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2011 J. Phys. A: Math. Theor. 44 475305

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Graphene tests of Klein phenomena

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Received 11 July 2011, in final form 27 September 2011

Published 4 November 2011

Online at stacks.iop.org/JPhysA/44/475305

Abstract

Graphene is characterized by chiral electronic excitations. As such it provides a perfect testing ground for the production of Klein pairs (electron/holes). If confirmed, the standard results for barrier phenomena must be reconsidered with, as a byproduct, the accumulation within the barrier of holes.

PACS number: 03.65.-w

1. Introduction

Graphene is a subject of intense interest in the scientific community. After the assignment of the 2010 Nobel prize in Physics, for the experimental realization of graphene obtained by extracting single atomic thick crystallites from bulk graphite, to Geim and Novoselov [1, 2], many papers appear every day with new and interesting discussions about the properties of this intriguing material. Due to this vast amount of literature, periodic updates are needed to cover the recent progress. The most explored aspects of graphene physics are related to its electronic properties. Due to the fact that electrons propagating through graphene lose their effective mass, they are described by a Dirac-like equation rather than the Schrödinger equation. This opens the doors to new possibilities of exploring effects that were previously inaccessible. The massless Dirac equation in graphite intercalation compounds was first pointed out in 1984 [3]. Nevertheless, the first observation of the Dirac fermion nature of electrons in graphene [4, 5] was only provided when graphene was mechanically exfoliated on SiO₂ [1, 2]. Relativistic phenomena related to Zitterbewegung [6], chirality and minimal conductivity [7, 8], Klein tunneling [9], quantum Hall effect [10, 11], Schwinger production [12], Casimir interactions [13] and transformations of the discrete Landau level spectrum to a continuum of extended states in the presence of a static electric field [14] have been investigated and when possible tested by using this rich and surprising material. For an extensive theoretical review of the properties of electron transport in graphene, we refer the reader to the report of Castro [15].

In the last year, as observed by Geim [16], the initial skepticism with respect to graphene applications was gradually evaporating and graphene has rapidly changed its status from newcomer to star. The study presented in this paper was inspired by the possibility of

understanding, by an experiment with graphene, the physics which governs a well-known phenomenon of the Dirac equation known as Klein paradox [17], i.e. for the step potential the reflected flux can be larger than the incident one [18]. This relativistic effect is attributed to the fact that sufficiently strong potentials open the door to pair production and consequently to positrons inside the potential region. This result is generally accepted for a step potential but not always quoted for a barrier potential where plane wave solutions *seem* not to exhibit pair production [19]. Pair production at the discontinuity of square potentials has never been observed experimentally because its observation requires very strong electric fields [20]. The transmission of an electron through graphene heterojunctions [21–23] could now provide an experimental signature of the Klein pair production.

Graphene is a two-dimensional structure characterized by chiral (mass zero) electronic excitations one of whose equations of motion reads

$$-i \hbar v_F \boldsymbol{\sigma} \cdot \nabla \psi_F(\mathbf{r}) = E \psi_F(\mathbf{r}), \quad (1)$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, 0)$ and $v_F \approx 10^6 \text{ m s}^{-1}$ is the Fermi velocity. This equation mimics one of the two-dimensional free Weyl equations [18, 24] for a (Weyl) spinor if we substitute v_F by the velocity of light c . In the following, we shall present the results for the Weyl equation for a potential barrier via the well-trying step method [25–27]. Consequently, we ‘reconsider’ the hypothesis of Klein pair production [17] for the step potential. The step potential is actually a purely abstract construct, because of its infinite extension (same abstraction of plane waves). However, as we have demonstrated elsewhere with the Dirac equation [26], the step potential is a useful tool for general piece-wise potential calculations. Contrary to a common misconception, it is compatible with a very large barrier potential. We will have the opportunity to reassert this fact here with our results for the Weyl equation. Furthermore, and this is essential to our conclusions, if Klein pair production occurs for a step, it must *also* occur for a barrier potential [19].

