Localization of relativistic electrons in a one-dimensional disordered system

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Abstract. We address the question as to whether relativistic effects have any influence on localization phenomena in disordered systems. Starting from the Schrödinger and Dirac equations for Kronig–Penney potentials, we derive their discrete counterparts within the framework of the linear combination of atomic orbitals and tight-binding approaches. As a specific example we subsequently focus on substitutional binary alloys. We show that taking relativity into account leads to many important differences with respect to the results obtained in the non-relativistic approximation. The predicted behaviour of localization length can be very relevant in several experimental contexts.

1. Introduction

During the last few decades a considerable amount of work has been devoted to the study of relativistic effects in one-dimensional (1D) condensed-matter physics [1–10]. In fact, the proper treatment of electronic states in systems consisting of heavy atoms, whether crystalline or disordered, requires a substantial revision of the usual, non-relativistic approaches. Very recently, Roy and Basu [10] have considered the possible impact of relativistic effects on electrical conduction in disordered systems by means of a generalization of the Landauer approach [11] to the relativistic case. In this way, the relationship between transmission properties of relativistic electrons and electrical conduction in 1D systems has been accomplished. On the other hand, transmission of particles through 1D disordered systems can be related to the localization of quantum states, which is known to occur even for an infinitesimal amount of uncorrelated disorder. On the contrary, Kronig–Penney models with correlated disorder present a band of delocalized states [12]. The treatment of electron localization in disordered systems has so far been carried out on a non-relativistic footing. Nevertheless, the necessity of fully relativistic treatments has become widely recognized in recent years, as it has been shown that the introduction of relativity may lead to quantitatively as well as qualitatively new features. In particular, this work aims at a comparative study of relativistic and non-relativistic electron-localization phenomena, thus also expanding the available knowledge on this problem [10].

The rest of the paper is organized as follows. In section 2, we derive non-relativistic and relativistic discretized Hamiltonians by means of a linear combination of atomic orbitals (LCAO), within the tight-binding approximation (TBA). In section 3 we present a specific example to apply our general results and discuss our findings on localization-length effects arising from relativity. Finally, we summarize our conclusions and comment on the possible experimental relevance of this work.

2. General model

The system we study is a periodic lattice, in which a fraction ν of host atoms (called A) is replaced by impurity atoms (called B), randomly distributed over the sample. For simplicity, we suppose that interatomic distances remain unchanged in this substitutional alloy, although this is not essential in our calculations and more complex situations can be easily handled.

We first consider a non-relativistic electron of mass m under the action of a one-dimensional potential and assume that this potential is the superposition of atomic potentials $v_j(x)$. Hence we are concerned with the Schrödinger equation (we use units such that $m = \hbar = c = 1$ throughout the paper),

$$\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_j v_j(x - ja) \right)\Psi(x) = E\Psi(x) \tag{1}$$

where a is the nearest-neighbour atomic distance. In order to solve (1), we shall take atomic potentials of the form $v_j(x) = -\lambda_j\delta(x)$. In fact, this replacement is not so restrictive; it has been recently demonstrated [14] that the 1D Schrödinger equation for an arbitrary potential can be mapped onto a 1D Schrödinger equation for an array of δ-function potentials, and that this assertion also holds for the 1D Dirac equation. Hereafter we restrict ourselves to attractive potentials ($\lambda_j > 0$). Then we express the electron wavefunction as a LCAO of the form

$$\Psi(x) = \sum_k C_k\phi_k(x - ka) \tag{2}$$

where $\phi_k(x) = \sqrt{\lambda_k}\exp(-\lambda_k|x|)$ is the normalized eigenfunction for a single δ-function potential. Neglecting the overlap between different orbitals and assuming that only nearest-neighbour interactions are significant (this may be accomplished by considering large a), we obtain the following tight-binding equation for the amplitudes:

$$(E - \varepsilon_k^{\mathrm{NR}})C_k = t_{k,k+1}^{\mathrm{NR}}C_{k+1} + t_{k,k-1}^{\mathrm{NR}}C_{k-1} \tag{3}$$

where the on-site energies and hopping integrals are given by

$$\varepsilon_k^{\mathrm{NR}} = -\tfrac{1}{2}\lambda_k^2 \qquad t_{k,k\pm1}^{\mathrm{NR}} = -\lambda_k\lambda_{k\pm1}\mathrm{e}^{-(\lambda_k+\lambda_{k\pm1})a/2}. \tag{4}$$

For convenience, we introduce the superscript NR, meaning non-relativistic approach, in order to facilitate the comparison with the corresponding relativistic expressions. Notice that in our approach on-site energies and hopping integrals are mutually related and depend on the nature of neighbouring atoms. This means that these matrix elements are calculated *ab initio* and no semi-empirical approximations are required.

