LCAO approach to non-relativistic and relativistic Kronig–Penney models

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Abstract

We have reported a comparative study of dynamics of non-relativistic and relativistic electrons in Kronig–Penney models with the use of discretized Hamiltonians in the context of the linear combination of atomic orbitals approach. We have carried out general formulations of both non-relativistic and relativistic cases, by taking the atomic potentials appropriately as δ-function potentials; then, we have applied these general formulations to obtain significant results regarding relativistic impacts on certain important aspects of the electronic energy spectrum of periodic, quasiperiodic and disordered systems.

1. Introduction

Point interaction potentials in one space dimension are widely used in condensed matter physics to approximate more structured and more complex short-ranged potentials. A point interaction potential means any sharply peaked potential approaching the δ-function limit. The rigorous mathematical basis of such a definition may be found in the monograph of Albeverio et al. [1]. One of the most successful applications of the point interaction potentials is the well-known Kronig–Penney model [2]. In this model the interaction of one electron with the solid is replaced by an array of square barrier potentials and then the δ-function limit is considered. The energy spectrum of the electron

was found to consist of allowed bands and forbidden gaps as in the case in real crystals. Since the Kronig–Penney model was introduced, it has been applied to many fields of physics, like band structure and electron dynamics in ordered solids, impurity levels, localization phenomena in disordered solids and liquids [3], microelectronic devices [4,5], properties of layered superconductors [6], electronic transport in spontaneously dimerized solids (Peierls transition) [7], or relativistic quark tunnelling in one-dimensional nuclear models [8]. In addition, the capabilities of the Kronig Penney model in describing relativistic electrons in condensed matter have been explored during the last decades. The issues which have been studied within the relativistic framework are: bulk states in crystalline solids [9–12], surface states [13,14], interface states [15], electron states in disordered [16–20] and quasiperiodic [21] solids, and tunnelling

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phenomena [22, 23]. Moreover, it has been recently demonstrated [24] that the discretized forms of both the Schrödinger and the Dirac equations for any arbitrary potential in one dimension are equivalent to a generalized Kronig–Penney model. Hence it is clear that this model is more than a naive approach and it can take care of many physical situations.

The transfer matrix method provides a valuable help to solve the scattering problem of electrons by an array of δ-function potentials. This method is particularly simple in the absence of any other potential, such as those related to external electric or magnetic fields. In this case the wave function in the field-free region is a combination of plane waves, which are the solutions of the free-particle wave equation. However, one must solve the corresponding wave equation in the interatomic regions when external fields are applied, and the transfer matrix could be more complex; for instance, Airy functions appear when a uniform electric field is applied to the solid. The transfer matrix method is a *continuous* method, in the sense that the solution of the problem is obtained by solving a differential equation. An alternative (discrete) method was proposed by Bellisard et al. [25] for the non-relativistic wave equation. This method is based on the Poincaré map associated to the Schrödinger equation. The generalization of the Poincaré map to the case of the Dirac equation has been recently given by Méndez et al. [24]. This map relates the value of the electron wave function at three consecutive lattice sites by means of a three-term recurrence relation. Dynamical systems techniques are then used to find the electronic energy spectrum. Although this approach becomes exact and no information is lost in passing from the wave equation to the Poincaré map, the three-term recurrence relations involve the electron energy in a rather complex fashion. Therefore direct tridiagonalization is not possible and the electron wave function is difficult to obtain in an accurate manner; for instance, in the case of disordered systems with no external fields it is difficult to separate the exponentially decreasing function from the exponentially growing solution, which is unphysical.

The aim of this paper is to report a comparative study of dynamics of non-relativistic and relativistic electrons in Kronig–Penney models, on the basis of discretized Hamiltonians in the context of the linear combination of atomic orbitals (LCAO) approach, avoiding numerical shortcomings of the Poincaré map. The formulations for both non-relativistic (Section 2) and relativistic (Section 3) cases are first carried out generally for arbitrary atomic potentials which are finally replaced by appropriate δ-function limits. The general formulation with respect to δ-function potentials is then applied to study relativistic impacts on certain important aspects of the electronic energy spectrum for periodic (Section 4) and general lattices which include the cases of quasiperiodic and disordered systems (Section 5). Section 6 contains discussions and conclusions.