For the Dirac equation [18, 28], the so-called Klein energy zone (where Klein pair production is possible) requires a step potential height V_0 of at least $2m$ (m the mass of the fermion). For a free electron, this means $V_0 > 1 \text{ MeV}$, not a typical laboratory potential energy step. Not surprisingly, experimental verification of Klein pair production has not been achieved to date. Neutrinos are a possible alternative choice of particle since they are now known to have a very small mass, but the weak nature of their interactions introduces formidable experimental difficulties [29]. The best alternative ‘particle’ is that of electrons within a dielectric with effective masses m_* much smaller than the free electron mass. Graphene, with a null effective electron mass, is the most promising material of all to study. A step potential of any height could test the creation of Klein pairs (electron–hole) and as we have anticipated, this has consequences even for the barrier potential seen within the graphene structure.

In the next section, we calculate, in three dimensions for completeness, the chiral interaction with a step and subsequently in section 3 that with a barrier potential. The arguments require a discussion of an incoming wave packet and resolves the apparent paradox that a step has a single transmitted wave packet (both for the diffusion zone and the Klein zone), while a long barrier gives rise to infinite wave packets. We shall again argue that nevertheless the step and barrier results are perfectly compatible. In section 4, we discuss Klein pair production. We also show that for this case the transmission/reflection amplitude series are divergent. The finite standard (matrix) results are radically different. They do not involve pair production. The application to graphene is straightforward. We argue that the barriers within graphene act as a ‘well-trap’ for the created ‘antiparticles’. This should result in a growth in time of positive charge within the well/barrier. We suggest the detection of such an accumulating charge as a proof of Klein pair production.

2. Weyl interaction with a step potential

The spinor Weyl equation for a positive helicity (massless) state is [18]

$$-i \boldsymbol{\sigma} \cdot \nabla \Psi(\mathbf{r}, t) = i \partial_t \Psi(\mathbf{r}, t) / c. \quad (2)$$

Plane wave solutions of the kind $\psi(\mathbf{r}) = u(\mathbf{p}) \exp[i(\mathbf{p} \cdot \mathbf{r} - Et)/\hbar]$, where $E = |\mathbf{p}|c$ and \mathbf{p} is the particle three-momentum, result in the spinor equation

$$\boldsymbol{\sigma} \cdot \mathbf{p} u(\mathbf{p}) = E u(\mathbf{p}) / c, \quad (3)$$

the solution of which is

$$u(\mathbf{p}) = \sqrt{\frac{E + p_3c}{2E}} \begin{bmatrix} 1 & \frac{p_1c + ip_2c}{E + p_3c} \end{bmatrix}^t, \quad (4)$$

where the upper index t represents the transpose. Our step potential is chosen in the x variable. Without loss of generality, we set the discontinuity at $x = 0$,

$$V(x) = \{0 \text{ for } x < 0 \text{ region I, } V_0 > 0 \text{ for } x > 0 \text{ region II}\}.$$

In region I ($x < 0$), we have set the incoming momentum as $\mathbf{p} = (p_1, p_2, p_3)$ with

$$p_1c = \sqrt{E^2 - (p_2c)^2 - (p_3c)^2}.$$

In region II ($x > 0$), only p_1 changes. We call the new momentum $\mathbf{q} = (q_1, p_2, p_3)$ with

$$q_1c = \sqrt{(E - V_0)^2 - (p_2c)^2 - (p_3c)^2}.$$

The continuity equation for $\Psi(\mathbf{r}, t)$ at $x = 0$ is

$$\begin{aligned} & \begin{bmatrix} 1 & \frac{p_1c + ip_2c}{E + p_3c} \end{bmatrix}^t + r_0 \begin{bmatrix} 1 & \frac{-p_1c + ip_2c}{E + p_3c} \end{bmatrix}^t \\ &= \underbrace{\sqrt{\frac{E(E - V_0 + p_3c)}{(E - V_0)(E + p_3c)}}}_N t_0 \begin{bmatrix} 1 & \frac{q_1c + ip_2c}{E - V_0 + p_3c} \end{bmatrix}^t. \end{aligned} \quad (5)$$

After a straightforward calculation, we find

$$r_0 = \frac{1 - \alpha}{1 + \alpha} \quad \text{and} \quad t_0 = \frac{2}{N(1 + \alpha)}, \quad \text{with} \quad \alpha = \frac{q_1(E + p_3c) + ip_2V_0}{p_1(E - V_0 + p_3c)}. \quad (6)$$

Starting from the reflection probability,

$$|r_0|^2 = \frac{1 + |\alpha|^2 - 2 \operatorname{Re}[\alpha]}{1 + |\alpha|^2 + 2 \operatorname{Re}[\alpha]}, \quad (7)$$

there are specific cases to be considered.