Now we consider a relativistic electron obeying the Dirac equation

$$\left[-\mathrm{i}\sigma_x\frac{\mathrm{d}}{\mathrm{d}x} + \sigma_z + \sum_j v_j(x - ja) \right]\Psi(x) = (E + 1)\Psi(x) \tag{5}$$

where now Ψ is a two-component spinor, and σ_x and σ_z stand for the Pauli matrices. It should be mentioned that the electron energy E does not include the rest-mass energy, so that the relativistic energy is actually $E + 1$. We may directly compare this energy E with non-relativistic values. To solve (5), we also assume a LCAO solution similar to (2). Taking atomic potentials of the form $v_j(x) \rightarrow -\lambda_j \delta(x)$, the corresponding atomic orbitals are given by [15]

$$\phi_k(x) = \sqrt{\sin \lambda_k} \begin{pmatrix} \cos(\lambda_k/2) \\ i \sin(\lambda_k/2) \mathrm{sgn}(x) \end{pmatrix} \exp(-|x| \sin \lambda_k). \tag{6}$$

Following the LCAO-TBA as before, one obtains

$$(E - \varepsilon_k^R) C_k = t_{k,k+1}^R C_{k+1} + t_{k,k-1}^R C_{k-1} \tag{7}$$

where now

$$\varepsilon_k^R = -(1 - \cos \lambda_k) \qquad t_{k,k\pm1}^R = -\sin \lambda_k \sin \lambda_{k\pm1} e^{-(\sin \lambda_k + \sin \lambda_{k\pm1})a/2} \tag{8}$$

where the superscript R means relativistic approach. As expected, the values of ε_k^R and $t_{k,k\pm1}^R$ reduce in the weak-coupling limit to the non-relativistic expressions (4), obtained by directly solving the Schrödinger equation. This is clearly seen by expanding (8) in powers of the potential strength. Up to first-order corrections, one gets

$$\varepsilon_k^R = \varepsilon_k^{NR} \left(1 - \frac{\lambda_k^2}{12} \right) \tag{9a}$$

$$t_{k,k\pm1}^R = t_{k,k\pm1}^{NR} \left(1 - \frac{\lambda_k^2 + \lambda_{k\pm1}^2}{6} \right). \tag{9b}$$

In the case of a perfect lattice $\lambda_k \equiv \lambda$, equation (9b) leads to the following ratio r between relativistic and non-relativistic bandwidths in the weak-coupling limit (recall that the bandwidth is proportional to the corresponding hopping integral):

$$r = 1 - \frac{\lambda^2}{3}. \tag{10}$$

Hence, for small values of λ, the non-relativistic bandwidth is larger than the relativistic one. The occurrence of this *shrinkage* of allowed bands when relativity is taken into account is also found in more elaborate 1D models, e.g. the treatment of the Mathieu potential by the Dirac equation [14]. In addition, this *shrinkage* is in qualitative agreement with experimental and relativistic augmented plane-wave calculations in crystalline solids [16]. We would like to mention that such a shrinkage of the relativistic electronic spectrum is not restricted to periodic lattices. It is also found in quasi-periodic [7] and disordered [17] lattices.

The tight-binding equations of motion, (3) and (7), can be cast in the form

$$t_k C_{k-1} + (\varepsilon_k - E) C_k + t_{k+1} C_{k+1} = 0. \tag{11}$$

Here we have rewritten $t_{k+1,k} = t_{k,k+1} \equiv t_{k+1}$, and a superscript R or NR should be understood in all expressions. To compute the localization length for relativistic and non-relativistic electrons in disordered systems we follow the method proposed by Roman and Wiecko [13]. These authors found that the localization length l is given by

$$l = \lim_{n \to \infty} \langle S_n \rangle \tag{12}$$

where $\langle \cdots \rangle$ denotes ensemble average and the symbol

$$S_n \equiv \frac{n}{\ln |a_n|} \tag{13}$$

is introduced for a convenient discussion of results. This parameter is recursively evaluated from the knowledge of a_n using

$$a_n = -a_{n-1}\frac{\varepsilon_n - E}{t_n} + b_{n-1} \tag{14a}$$

$$b_n = -a_{n-1}\frac{t_{n+1}}{t_n} \tag{14b}$$

supplemented by the initial conditions $b_0 = 0$ and $a_0 = -t_1$. This recursive expression can be used to obtain both non-relativistic and relativistic localization lengths, which we will denote by l_{NR} and l_R, respectively.