2. Non-relativistic LCAO approach

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

$$\left(-\frac{1}{2m}\frac{d^2}{dx^2} + \sum_j v_j(x - x_j) \right) \Psi(x) = E\Psi(x), \quad (1)$$

where x_j is the position of the jth atom and the sum runs over all atoms in the chain. In order to solve Eq. (1) we take a LCAO solution of the form

$$\Psi(x) = \sum_i c_i \phi_i(x - x_i). \quad (2)$$

We have assumed that each atom only supports one bound state, as occurs in the case of the δ-function potential, although more complicated situations can be handled in a similar fashion. The atomic orbitals ϕ_i can be found by solving the corresponding Schrödinger equation

$$\left(-\frac{1}{2m}\frac{d^2}{dx^2} + v_i(x - x_i) \right) \phi_i(x - x_i) = \varepsilon_i \phi(x - x_i), \quad (3)$$

ε_i being the electron energy in the isolated ith atom. Inserting Eq. (2) in Schrödinger equation (1) and

using Eq. (3) we get

$$\sum_i \left[\varepsilon_i - E + \sum_{j \neq i} v_j(x - x_j) \right] c_i \phi(x - x_i) = 0. \quad (4)$$

We proceed in the standard fashion to obtain the electronic amplitude c_i at any site. We multiply Eq. (4) by $\phi_k^*(x - x_k)$ from the left and perform the integration along the whole chain. By doing so, we are led to the following algebraic equation for the amplitudes:

$$\sum_i \left[(\varepsilon_i - E) A_{ki} + \sum_{j \neq i} B_{kji} \right] c_i = 0, \quad (5)$$

where we have defined

$$A_{ki} = \int dx \, \phi_k^*(x - x_k) \phi_i(x - x_i), \quad (6)$$

$$B_{kji} = \int dx \, \phi_k^*(x - x_k) v_j(x - x_j) \phi_i(x - x_i), \quad i \neq j. \quad (7)$$

The above results become valid for non-relativistic electrons for any superposition of arbitrary atomic potentials v_j. Calculations are simplified by approaching these atomic potentials by δ-function potentials. In fact this approach is not so unrealistic as one could expect: as we mentioned earlier, the the δ-function potential is usually regarded as a good candidate to approximate more complex short-ranged potentials [26]. Hence we take

$$v_j(x - x_j) = -\lambda_j \delta(x - x_j). \quad (8)$$

We take the coupling constants λ_j to be positive, thereby restricting ourselves to attractive δ-function potentials. In this case the atomic levels and the atomic orbitals are found to be

$$\varepsilon_k = -\frac{m}{2} \lambda_k^2, \quad (9)$$

$$\phi_k(x) = \sqrt{m\lambda_k} \exp(-m\lambda_k |x|). \quad (10)$$

The explicit expressions for the coefficients A_{ki} and B_{kji} appearing in Eq. (5) are given by

$$A_{ki} = \delta_{ki} + (1 - \delta_{ki}) \left(\frac{2\sqrt{\lambda_k \lambda_i}}{\lambda_k^2 - \lambda_i^2} \right)$$
$$\times [\lambda_k \exp(-m\lambda_k |x_k - x_i|)$$

$$-\lambda_i \exp(-m\lambda_i |x_k - x_i|)] \quad (11)$$

and

$$B_{kji} = -m\lambda_j \sqrt{\lambda_k \lambda_i} \exp(-m\lambda_k |x_k - x_j|$$
$$-m\lambda_i |x_i - x_j|), \quad i \neq j, \quad (12)$$

where δ_{ki} is the Kronecker delta.

In order to find the electron wave function (2), one must solve the algebraic equation (5). Clearly this is prohibitive for systems of interest, where the number of atoms is very large. It is convenient to consider a suitable approximation to reduce the number of coefficients involved in the calculation. We suppose that electrons are tightly bound so that overlap between orbitals of neighbouring atoms is small. Whenever this condition is valid one can replace A_{ki} by δ_{ki}. Concerning the three centre integrals (7), we assume that the only non-vanishing coefficients are $B_{kkk \pm 1}$ since only nearest-neighbour interactions are significant.