The situation when $q_1^2 < 0$, i.e. when $p_2^2 + p_3^2 > [(E - V_0)/c]^2$, implies an imaginary q_1 and whence to ‘tunneling’ when penetration into the classically forbidden region II occurs. An imaginary momentum q_1 also implies $\operatorname{Re}[\alpha] = 0$; consequently, $|r_0| = 1$. We are not interested in evanescent solutions in this paper and henceforth consider only real momentum q_1 .

Diffusion occurs when $E > V_0 + \sqrt{p_2^2 + p_3^2} c$. In this case, $\text{Re}[\alpha] > 0$ and consequently $|r_0| < 1$. We treat this case in the next section. For $E < V_0 - \sqrt{p_2^2 + p_3^2} c$, we have again a real momentum q_1 but now $E - V_0 + p_3 c < E - V_0 + \sqrt{p_2^2 + p_3^2} c < 0$ and consequently $\text{Re}[\alpha] < 0$ which implies $|r_0| > 1$. This *Klein* energy zone is thus characterized by an oscillatory (free) plane wave in region II. The corresponding flux could, in principle, be interpreted as an *additional* incoming particle beam from $x = +\infty$, hence resulting in an excess of ‘reflected’ particles in region I, or in alternative as an antiparticle flux flowing in the positive x direction and ‘created’ at $x = 0$. The former choice contradicts our initial conditions of a sole incoming particle wave from the left ($x = -\infty$); it also implies the unpalatable concept of free *particles* that exist and propagate freely in the classically forbidden region below potential. The latter solution implies the creation of *Klein pairs*. The ‘antiparticles’ (energy $-E$) travel to the right, while the particles created (energy E) add to the reflected incoming particles and travel to the left, thus yielding $|r_0| > 1$. This latter interpretation is consistent with the fact that antiparticles see a potential of $-V_0$ and hence are above potential *free antiparticles*, since $-E > -V_0$. However, it must be recalled that this latter interpretation also implies that the particle/antiparticle number is not conserved (only *total* charge and other additive quantum numbers are conserved). Our spinor equation, as occurs for the Dirac equation, would thus no longer be a single-particle equation. Some have claimed this to be another positive feature of the Dirac equation since it anticipated pair creation in field theory.

3. Weyl diffusion with a barrier potential

The barrier potential $V(x) = \{V_0 \text{ for } 0 < x < L, 0 \text{ elsewhere}\}$ can be treated for calculational purposes as a two-‘step’ interaction. As we have shown in previous publications [25–27], it is also physically correct to consider it as such. A brief argument for this is as follows. Consider a numerical simulation of an incoming wave packet from the left, say with $E > V_0 + \sqrt{p_2^2 + p_3^2} c$ so that diffusion occurs. Upon reaching $x = 0$ (the barrier), the wave packet splits into two amplitudes: one the reflected wave, the other the transmitted wave moving in the region of the potential. The group velocity of the latter is of course lower than the incoming/reflected wave group velocity. When the wave packet reaches the end of the barrier, reflection and transmission occur anew. The very existence of a reflected wave for a downward step is the characteristic of quantum mechanics. This procedure repeats itself ad infinitum. Infinite reflected and transmitted wave packets are produced. If L is large compared to the wave packet size, the individual wave packets will be separated and interference effects are negligible. Incoherence reigns. Even when the barrier size is of order or smaller than the wave packets, this approach can be used except that now the overlapping wave packet amplitudes are coherent and must be summed. Separation into individual contributions may even be done for single plane waves which, of course, are totally coherent. The sum of the infinite contributions for plane waves yields exactly the same result as that deduced from a matrix calculation of the continuity equations. This argument can therefore be reversed. A wave packet convolution of a (matrix) barrier solution will yield infinite outgoing wave packets when L grows larger than the wave packet size. This is by no means obvious, but numerical calculations confirm this claim [25, 26].

We have called the above method of calculation the two-step approach to the barrier. However, it actually requires three-step results since the discontinuity at $x = 0$ receives waves impinging both from the left (the original wave) and from the right (reflected waves at $x = L$).

These three results are listed below. Any two can be derived from the third by implementing the momentum changes indicated, together with the appropriate plane wave phase changes.

