2}$. Since the Fermi level in these units is $e_F=2\pi=P$, we look for the spectrum near the value $e=\pm[k_x^2+(k_y+2n\pi)^2]^{1/2}$. Although these bands seem to fulfill our demands because the dispersion looks rather flat in the $k_x$ direction, the concern is that we would obtain the same dispersion for $P=0$ and $e_F=2\pi$ but never by folding the conelike dispersion of graphene and results simply from working in the reduced-zone scheme. Consequently no new fundamental physics should be attached to it. Further, from this correspondence we expect and found that for square barriers with $P=2mn$, the situation is more favorable for the occurrence of collimation. It follows that the collimation effect is also obtainable for barriers that are lower than the unusually high ones of Ref. 9 if one uses longer unit-cell periods.

V. EXTENDED KRONIG-PENNEY MODEL

The square barriers are replaced by alternating-in-sign $\delta$-function barriers. The unit cell of the periodic potential contains one such barrier up, at $x=0$, followed by a barrier down, at $x=1/2$. The resulting transfer matrix leads to

$$e=\cos\phi=k_x=\cos\lambda-(2k_x^2/\lambda^2)\sin^2(\lambda/2)\sin^2 P,$$  

where $\tan \phi=k_x/\lambda$. From Eq. (15) we deduce that the dispersion is periodic in $P$, with period $\pi$, and has the following properties:

1. it is invariant for $e \rightarrow -e$ and $P \rightarrow \pi - P$,

2. $P=\pi n \rightarrow e=\pm[k_x^2+(k_y+2n\pi)^2]^{1/2}$,

3. $P=\pi/2 \rightarrow (e,k_x,k_y)=(0,0,k_y)$.  

In Fig. 6(a) we show the spectrum for $P=\pi/2$. As seen, it is almost independent of $k_y$ for small energies while in the $k_x$ direction the bands are linear; this is an advantageous situation for self-collimation. For $k_x=0$ we obtain the linear spectrum

$$e=\pm|k_x|+2n\pi,$$  

with the Dirac point at $e=0$. We can also find an explicit expression for $k_x=0$. Solving Eq. (15) gives

$$e=\pm|k_x|\cos P.$$  

Then the group velocity $v_x=\partial e/\partial k_x$ becomes small if $P=\pi/2+2n\pi$. Figure 6(b) shows the energy spectrum for $P=\pi/4$, the Dirac cone becomes anisotropic, as the spectrum flattens in the $k_y$ direction.

We now consider the case where $k_x$ and $k_y$ are nonzero. If $e \ll 1$ then the right-hand side of Eq. (15) can be expanded in $e$. This leads to a quadratic equation for $e$ with solutions

$$e=\pm|k_x|[\cosh k_x\cos k_y-f]/(k_x/2)\cos^2 P \sinh k_y+f$$

$$\pm|k_x|\sin|k_x|/2)/\sinh|k_x|/2)$$  

where $f=2\sin^2 P \sin^2(k_x/2)$. For $k_y=0$ we find the result given by Eq. (13), that is, $e=\pm 2\sin|k_x|/2$ which is linear for small $k_x$.

VI. CONCLUSIONS

In summary, we studied the transmission and conductance of fermions, with energy linear-in wave vector, through one and two $\delta$-function barriers and the energy spectrum of a KP superlattice. For very high ($V_0 \rightarrow \infty$) and very thin ($W \rightarrow 0$) barriers we showed that they are periodic functions of their strength $P=WV_0/\hbar v_F$, where $v_F$ is the Fermi velocity. Further, we showed that a KP superlattice has an energy spectrum that is a periodic function of $P$, which is in sharp contrast with that obtained from the Schrödinger equation. An important consequence of that is collimation of an incident electron beam that here occurs for $P=2\pi n$ with $n$ an integer. We also obtained various explicit but approximate dispersion relations, e.g., for small wave vector $k=|k_x,k_y|$. Given the intense research activity in graphene and the very recent experimental verification of Klein tunneling, we expect that this periodic dependence on the strength $P$ will be tested in a near future.

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