Taking into account these approximations, the equation for the amplitudes is reduced to the following tridiagonal system:

$$(E - \varepsilon_k) c_k = B_{kkk+1} c_{k+1} + B_{kkk-1} c_{k-1}. \quad (13)$$

Unfortunately the tridiagonal matrix is not Hermitian. This is expected in view of the asymmetric role of the ith and jth atoms in Eq. (12), although the electron eigenenergies are real because Eq. (13) is related to the Schrödinger equation (1). This shortcoming occurs in LCAO treatments using a non-orthogonal basis for expanding the electron wave function. An approximate way to make the matrix Hermitian is to define new non-diagonal elements as follows [27]:

$$t_{kk \pm 1}^{NR} = t_{k+1k}^{NR} = -\sqrt{B_{kkk \pm 1} B_{k \pm 1k \pm 1k}}. \quad (14)$$

For convenience we introduce the superscript NR, meaning non-relativistic approach, in order to facilitate the comparison with the corresponding relativistic expressions (Section 3). The equation of motion for the amplitudes now reads

$$(E - \varepsilon_k^{NR}) c_k = t_{kk+1}^{NR} c_{k+1} + t_{kk-1}^{NR} c_{k-1}, \quad (15)$$

and the explicit expressions of the matrix elements are

$$\varepsilon_k^{NR} = -\frac{m}{2}\lambda_k^2,$$

$$t_{kk\pm1}^{NR} = -m\lambda_k\lambda_{k\pm1}$$

$$\times \exp\left[-\frac{m}{2}(\lambda_k + \lambda_{k\pm1})|x_k - x_{k\pm1}|\right]. \quad (16)$$

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.

3. Relativistic LCAO approach

In this section we deal with the LCAO approach to the one-dimensional Dirac equation. We consider a relativistic electron obeying the equation

$$\left[-i\alpha\frac{d}{dx} + \beta m + \sum_j v_j(x - x_j)\right]\Psi(x)$$

$$= (E + m)\Psi(x), \quad (17)$$

where now Ψ is a two-component spinor. α and β denote 2×2 traceless, Hermitian matrices; the squares of these matrices are unity and they satisfy the anticommuting relation $\alpha\beta + \beta\alpha = 0$. It should be mentioned that the electron energy E does not include the rest mass energy, so that the relativistic energy is actually $E + m$. We may directly compare this energy E with non-relativistic values. To solve Eq. (17), we assume a LCAO solution (2), where now the atomic orbitals are two-component spinors satisfying the equations

$$\left[-i\alpha\frac{d}{dx} + \beta m + v_k(x - x_k)\right]\phi_k(x - x_k)$$

$$= (\varepsilon_k + m)\phi_k(x - x_k). \quad (18)$$

We follow the tight-binding approach of the previous section in order to obtain an algebraic equation for the amplitudes similar to Eq. (13). Within this approximation we assume that the overlap between orbitals different atoms vanishes so that

$\int dx\, \phi_k^\dagger(x - x_k)\phi_i(x - x_i) = \delta_{ki}$ († denotes Hermitian conjugates). Restricting ourselves to nearest-neighbour interactions the (non-zero) hopping integrals in the present case are given by

$$B_{kk\pm1} = \int dx\, \phi_k^\dagger(x)v_k(x)\phi_{k\pm1}(x - x_{k\pm1} + x_k).$$

$$(19)$$

The presence of a product involving the atomic orbital and the atomic potential at the same site in Eq. (19) gives rise to some problems when the δ-function limit is taken (see Ref. [28] and the references therein). As pointed out by Sutherland and Mattis [29], some ambiguities appear in taking the limit $v_k(k) \to -\lambda_k\delta(x)$ at the outset in the Dirac equation, because potentials of different shapes approaching the δ-function limit give wave functions reaching different values at the point of discontinuity. The origin of these ambiguities was clarified by McKellar and Stephenson [30], and it is related to the fact that the Dirac equation is linear in momentum rather than quadratic. Due to this linearity in momentum, the wave function itself must be discontinuous at $x = 0$ in order to account for the singularity of the potential term. However, the product $\delta(x)\theta(x)$, θ being the step function, is not well defined in the sense of a strict distribution-theory, so that there exists arbitrariness regarding the definition of relativistic point interaction potentials. To avoid these problems we solve Eq. (19) for any sharply peaked potential $v_k(x) \equiv v_k(x, \varepsilon)$ satisfying the condition

$$\int_{-\varepsilon}^{\varepsilon} dx\, v_k(x, \varepsilon) = -\lambda_k, \quad (20)$$