- Step 1 [$x = 0$] (see section 2 for derivation):

incoming momentum $(E/c, p_1, p_2, p_3)$, reflected $(E/c, -p_1, p_2, p_3)$, transmitted $[(E - V_0)/c, q_1, p_2, p_3]$,

$$\begin{aligned} r_0 &= \frac{1 - \alpha}{1 + \alpha}, & \text{with } \alpha &= \frac{q_1(E + p_3c) + ip_2V_0}{p_1(E - V_0 + p_3c)}. \\ t_0 &= \frac{2}{N(1 + \alpha)}. \end{aligned} \quad (8)$$

- Step 2 [$x = L$]:

incoming momentum $[(E - V_0)/c, q_1, p_2, p_3]$, reflected $[(E - V_0)/c, -q_1, p_2, p_3]$, transmitted $(E/c, p_1, p_2, p_3)$,

$$\begin{aligned} r_L &= \frac{1 - \beta}{1 + \beta} e^{2iq_1L/\hbar}, & \text{with } \beta &= \frac{p_1(E - V_0 + p_3c) - ip_2V_0}{q_1(E + p_3c)}. \\ t_L &= \frac{2N}{1 + \beta} e^{i(q_1 - p_1)L/\hbar}. \end{aligned} \quad (9)$$

- Step 3 [$x = 0$]:

incoming momentum $[(E - V_0)/c, -q_1, p_2, p_3]$, reflected $[(E - V_0)/c, q_1, p_2, p_3]$, transmitted $(E/c, -p_1, p_2, p_3)$,

$$\begin{aligned} \tilde{r}_0 &= \frac{1 - \gamma}{1 + \gamma}, & \text{with } \gamma &= \frac{-p_1(E - V_0 + p_3c) - ip_2V_0}{-q_1(E + p_3c)} = \beta^*. \\ \tilde{t}_0 &= \frac{2N}{1 + \gamma}, \end{aligned} \quad (10)$$

Observing that $1 + \beta^* = (1 + \alpha)/\text{Re}[\alpha]$ and $1 - \beta = (\alpha - 1)/\text{Re}[\alpha]$, we can rewrite all the previous amplitudes in terms of α ,

$$\begin{aligned} r_0 &= \frac{1 - \alpha}{1 + \alpha}, & r_L &= \frac{\alpha - 1}{1 + \alpha^*} e^{2iq_1L/\hbar}, & \tilde{r}_0 &= \frac{\alpha^* - 1}{1 + \alpha}, \\ t_0 &= \frac{2}{N(1 + \alpha)}, & t_L &= \frac{2N \text{Re}[\alpha]}{1 + \alpha^*} e^{i(q_1 - p_1)L/\hbar}, & \tilde{t}_0 &= \frac{2N \text{Re}[\alpha]}{1 + \alpha} \end{aligned} \quad (11)$$

The total transmitted wave beyond the barrier ($x > L$) is then given by

$$t = t_0 t_L \sum_{s=0}^{\infty} (r_L \tilde{r}_0)^s = \frac{t_0 t_L}{1 - r_L \tilde{r}_0} = 4 \text{Re}[\alpha] \frac{e^{-ip_1L/\hbar}}{e^{-iq_1L/\hbar} |1 + \alpha|^2 - e^{iq_1L/\hbar} |1 - \alpha|^2},$$

which incidentally is normalization independent. After simple algebraic manipulations, we find

$$t = e^{-ip_1L/\hbar} \left/ \left[\cos(q_1L/\hbar) - i \frac{1 + |\alpha|^2}{2 \text{Re}[\alpha]} \sin(q_1L/\hbar) \right] \right. \quad (12)$$

Similarly, for the total reflected amplitude, we have

$$r = r_0 + t_0 r_L \tilde{t}_0 \sum_{s=0}^{\infty} (r_L \tilde{r}_0)^s = r_0 + \frac{r_L \tilde{t}_0}{t_L} t = \frac{1 - \alpha}{1 + \alpha} [1 - e^{i(p_1 + q_1)L/\hbar} t],$$

which results in

$$r = -i \frac{(1 - \alpha)(1 + \alpha^*)}{2 \operatorname{Re}[\alpha]} \sin(q_1 L / \hbar) \left/ \left[\cos(q_1 L / \hbar) - i \frac{1 + |\alpha|^2}{2 \operatorname{Re}[\alpha]} \sin(q_1 L / \hbar) \right] \right. . \quad (13)$$

