Dirac comb with a periodic mass jump

J.J. Alvarez
E.U. de Informática de Segovia,
University of Valladolid, Spain.
jjalvarez@infor.uva.es

M. Gadella
Departamento de Física Teórica, Atómica y Optica, Universidad de Valladolid,
Facultad de Ciencias, Paseo Belén 9, 47011, Valladolid, Spain.
e-mail: manuelgadella1@gmail.com

L.M. Nieto
Física Teórica, Atómica y Optica, Universidad de Valladolid, Facultad de Ciencias,
Paseo Belén 9, 47011, Valladolid, Spain.
e-mail: luismi@metodos.fam.cie.uva.es

Received 3 June 2013; accepted 26 July 2013

We discuss some of the properties of the spectrum of a Dirac comb with periodic mass discontinuity. Based on the relationship between the two different masses, we derive the general behavior of the spectra for both cases $E > 0$ and $E < 0$. The relationship with the constant mass model for the Dirac comb and the generalization to periodic quantum chains with n different masses are also discussed.

Keywords: Delta interactions; mass jumps; periodic potentials; energy band structures.

Se discuten algunas de las propiedades del espectro del peine de Dirac con una discontinuidad periódica en la masa. Deducimos el comportamiento general del espectro para los casos $E > 0$ and $E < 0$, basándonos en la relación entre las diferentes masas. También se discute la correspondencia entre nuestros resultados y los obtenidos para el peine de Dirac con masa constante, así como la generalización a cadenas periódicas con n masas diferentes.

Descriptores: Interacciones tipo delta; saltos de masa; potenciales periódicos; estructuras de bandas de energía.

PACS: 03.65.-w; 03.65.Ge

1. Introduction

One dimensional Hamiltonians with singular potentials have recently received a lot of attention as they provide examples of exactly solvable models [1–6]. Independently, systems with variable mass have lately acquired some attention in the literature [7–9]. The simplest one dimensional systems with variable mass are those in which the mass is constant except for a discontinuity or jump at a given point. This kind of abrupt discontinuity is interesting from the physicist point of view since it can be used to represent an abrupt heterojunction between two different materials [7].

In the present example, we study a one dimensional system with an interaction in the form of Dirac's comb with two alternating different masses. At the points supporting the deltas the mass is discontinuous and undergoes a jump, it is constant at any other point. The purpose of this article is to discuss the spectral phenomena produced by this kind of periodic systems, an analysis inspired on the study of the Kronig-Penney model.

Here, the Hamiltonian for the system under our consideration can be splitted in the sum of two terms: an unperturbed Hamiltonian H_0 plus a singular potential. In its most general form, H_0 can be written as

$$H_0 = \frac{1}{2}\, m^\alpha(x)\, p\, m^\beta(x)\, p\, m^\alpha(x)\,, \tag{1}$$

with $2\alpha + \beta = -1$ and $m(x)$ is an arbitrary function given the mass in terms of the position. Consequently, $m(x)$ in (1) should be represented as an operator which in general does not commute with the momentum p as is a function of the variable x. In this paper, we shall use some particular form of $m(x)$ as well as a particular choice of α and β. This is the purely kinetic term of the Hamiltonian. The total Hamiltonian is of the form $H = H_0 + V$, where V is a singular potential, the Dirac comb that will be defined in precise terms later.

This paper is organized as follows: in Sec. 2, we summarize the results in the case of one delta barrier and one mass jump. The case of Dirac's comb with periodic mass jumps is discussed in Section III, along some ideas concerning generalizations to periodic systems with more different masses. The article is closed with some concluding remarks.

2. One Dirac delta with a mass jump at $x = a$

The simplest system of the type discussed in the Introduction includes one delta barrier supported at the point $x = a > 0$ plus a mass jump at the same point. As was stated in the Introduction, situations with variable mass simulate nonhomogeneous media and, in particular, a mass jump mimics a sudden change in the media. Here, the idea is to combine the mass discontinuity with a delta interaction. This system, which has been already introduced in Ref. 10, is essential for any further generalization. In addition, its inclusion here makes the present article self contained. Then, let us first consider the Hamiltonian H_0 as in (1) with a mass jump at the point $a > 0$. Thus, it seems natural to choose the function of the mass in terms of the position $m(x)$ to be:

$$m(x) = \begin{cases} m_1 & \text{if} \quad x < a \\ m_2 & \text{if} \quad x > a \end{cases} . \tag{2}$$

