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Effects of strong electric fields in a polyacetylene chain

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ABSTRACT

In this work, we study the effects related to the creation of electron/hole pairs via application of an external electric field that acts on a pristine *trans*-polyacetylene molecular chain at zero-temperature. This phenomenon is termed Schwinger–Landau–Zener (SLZ) effect and arises when a physical system, which can even be the vacuum, is under the action of a strong, static and spatially homogeneous electric field. Initially, we investigate how the electrical conductivity of the polyacetylene changes with the applied field, by considering the carriers production as well as the variation of the interband gap according to certain *ab initio* models. Next, we analyse the competition between the SLZ effect and another one associated with the incidence of an uniform electric field on one-dimensional crystals – the Bloch oscillations. We evaluate the conditions in which these latter can be destroyed by the particles created through the same field that induces them, and verify the possibility of occurrence of the Bloch oscillations inside the *trans*-polyacetylene with frequencies equal to or higher than the terahertz scale.

1. Introduction

In the early 1950s of the last century, J. Schwinger showed that an intense, static and spatially homogeneous electric field can disrupt the quantum vacuum in such a way to cause the generation of electron/positron pairs [1]. He used the theoretical framework of quantum electrodynamics in order to find the non-perturbative exact amplitude of transition vacuum-to-vacuum, or vacuum persistence, for that physical process. At an instant t and within certain volume V, the correspondent probability is

$$P_{vac} = |\langle 0|U(t)|0\rangle|^2 = \exp(-\omega Vt), \tag{1}$$

where $U(t)$ is the time evolution operator and

$$\omega = \frac{(eE)^2}{4\pi^3\hbar^2 c}\sum_{n=1}^{\infty}\frac{1}{n^2}\exp\left(-\frac{n\pi E_{cr}}{E}\right). \tag{2}$$

Here, e is the electronic charge and E is the magnitude of the applied electric field, and

$$E_{cr} = \frac{m_e^2 c^3}{\hbar e}, \tag{3}$$

is the electric field needed to create abundant electron/positron pairs in the vacuum, as we will see below. This critical field can be thought of as that one required for realize the work to separate a virtual pair of particle/antiparticle of electronic mass m_e by a distance equal to its Compton wavelength. It is also possible to calculate the production of pairs per unit time per unit volume, which is given by [2,3]

$$\frac{d^2N}{dVdt} = \frac{(eE)^2}{4\pi^3\hbar^2 c}\exp\left(-\frac{\pi E_{cr}}{E}\right). \tag{4}$$

This expression is the first term of the sum in Eq. (2). Notice that an applied electric field greater than or equal to the critical one neutralizes the exponential in Eq. (4), with the pair production rate growing approximately as a function of the square of the electric field when E is very high.

The value of the critical electric field is $E_{cr} \approx 10^{18}$ V/m and exceeds quite the current technological capability of generation of these fields. The most powerful electric field produced in our laboratories oscillates in certain laser beams, reaching 10^8 V/m [4], eliminating any hope of presently detecting the Schwinger effect, at least in the vacuum. It is worth notice in here that the Schwinger effect may also occur through action of variable electric fields [5].

However, in the context of condensed matter physics, in semiconductors of low-dimensionality at zero-temperature, the limit velocity of the carriers is much lower than one of the light in vacuum. For example, the Fermi velocity (v_F) in the molecular polyacetylene, an one-dimensional system, or in the graphene, a planar crystalline system, is *circa* 1000 times lower than c [6].

In principle, one could detect an analogue of the Schwinger

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effect in such condensed matter systems, where the external electric field would generate electron/hole pairs in a way quite similar to the Landau–Zener effect in semiconductors. In this phenomenon, the presence of an external field induces the transition via quantum tunneling of an electron from the valence band to the conduction one [7]. Thus, in the graphene sheet, the rate of pair production per unit area per unit time is given by [8]

$$\frac{d^2N}{dAdt} = \frac{(eE)^{3/2}}{4\pi^2\hbar^{3/2}c^{1/2}} \exp\left(-\frac{\pi E_{cr}}{E}\right). \tag{5}$$

In the case of one-dimensional systems (polyacetylene, for instance), one gets the rate of pair production per length unit per time unit [18]

$$\frac{d^2N}{dLdt} = \frac{eE}{2\pi\hbar} \exp\left(-\frac{\pi E_{cr}}{E}\right). \tag{6}$$

In Eqs. (5) and (6), the critical electric field E_{cr} is yet given by Eq. (3), with the change $c \to v_F$, and then we have $E_{cr} \sim 10^{11}$ V/m, a value that is not so far from our current technological possibilities. The abundance of pairs produced by this electric field would be about 10^{24} per meter per second in the molecular chain.

The polyacetylene is a long molecular chain, a conjugated polymer that presents a behavior of semiconductor. When it is richly doped, presents the properties of a metal, but the transition to metallic state occurs in an unconventional way due to its low-dimensionality [9]. Its simpler form *trans*-polyacetylene has alternating single and double bonds which have lengths of 1.44 and 1.36 Å, respectively, which confer high stability to the polymer [10,11]. Th energy gap of the polyacetylene can be written as

$$\Delta = 2m_e v_F^2, \tag{7}$$

which is equivalent to the minimal energy needed to create an electron/positron pair in the vacuum, if $v_F \to c$. Some values for the polyacetylene gap energy are found in [12].