For diffusion, the single plane wave reflection and transmission probabilities are $|r|^2$ and $|t|^2$ and of course satisfy

$$|r|^2 + |t|^2 = 1 . \quad (14)$$

The above results coincide with those calculated by solving the coupled continuity equations. However, it must be recalled, because often forgotten, that even for diffusion, $|t|^2$ is the transmission probability (i.e. has a physical meaning) *only* for a single plane wave. For wave packets small compared to the barrier width, incoherence dominates. The transmission probability is then an infinite sum of squares and *not* the square of an infinite sum. In the limit of *total incoherence*, the probabilities become

$$\begin{aligned} \text{incoherent T-probability : } |t_0 t_L|^2 \sum_{s=0}^{\infty} |r_L \tilde{r}_0|^{2s} &= (1 - |r_0|^2)^2 \sum_{s=0}^{\infty} |r_0|^{4s} \\ &= \frac{1 - |r_0|^2}{1 + |r_0|^2} , \\ \text{incoherent R-probability : } |r_0|^2 + |t_0 r_L \tilde{t}_0|^2 \sum_{s=0}^{\infty} |r_L \tilde{r}_0|^{2s} &= |r_0|^2 + |r_0|^2 \frac{1 - |r_0|^2}{1 + |r_0|^2} \\ &= \frac{2|r_0|^2}{1 + |r_0|^2} , \end{aligned} \quad (15)$$

with again probability conservation.

Now the apparent conundrum, the step potential, has only a single reflected and transmitted wave. How can this be reconciled with the infinite contributions (for large L) described above? The answer is very simple. *The first contributions at $x = 0$ are, obviously, the step results.* The others require a time for their appearance which are multiples of L/v_g , where v_g is the group velocity of the wave packet in the barrier region. As $L \rightarrow \infty$, this time interval goes to infinity. Formally, even for the step, the other contributions exist but one must attend an infinite-time interval to see even the second contribution and so forth. This feature is ‘hidden’ when using (unconvoluted) plane waves since no barrier size exceeds the size of a plane wave.

An interesting observation is that the standard resonance condition, $q_1 L = n\pi \hbar$, is only valid in the limit of total coherence. However, another resonance condition is brought to light in the above results. The total transmission amplitude equals unity when there is ‘head on’ diffusion, $p_2 = p_3 = 0$. This resonance condition does not depend upon the incoming energy value. Furthermore, it is independent of coherence requirements. The result occurs *step by step* for the head-on collision. This latter resonance condition is a consequence of zero mass. It does not appear for a massive Dirac particle.

4. Klein pair production

In the previous section, we used the two-step method for the calculation of the total transmission and reflection amplitudes. Both can be expressed as infinite sums of amplitudes. Each term in the sum represents a wave packet source (once convolution is performed). The series are convergent. The total amplitudes can be calculated either by the two-step method or by the

matrix method based upon continuity at both $x = 0$ and $x = L$. Which one uses is a matter of taste.

Note that there is always oscillatory behavior for the y and z axes. It is only the x -axis (that of potential discontinuity) where q_1 may be either real (oscillatory behavior) or imaginary (evanescent behavior). Bypassing, as previously anticipated, the evanescent case (tunneling) which exists even for mass-zero particles when there is a transverse momentum component, we now pass to the Klein energy region, $E < V_0 - \sqrt{p_2^2 + p_3^2} c$.

We have argued for the step result $|r_0| > 1$. This means that the first contribution to the total reflection amplitude for a barrier exceeds unity. This is already incompatible with the matrix solution which always satisfies $|r| < 1$.

The situation is even more radical. The holes (antiparticles) produced at $x = 0$ have energy $-E$. They travel within a well potential $V(x) = -V_0$ for $0 < x < L$ and zero beyond. At $x = L$, they are within their own Klein zone. Thus, they also create Klein pairs, holes/electrons. The holes are reflected to the left. Consequently, all holes are *entrapped* within the barrier/well region. Pair creation occurs at each potential discontinuity and hence with time the hole density within the barrier/well increases.