ε being a small positive parameter. We closely follow the method of Méndez et al. in dealing with a Green function approach to the level shift under the influence of relativistic point interaction potentials [31]. Since atomic orbitals are continuous functions of the variable x everywhere except at $x = 0$, we can write

$$B_{kk\pm1} = \left[\int_{-\varepsilon}^{\varepsilon} dx\, \phi_k^\dagger(x)v_k(x, \varepsilon)\right]\phi_i(x_k - x_{k\pm1}).$$

$$(21)$$

To find the integral appearing in Eq. (21) we consider the Hermitian conjugates of Eq. (18),

$$-i\frac{d\phi_k^\dagger(x)}{dx}\alpha - \phi_k^\dagger(x)(\beta m - \varepsilon_k - m) = \phi_k^\dagger v_k(x,\varepsilon),$$

(22)

and perform the integration on both sides along the interval $[-\varepsilon,\varepsilon]$. The integral of the second term on the left-hand side of Eq. (22) vanishes in the limit $\varepsilon \to 0$ since the elements of $\phi_k^\dagger$ are not singular. The integral of the first term can be found after integration by parts. Thus we find

$$\lim_{\varepsilon\to 0}\left[\int_{-\varepsilon}^{\varepsilon} dx\,\phi_k^\dagger(x)\,v_k(x,\varepsilon)\right]$$
$$= -i[\phi_k^\dagger(0^+) - \phi_k^\dagger(0^-)]\alpha,$$

(23)

and finally from Eq. (21),

$$B_{kkk\pm 1} = -i[\phi_k^\dagger(0^+) - \phi_k^\dagger(0^-)]\,\alpha\phi_k(x_k - x_{k\pm 1}).$$

(24)

Notice that the result becomes independent of how the δ-function limit is taken, thus avoiding the arbitrariness discussed earlier.

The one-dimensional Dirac equation can be exactly solved for a single point interaction potential satisfying Eq. (20). The explicit expression depends on the representation for the matrices α and β. In the case $\alpha = \sigma_x$ and $\beta = \sigma_z$, σ's being the Pauli matrices, the atomic orbitals are given [32] by

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

(25)

and the atomic energy is

$$\varepsilon_k = -m(1-\cos\lambda_k).$$

(26)

In the non-relativistic limit and for weak coupling (small λ_k), the upper component and the energy reduce to the non-relativistic atomic orbital (10) and the non-relativistic energy (9), respectively. Inserting Eq. (25) in Eq. (24) we obtain the expression for the coefficients $B_{kkk\pm 1}$ straightforwardly. As occurs in the non-relativistic case, the tridiagonal matrix is not Hermitian and we therefore define new hopping integrals by means of a relation similar to Eq. (14).

Thus one finally gets the equation of motion of the amplitudes in the relativistic case:

$$(E - \varepsilon_k^R)c_k = t_{kk+1}^R c_{k+1} + t_{kk-1}^R c_{k-1},$$

(27)

where the superscript R means the relativistic approach and

$$\varepsilon_k^R = -m(1 - \cos\lambda_k),$$

$$t_{kk\pm 1}^R = -m\sin\lambda_k\sin\lambda_{k\pm 1}$$

$$\times\exp\left[-\frac{m}{2}(\sin\lambda_k + \sin\lambda_{k+1})|x_k - x_{k\pm 1}|\right].$$

(28)

As expected, the values of ε_k^R and $t_{kk\pm 1}^R$ reduce in the weak coupling limit (small λ_k) to the non-relativistic expression (16) obtained by directly solving the Schrödinger equation. This is seen by expanding Eq. (28) in powers of the potential strength. Up to first-order corrections, one gets

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

$$t_{kk\pm 1}^R = t_{kk\pm 1}^{NR}\left(1 - \frac{\lambda_k^2 + \lambda_{k\pm 1}^2}{6}\right).$$

(29)

In particular we find that the absolute values of relativistic on-site energies and hopping integrals are smaller than the corresponding non-relativistic ones. This result will be used later.

4. Periodic lattices

In the case of periodic lattices the Bloch theorem allows us to find the electronic energy spectrum analytically. For monoatomic lattices all the atomic potentials and nearest-neighbour distances are the same we take $\lambda_k \equiv \lambda$ and $|x_k - x_{k+1}| \equiv d$. Hence the equations of motion (15) and (27) admit a Bloch solution of the form

$$c_k = C\exp(i\kappa kd),$$

(30)

where κ is the crystal momentum and C is a constant. The dispersion relation is

$$\cos\kappa d = -\frac{\exp(md\lambda)}{2m\lambda^2}\left(E + \frac{m}{2}\lambda^2\right)$$