Bloch oscillations are another interesting phenomenon associated with the incidence of electric fields on one-dimensional crystalline lattices. F. Bloch demonstrated in 1928 the existence of electronic oscillations within one-dimensional crystals when these latter are subjected to a static and spatially homogeneous electric field generated externally [19]. Such oscillations occur with a period inversely proportional to both the field magnitude and the distance between the atoms that form the polymer (lattice parameter). The Bloch oscillations have been tested in some laboratories after its theoretical elucidation, but they are very difficult to observe due to their short duration, of the order of 10^{-12} s, because thermal and acoustic disturbances, as well as impurities and defects in the crystals, tend to scatter the electrons within them, undoing the coherence of the oscillations.

It is worth point out that the occurrence of the Bloch oscillations is not exclusive of 1-D systems. They may exist in 2-D lattices, with the concomitant transport of the electronic wave packet, as it was theoretically shown in [14]. The observation of those two effects combined, namely Landau–Zener and Bloch oscillations, in photonic 2-D lattices was reported in [21]. Bloch oscillations were also observed in semiconductor superlattices [22,23]. But it remains an unsolved question whether electronic Bloch oscillations can occur in a bulk crystal [24].

In this paper, we will analyze the behavior of the electrical conductivity of the undoped *trans*-polyacetylene molecular chain while a static and spatially homogeneous electric field is applied on the polymer. In this analysis, the production of electron/hole pairs via Schwinger–Landau–Zener (SLZ) effect will be studied and how the generated carriers affect the polyacetylene electrical conductivity will be investigated, considering the modification of the gap width caused by the electric field action according to an *ab initio* model found in the literature. In our study, we will neglect the possibility of appearance in such molecular chain the bound electron/hole pairs (excitons) and their possibility of self-trapping [25].

We will also study how the Bloch oscillations induced by the external electric field are disturbed by the carriers produced via SLZ effect, investigating the possibility of the induction of Bloch oscillations with terahertz frequency or beyond within the undoped *trans*-polyacetylene and indicating a possible mechanism for their protection.

The paper is organized as follows: in Section 2, we do the analysis of the polyacetylene conductivity under the action of the electric field in light of the SLZ effect. In Section 3, we study the effects of the SLZ dynamics on the Bloch oscillations within the polymer and in Section 4 we discuss the results.

2. SLZ Effect and the Polyacetylene Electric Conductivity

In certain *ab initio* models, the gap width of the polyacetylene vanishes when one applies a static and spatially homogeneous electric field sufficiently strong [13,20]. According to these models, the gap varies quadratically with the applied field as (in SI units)

$$\Delta = a - bE^2, \tag{8}$$

where $a = 1.3 \times 10^{-18}$ J and $b = 2.5 \times 10^{-38}$ J/V^2. This expression must yield the gap value compatible with Eq. (7) when the electric field is turned off. On the other hand, the gap energy vanishes for a field magnitude equal to $E_{db} \sim 10^{10}$ V/m, meaning that at this point the state of dielectric breakdown (db) is reached, and the transition insulator–metal occurs without the need to dope it. Notice that the value of the field required for the dielectric breakdown is one order of magnitude below that necessary for generating abundant electron/hole pairs via SLZ effect.

Let us now write just the electron creation rate, according to (3) and (5), as a function of the gap width (7) and integrated in the time, which yields

$$n_e = \frac{eEt}{4\pi\hbar} \exp\left(-\frac{4\pi m_e^2 v_F^4}{4v_F\hbar eE}\right) = \frac{eEt}{4\pi\hbar} \exp\left(-\frac{\pi\Delta^2}{4v_F\hbar eE}\right), \tag{9}$$

allowing to analyze the production of free electrons in terms of the gap variation with the applied field, according to Eq. (7). n_e is the linear density of these carriers. We can express the one-dimensional electric current density as

$$j_x = en_e v_F = \frac{e^2 v_F Et}{4\pi\hbar} \exp\left(-\frac{\pi\Delta^2}{4v_F\hbar eE}\right), \tag{10}$$

where we remark the presence of the factor that determines the linear-response, Et, which does not lead in any field regime, even considering the variation of the gap width with the electric field, according to Eq. (7). This feature seems to be typical of low-dimensional systems, since the same occurs, for example, in the graphene, at least in the context of the SLZ effect [16].

The polyacetylene is an ohmic material, just presenting a non-ohmic behavior when is highly doped, as, for example, with iodine [15]. First we are analysing here the non-doped polyacetylene, then we can find its classical electrical conductivity σ, by dividing Eq. (10) by Ev_{Ft}, arriving at

$$\sigma = \frac{e^2}{4\pi\hbar} \exp\left(-\frac{\pi\Delta^2}{4v_F\hbar eE}\right). \tag{11}$$

If Δ has the form given in Eq. (8), then one can show that the conductivity, starting from zero, reaches a maximum value when