3. Substitutional alloy

In order to elucidate the extent of relativistic impact on localization length from a quantitative point of view, we consider a substitutional alloy in which a fraction nu of host atoms have been replaced by impurity atoms. For this system λ_k takes on two values, λ_A and λ_B, representing, respectively, the potential of host atoms and impurity atoms. The ratio λ_B/λ_A measures, in fact, the degree of chemical diversity of the alloy (the more distant from unity, the more different the chemical species). In addition, the interatomic distance is taken to be $a = 2$ in our calculations. With these parameters, the non-relativistic allowed band for the perfect A lattice for $\lambda_A = 1$ is $[-0.770, -0.229]$, whereas the corresponding relativistic allowed band is $[-0.723, -0.196]$. We will average over ensembles comprising a number of 50 realizations. We have checked that this number suffices to ensure a satisfactory convergence of the computed mean values of the localization length.

In figure 1 we show the variation of $\langle S_n \rangle$ with the number of atoms in the chain n, for both the non-relativistic and relativistic cases, at a fixed electron energy ($E = -0.5$), two different concentrations of impurity atoms (10 and 20%), $\lambda_A = 1.0$ and $\lambda_B = 1.2$. The graphs in figure 1 clearly show that $\langle S_n \rangle$ starts becoming nearly constant beyond a certain value, n_m, of the system size. The localization length can then be taken as $\langle S_n \rangle_{n=n_m}$, according to (12). We have observed that, for a wide range of relevant system parameters (λ_A, λ_B, concentration of impurity atoms), the values of n_m for the relativistic and non-relativistic cases are nearly the same.

Figure 2 shows l_{NR} and l_R over a wide range of energy, for the same system parameters as in figure 1 and a system size of 10 000. From a comparison of curves I and II, it is apparent that both l_{NR} and l_R decrease upon increasing the impurity concentration, as expected. The most salient aspect of this figure appears in comparing l_{NR} and l_R for the same concentration of impurities: there exists a *critical energy* for which both relativistic and non-relativistic localization lengths take the same value. The exact value of this critical energy depends slightly on the impurity concentration and, for the system parameters we have considered, is located at about $E = -0.65$ (see figure 2). As a consequence, relativistic electrons become less localized than non-relativistic ones for a wide range of energies ($E > -0.65$) whereas in the range $E < -0.65$ the situation is completely reversed. The physical implications of this result should be clear: if the Fermi energy is below the critical energy, the conductance of the sample should decrease as soon as relativistic effects become to be important. On the contrary, if the Fermi level is above the critical energy, the conductance should be enhanced. Looking again at figure 2, we observe that non-relativistic states with energies close to -0.5 (the energy of the unperturbed A atom levels) are more localized than neighbouring states, in agreement with non-relativistic tight-binding calculations in binary alloys with *diagonal disorder* [18]. It is known, however, that *off-diagonal* disorder yields infinite localization
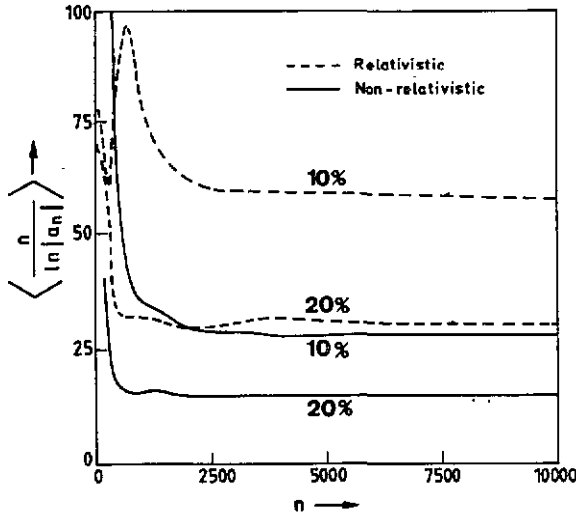
Figure 1. Variation of $\langle S_n \rangle$ with n for $\lambda_A = 1.0$, $\lambda_B = 1.2$ and $E = -0.5$ for relativistic (broken curves) and non-relativistic (full curves) electrons. The concentration of impurity atoms in the alloy are $\nu = 0.1$ and 0.2.