We have seen that the kinetic term H_0 in (1) depends on the parameter α (note than if we determine α, β is automatically determined). Among all possible choices, $\alpha = 0$ and $\beta = -1$ is the most natural and, in addition, it has been proven to be Galilei invariant [8]. In Ref. 11 we have proven that a domain of self adjointness for H_0 can be provided by the space of square integrable functions $\psi(x)$ continuous at $x = a$ and with the following matching conditions for the first derivative:

$$\frac{1}{m_2}\,\psi'(a+) - \frac{1}{m_1}\,\psi'(a-) = 0\,. \tag{3}$$

In this case, the kinetic term H_0 can be written as [11]:

$$H_0 := \begin{cases} -\dfrac{\hbar^2}{2m_1}\dfrac{d^2}{dx^2}\,, & x < a\,, \\ -\dfrac{\hbar^2}{2m_2}\dfrac{d^2}{dx^2}\,, & x > a\,. \end{cases} \tag{4}$$

A thoroughly discussion of the self adjoint versions of (4) is given in Ref. 12. Another possibility is introduced in Ref. 10. Also, a discussion on the self adjointness of H_0 with mass jump and arbitrary values of α can be carried out analogously. However, this is not the relevant discussion in here, where we have in addition to the mass jump, a Dirac delta at the same point $x = a$, so that the total Hamiltonian becomes

$$H = H_0 + \lambda\delta(x-a)\,, \quad a > 0\,. \tag{5}$$

As done with H_0 in Ref. 12, a self adjoint version of (5) should be constructed using the von Neumann formalism of self adjoint extensions of symmetric operators with equal deficiency indices [1,2]. We shall present a brief discussion of this in the next subsection.

2.1. Self adjoint determination of H through matching conditions

According to the theory of self adjoint extensions of symmetric operators, in order to define the total Hamiltonian given in (5), we need to specify a domain, $\mathcal{D}(H)$ for H. This domain is a subspace of the space of square integrable functions fulfilling certain conditions plus given matching conditions at $x = a$. Thus the functions in the domain of H belong to the Sobolev space $W(\mathbb{R}/\{0\})$ [13] and fulfill the following matching conditions at $x = a$ [11]:

$$\begin{pmatrix} \varphi(a+) \\ \varphi'(a+) \end{pmatrix} = \mathcal{T} \begin{pmatrix} \varphi(a-) \\ \varphi'(a-) \end{pmatrix}, \tag{6}$$

where $\varphi(a+)$ and $\varphi(a-)$ are the boundary values at $x = a$ of the function $\varphi \in \mathcal{D}(H)$ to the right and to the left respectively. The 2×2 matrix $\mathcal{T}$ gives the matching conditions at $x = a$ and the prime denotes derivative with respect x.

As was proven in a previous article [11], boundary conditions given by $\mathcal{T}$ define a domain for which H is self adjoint if and only if [14]

$$M_1 = \mathcal{T}^\dagger M_2 \mathcal{T}\,, \tag{7}$$

where,

$$M_i := \frac{\hbar^2}{2m_i}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad i = 1, 2 \tag{8}$$

The matching conditions that determine the Hamiltonian H in (5) are [11]

$$\psi(a-) = \psi(a+) = \psi(a)\,,$$

$$\frac{1}{m_2}\psi'(a+) - \frac{1}{m_1}\psi'(a-) = \frac{2\lambda}{\hbar^2}\,\psi(a)\,, \tag{9}$$

which is a simple generalization of (3). Note that the wave functions on this domain are continuous. The discontinuity in the derivative is the minimal generalization of the discontinuity defining the delta potential allowing for a mass jump. In this particular situation, matrix $\mathcal{T}$ as in (6) is given by

$$\mathcal{T} = \begin{pmatrix} 1 & 0 \\ \frac{2m_2\lambda}{\hbar^2} & \frac{m_2}{m_1} \end{pmatrix}. \tag{10}$$

Thus far the discussion on the construction of the Hamiltonian H in (5).