The series for t and r contains the loop factor

$$r_L \tilde{r}_0 = \frac{1 + |\alpha|^2 - 2\text{Re}[\alpha]}{1 + |\alpha|^2 + 2\text{Re}[\alpha]} e^{2iq_1 L/\hbar}.$$

The energy zone for diffusion is

$$E > V_0 + \sqrt{p_2^2 + p_3^2} c \implies E > V_0 - p_3 c \implies \text{Re}[\alpha] > 0 \implies |r_L \tilde{r}_0| < 1.$$

In this case, the series for t and r can be summed, see equations (12) and (13). However, in the Klein energy zone,

$$E < V_0 - \sqrt{p_2^2 + p_3^2} c \implies E < V_0 - p_3 c \implies \text{Re}[\alpha] < 0 \implies |r_L \tilde{r}_0| > 1.$$

Thus, the two-step series in the Klein energy zone cannot be summed. The matrix method is here *incompatible* with the two-step calculation. Holes entrapped within the potential well (barrier) will bounce back and forth an infinitum increasing at each reflection their number. Thus, the number of pairs created grows without limit in time. This is of course only theoretical since we expect the corresponding growth in (antiparticle) charge to eventually modify the potential itself.

5. Conclusions

In the previous sections, we have presented the results of the three-dimensional interaction of a chiral (Weyl) fermion with first a step and consequently (using the step results) with a barrier. We have considered separately the case of diffusion, $E > V_0 + \sqrt{p_2^2 + p_3^2} c$, and Klein zone, $E < V_0 - \sqrt{p_2^2 + p_3^2} c$. We have bypassed tunneling in this work.

Now for graphene, we must set $p_3 = 0$ so that our solutions apply to a physical plane (x, y) . We must also allow for the Fermi velocity by the substitution $c \rightarrow v_F$. In this limit

$$\frac{1 + |\alpha|^2}{2\text{Re}[\alpha]} = \frac{E(E - V_0)/c^2 - p_2^2 - p_3^2}{p_1 q_1} \longrightarrow \frac{E(E - V_0)/v_F^2 - p_2^2}{p_1 q_1}.$$

It is convenient to introduce the angles $\phi = \arctan(p_2/p_1)$ and $\theta = \arctan(p_2/q_1)$. In terms of these angles,

$$\left(\frac{E}{p_1 v_F}, \frac{E - V_0}{q_1 v_F}, \frac{p_2^2}{p_1 q_1} \right) = \left(\frac{\text{sign}[E]}{\cos \phi}, \frac{\text{sign}[E - V_0]}{\cos \theta}, \tan \phi \tan \theta \right).$$

Thus, from equation (12), we find the formulas standard to the graphene literature [9, 15],

$$|t|^2 = 1 \left/ \left[\cos^2(q_1 L/\hbar) + \left(\frac{\text{sign}[E] \text{sign}[E - V_0] - \sin \phi \sin \theta}{\cos \phi \cos \theta} \right)^2 \sin^2(q_1 L/\hbar) \right] \right. \quad (16)$$

This equation clearly shows that beyond the standard resonances, $q_1 L = n\pi\hbar$, there are additional head-on resonances for chiral fermions which are absent for massive particles.

We now recall some of our results.

- For diffusion, in the limit of total coherence (wave packets large if compared to the barrier width), the transmission probability is given by equation (12). For wave packets small compared to the barrier width, incoherence dominates and the transmission probability is given by equation (15). The first term in the infinite sum reproduces the step result.
- As for the Klein zone, we have reiterated our belief in Klein pair production, obligatory, and generally accepted for a step potential, but not always the result quoted for a barrier potential. Our claim is that this is the consequence of unwittingly summing a divergent series. The coherent diffusion amplitudes *cannot* be extended to the Klein energy zone.
- The holes created via pair production are trapped within the potential region and these localized holes have a continuous energy spectrum.

The question of Klein pair production is one more hypothesis that graphene could help to test. If valid it implies a very different physics for ‘above potential’ (Dirac/Weyl diffusion) and ‘below potential’ (Klein diffusion) phenomena. As always we leave the final judgement to experiment.

Acknowledgments

The authors thank anonymous referees for drawing the attention to interesting papers, for their constructive comments and for their useful suggestions. One of the authors (SdL) also thanks the Department of Physics, University of Salento (Lecce, Italy), for the hospitality and the FAPESP (Brazil) for financial support by the grant no 10/02213-3.

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