length at the middle of the band [19]. Since our results clearly show an absence of reduction of the localization length at the middle of the band in the relativistic case, it seems that our relativistic discrete Hamiltonian (7) is more similar to off-diagonal ones.
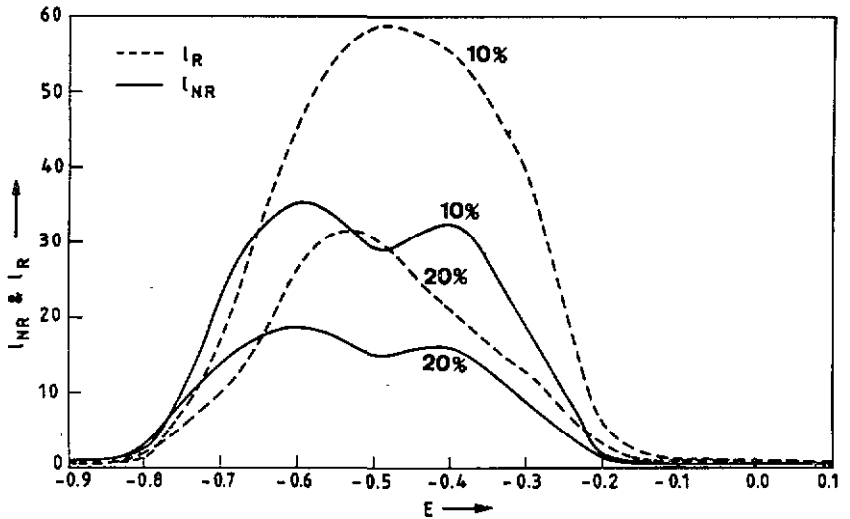

Figure 2. Variation of l_{NR} and l_R with energy E for the same system parameters indicated in figure 1.

Localization length as a function of the ratio λ_B/λ_A is shown in figure 3, for two different values of λ_A, electron energy $E = -0.7$, and impurity concentration $\nu = 0.2$. The non-relativistic as well as the relativistic localization length diverges as $\lambda_B/\lambda_A \to 1$ (perfect lattice), whereas they tend to decrease on increasing the chemical diversity of the alloy. We can observe that l_R is smaller than l_{NR} in almost the whole range of this ratio

for $\lambda_A = 1.0$. The contrary is found for $\lambda_A = 1.2$. Therefore, we conclude that relativistic effects on the conductance at zero temperature depend not only on the Fermi energy but also on the potential strength of individual atoms. This gives rise to a rich variety of conductance behaviour when relativistic effects are taken into account in disordered systems.
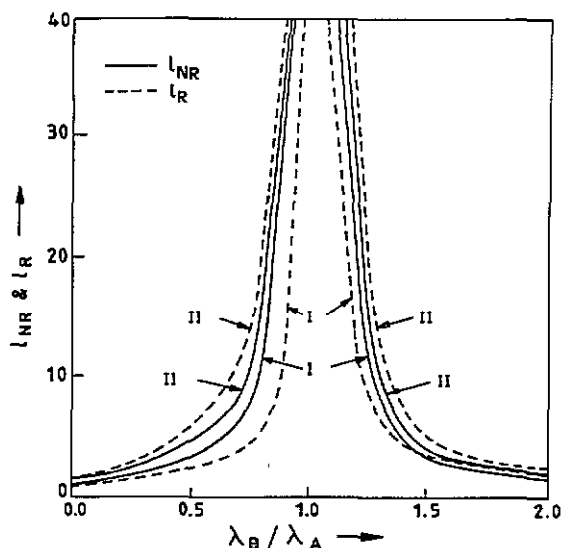

Figure 3. Variation of l_R (dashed lines) and l_{NR} (full lines) as a function of λ_B/λ_A, with $\lambda_A = 1.0$ (curves I) and $\lambda_A = 1.2$ (curves II). The electron energy is $E = -0.7$ and the impurity concentration is $\nu = 0.2$.

4. Concluding remarks

To conclude, we have compared Kronig–Penney models with and without relativistic effects via the Schrödinger and Dirac equations, respectively. We have shown how, in both cases, the same tight-binding equation is obtained in the LCAO approximation, but with different parameters that indicate the shrinkage of the bands when relativity is taken into account. We have then particularized our results for the substitutional alloy to obtain specific results on this comparison. We have found that relativistic effects show up in a variety of ways that depend generally on most parameters of the system, but predominantly on the electron energies and the on-site energies. Actually, which the localization length is larger, the relativistic or the non-relativistic one, depends crucially on the on-site energy.

Although we have only considered one particular model, it seems reasonable to believe that other systems that can be described by equations similar to those we deal with here will show a comparable richness of behaviour depending on the relevance of relativity to them. The conductance and transport properties, in general, of a given system will then be rather different, as they are directly related to localization phenomena. Complete, three-dimensional calculations for the purpose of relativistically investigating electron localization is expected to involve enormous intricacies. Therefore, analytical results in one dimension acquire an additional importance, as they may be the only ones available without prohibitively cumbersome calculations. This importance may only be ascertained by comparison with experimental results. In this respect, we would like to suggest that materials like amorphous semiconductors with heavy atoms (PbTe is a particular example),

often found in practice for application purposes, can be the suitable ones to test the validity of our calculations, and to decide whether it is actually necessary to go to three-dimensional calculations to correctly compare with physical systems. We hope this paper will encourage experimental effort in that direction.

Acknowledgments

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