3. The Dirac comb with mass jumps

Now, we investigate the Dirac comb with mass jumps at the points supporting the deltas. As is well known, the one dimensional Dirac comb is a one dimensional Hamiltonian of the form $H = -\hbar^2/(2m)\; d^2/dx^2 + V(x)$, where $V(x)$ is a singular potential given by

$$V(x) = \sum_{n=-\infty}^{\infty} \gamma\delta(x - na)\,. \tag{11}$$

If the constant mass in the kinetic term of the Hamiltonian is replaced by a function of the position $m(x)$, we have to determine this function first. The simplest possible choice is the following:

$$m(x) := \begin{cases} \cdots & \cdots & \cdots\cdots \\ m_1 & \text{if} & 0 < x < a \\ m_2 & \text{if} & a < x < 2a \\ m_1 & \text{if} & 2a < x < 3a \\ m_2 & \text{if} & 3a < x < 4a \\ \cdots & \cdots & \cdots\cdots \end{cases} . \tag{12}$$

Now, the situation is the following: at each point of the infinite sequence na with $n \in \mathbb{Z}$, where $\mathbb{Z}$ is the set of the entire numbers, we have a Dirac delta, either attractive or repulsive, plus a mass jump. The function giving the mass in terms of the position is the simplest possible compatible with the existence of a mass jump at each point supporting a delta. This implies that the only possible values of the mass are just two: m_1 and m_2.

In order to define the Hamiltonian $H = H_0 + V(x)$, we follow the procedure suggested in the previous section. Then, we shall determine matching conditions at the points $x_n = na$, $n \in \mathbb{Z}$. These matching conditions will be given by the following relations on the wave functions $\psi(x)$:

$$\begin{pmatrix} \psi_{n+1}(na) \\ \psi'_{n+1}(na) \end{pmatrix} = \mathcal{T}_n(na) \begin{pmatrix} \psi_n(na) \\ \psi'_n(na) \end{pmatrix} , \tag{13}$$

were $\psi_n(x)$ represents the function $\psi(x)$, solution of the Schrödinger equation, on the interval $[(n-1)a, na]$. Note that $\psi_n(x) = A_n\, e^{ik_n x} + B_n\, e^{-ik_n x}$, where $k_n = \sqrt{2m_n E/\hbar^2}$.

3.1. Determination of the spectrum

Once we have established the matching conditions for the above situation (11), we would like to obtain its spectrum. The band structure of the spectrum of the Dirac comb is well known [15] and it is depicted in Figs. 1 and 2, where the energy band structure is given by:

$$|\cos ka + \frac{\gamma}{k} \sin ka \,| \leq 1 \,. \tag{14}$$

Thus far, we have not distinguished between a comb with repulsive ($\gamma > 0$) or attractive ($\gamma < 0$) deltas. In the case of repulsive deltas, the expression (14) can be written as

$$|\cos(ka - \alpha)\,| \leq \frac{1}{\sqrt{1 + \frac{\gamma^2}{k^2}}} \tag{15}$$

with $\tan\alpha = \gamma/k$.

When all deltas are attractive ($\gamma < 0$ and $E < 0$), there is only one permitted energy band, which is given by

$$|\cosh ka - \frac{\gamma}{k} \sinh ka \,| \leq 1 \,. \tag{16}$$

This is is shown in Fig. 2.

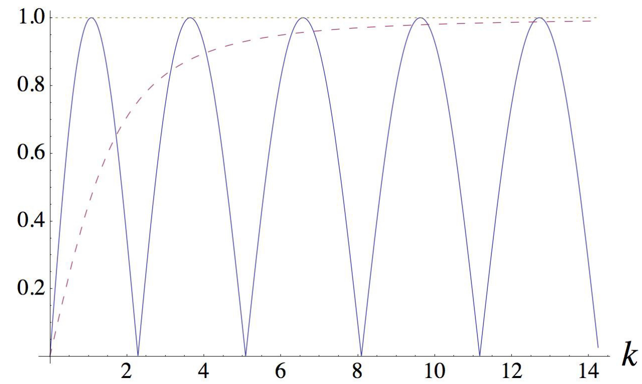

FIGURE 1. Dirac comb with constant mass and $\gamma = 2$. Repulsive case.