(31)

in the non-relativistic case and

$$\cos \kappa d = -\frac{\exp(md \sin \lambda)}{2m \sin^2 \lambda}(E + m - m \cos \lambda) \qquad (32)$$

in the relativistic case. These expressions are to be compared with those obtained by directly solving the non-relativistic (1) and relativistic (17) wave equations for a periodic array of δ-function potentials [10]. The exact dispersion relation for negative energies is

$$\cos \kappa d = \cosh q^{NR} d - md\lambda \frac{\sinh q^{NR} d}{q^{NR} d} \qquad (33)$$

in the non-relativistic case, where $q^{NR} = \sqrt{-2mE}$, and

$$\cos \kappa d = \cosh q^{R} d \cos \lambda - (E + m) md \sin \lambda \frac{\sinh q^{R} d}{q^{R} d} \qquad (34)$$

in the relativistic case, where $q^{R} = \sqrt{-2mE - E^2}$. Fig. 1 shows the exact and LCAO dispersion relations in the non-relativistic case, where the on-site energy is -13.6 eV (λ equals the fine structure constant) and $d = 3$ Å. With these parameters relativistic dispersion relations are similar to non-relativistic ones and plots are actually superimposed.
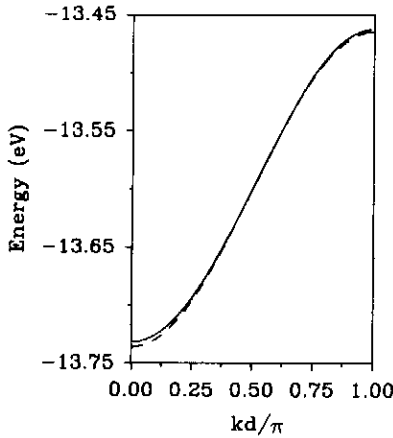

Fig. 1. Exact (full line) and LCAO (dashed line) non-relativistic dispersion curves for a monoatomic chain with atomic energy -13.6 eV and lattice parameter $d = 3$ Å.

We observe that our LCAO approach gives excellent results in the central region of the Brillouin zone. At the edges of the Brillouin zone diffraction effects become important and one should include more terms in the LCAO matrix to account for multiple scattering. However, we can see that the results are rather good within the tight-binding approach even at the edges of the Brillouin zone. For instance, the difference between exact and LCAO energies at the bottom of the band is only 4 meV.

For monoatomic chains, the non-relativistic and relativistic bandwidths are directly proportional to $|t^{NR}|$ and $|t^{R}|$, respectively (we drop the subscript since all atomic potentials are identical). In the case of weak coupling, which is of interest in solids, we can use Eq. (29) to find the ratio between relativistic and non-relativistic bandwidths:

$$\frac{|t^{R}|}{|t^{NR}|} = 1 - \frac{\lambda^2}{3}. \qquad (35)$$

This value indicates that a *shrinkage* occurs when relativistic effects are taken into account. This effect is also found when the exact dispersion relations are used [9]. In addition, other atomic potentials, such as non-local separable potentials [33] and Mathieu potential [24,31], present a decrease of the bandwidth when relativity is *switched* on.

When two kinds of atoms are arranged periodically (diatomic lattices), a gap is open. We now study the relativistic effects on this gap within the LCAO approach. Let us consider a chain in which the unit cell consists of two different atoms with coupling constants λ and λ', separated by a distance d, and the lattice period is assumed to be $2d$. Starting from the equation of motion for the amplitudes and using a Bloch solution of the form

$$c_k = C \exp(2i\kappa kd), \qquad (36)$$

the non-relativistic dispersion relation is found to be

$$\cos \kappa d =$$

$$-\frac{\exp[m(\lambda + \lambda')d/2]}{2m\lambda\lambda'} \sqrt{\left(E + \frac{m}{2}\lambda^2\right)\left(E + \frac{m}{2}\lambda'^2\right)} \qquad (37)$$

and the relativistic one is

$$\cos \kappa d = - \frac{\exp[m(\sin \lambda + \sin \lambda')\, d/2]}{2m \sin \lambda \sin \lambda'}$$

$$\times \sqrt{(E + m - m \cos \lambda)(E + m - m \cos \lambda')}. \quad (38)$$

The energy gap E_g is the difference between the two roots of the dispersion relation at the Brillouin zone edge ($\kappa = \pi/2d$). Using Eq. (29) one obtains in the case of weak coupling

$$\frac{E_g^R}{E_g^{NR}} = 1 - \frac{\lambda^2 + \lambda'^2}{6}, \quad (39)$$

meaning that relativity causes a decrease of the band gap.

5. General lattices

In this section we aim to study relativistic effects on the electronic energy spectrum in general lattices; they include disordered and quasiperiodic lattices which are subjects of a great deal of work. We will concern ourselves with the density of states (DOS) when translational symmetries are absent. A widely used method of approximating the DOS is based on calculating its moments [34]. It is known that the exact computation of the DOS from its moments requires the knowledge of all of them. In addition, this calculation is unstable (the accuracy of the computation must increase exponentially with the number of moments used [35]). However, some valuable information of the energy spectrum is obtained from the knowledge of the first few moments, as we will show below.

Let $\mathscr{H}$ be the tridiagonal Hamiltonian matrix whose elements are given by Eq. (16) in the non-relativistic case and by Eq. (28) in the relativistic case. The moment of order p of the density of eigenvalues of $\mathscr{H}$ is

$$\mu_p = \frac{1}{N} \mathrm{Tr}(\mathscr{H}^p), \quad (40)$$

N being the number of atoms in the chain. In the weak coupling limit we can use Eq. (29) to write

$$\mathscr{H}_R = \mathscr{H}_{NR} - H, \quad (41)$$

where H is a tridiagonal matrix whose elements are given by

$$H_{kk} = \frac{1}{12} \varepsilon_k^{NR} \lambda_k^2,$$

$$H_{kk \pm 1} = \frac{1}{6} t_{kk \pm 1}^{NR} (\lambda_k^2 + \lambda_{k \pm 1}^2). \quad (42)$$

Note that this matrix is of the order of λ^2 with respect to $\mathscr{H}_{NR}$ and consequently a perturbation treatment is justified. Moreover, it should be noticed that all matrix elements of $\mathscr{H}_R$, $\mathscr{H}_{NR}$ and H are negative. This means that moments of even (odd) order are positive (negative) in the relativistic as well as in the non-relativistic case.

Inserting Eq. (41) in Eq. (40), one has up to first-order corrections

$$\mu_p^R = \mu_p^{NR} - \frac{p}{N} \mathrm{Tr}(\mathscr{H}_{NR}^{p-1} H), \quad (43)$$

where we have used the fact that $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$. Since $\mathrm{Tr}(\mathscr{H}_{NR}^p H)$ is positive (negative) for p even (odd), the following relations hold:

$$0 < \mu_p^R < \mu_p^{NR}, \quad p \text{ even},$$

$$0 > \mu_p^R > \mu_p^{NR}, \quad p \text{ odd}. \quad (44)$$

These results are general, in the sense that they are valid for any kind of lattice we may consider. We now comment on the physical meaning of Eq. (44). The first moment ($p = 1$) gives the centroid of the DOS, and Eq. (44) demonstrates that relativity raises the whole spectrum. This result is also indicated clearly by the fact that $\varepsilon_k^R > \varepsilon_k^{NR}$. The second moment ($p = 2$) gives an estimation of the width of the spectrum, and Eq. (44) indicates that the relativistic spectrum is shrunk with respect to the non-relativistic one. This conclusion agrees well with the results we have obtained in the case of the periodic lattices. In addition, a shrinkage of the spectrum has also been observed in Kroning–Penney models on quasiperiodic lattices [21].

6. Discussions and conclusions

As we have seen earlier, the general formulations of Sections 2 and 3 lead to many important results concerned with the electronic energy spectrum of periodic, quasiperiodic and disordered systems, within the framework of discretized Hamiltonians;

Section 2 is pertinent to non-relativistic electrons while Section 3 takes care of relativistic electrons. As regards the periodic case, the results collected in Eqs. (35) and (39) are quite significant. These results express the relativistic impacts on bandwidths and gaps of monoatomic and diatomic chains; they are likely to throw light upon relativistic effects on electrical conduction and optical absorption of corresponding systems. With regard to general lattices which include quasiperiodic and disordered systems, the result expressed by Eq. (44) is a very important one; this result shows the relativistic impact on DOS, which is a vital entity in connection with electronic spectrum in condensed matter.

Finally, we would like to remark that, besides yielding the above-mentioned important results, the formulations of Sections 2 and 3 are capable of providing us with information about relativistic impact on *localization length* in disordered systems where Anderson localization plays a major role; we hope to report in the future our treatment of this issue.

Acknowledgements

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