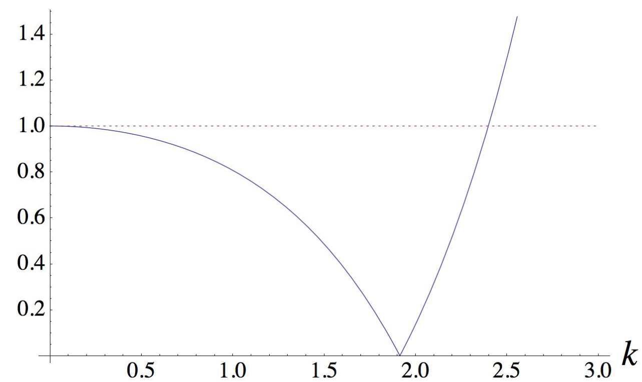

FIGURE 2. Diracs comb with constant mass and $\gamma = 2$. Atractive case.

This infinite chain of deltas with mass jumps described so far can be represented in terms of a one dimensional Bravais lattice as follows:

Here the black circles represent the regions with m_1 and the white circles the regions with m_2. Between them, we draw linking lines representing the matching conditions between two regions. This one dimensional lattice has a periodicity $2a$.

If we allocate one black circle at the origin of coordinates and we apply the Bloch theorem, we obtain three wave functions that are the minimal set of solutions of the Schrödinger equation that solve the Bravais lattice:

$$\begin{aligned} \psi_I(x) &= A_1\, e^{ikx} + B_1\, e^{-ikx}, \quad 0 \leq x \leq a \\ \psi_{II}(x) &= A_2\, e^{i\xi kx} + B_2\, e^{-i\xi kx}, \quad a \leq x \leq 2a \\ \psi_{III}(x) &= (A_1\, e^{ik(x-2a)} + B_1\, e^{-ik(x-2a)}) e^{iK2a}, \\ & \qquad 2a \leq x \leq 3a \,. \end{aligned} \tag{17}$$

Then, applying the matching conditions given by (9) to this set of solutions we get a homogeneous linear system in the variables A_1, A_2, B_1, B_2, whose coefficients are given by the following matrix:

$$\begin{pmatrix} e^{ika} & e^{-ika} & -e^{-i\xi ka} & -e^{i\xi ka} \\ \frac{-ie^{ika}(k-2im\gamma)}{m} & \frac{ie^{-ika}(k+2im\gamma)}{m} & \frac{-ie^{-ik\xi a}k}{m\xi} & \frac{ie^{ik\xi a}k}{m\xi} \\ e^{iK2a} & e^{iK2a} & -e^{-2ik\xi a} & -e^{2ik\xi a} \\ \frac{-e^{iK2a}(-ik+2m\gamma)}{m} & \frac{-e^{iK2a}(ik+2m\gamma)}{m} & \frac{ie^{-2ik\xi a}k}{m\xi} & \frac{-ie^{2ik\xi a}k}{m\xi} \end{pmatrix}, \tag{18}$$

where

$$\xi^2 = \frac{m_2}{m_1}, \qquad \xi = \frac{k_2}{k_1}, \qquad m = m_1 \qquad k = k_1 \,. \tag{19}$$

The constant K appears as a consequence of the Bloch theorem. In fact, the Bloch theorem states that our wave functions must satisfy the relation $\psi(x + 2a) = \mu\,\psi(x)$, where $|\mu| = 1$. Then, the relation $\mu = e^{i2aK}$ defines K.

In order to obtain a nontrivial solution of the above system (17), the determinant of (18) must be zero. If we impose this condition and after some algebra, we arrive to the following condition:

$$\cos K2a = \frac{1}{2k^2\xi}(2k\xi\cos ka(k\cos\xi ka + 2m\gamma\xi\sin\xi ka) - \sin ka(-4km\gamma\xi\cos\xi ka + (-4m^2\gamma^2\xi^2 + k^2(1+\xi^2))\sin\xi ka))\,. \tag{20}$$

In (20) the periodicity is expressed in terms of the energy and all the other parameters. As a consequence, we shall obtain a band spectrum for both the attractive ($\gamma < 0$) and the repulsive ($\gamma > 0$) cases.

Our results show that the dependency on ξ is rather complicated as is shown in Figs. 3 and 4.

In the repulsive case (Fig. 3), we can observe that the band structure including the mass jumps does not differs much from the band structure that appears in the constant mass case. See Fig. 1.

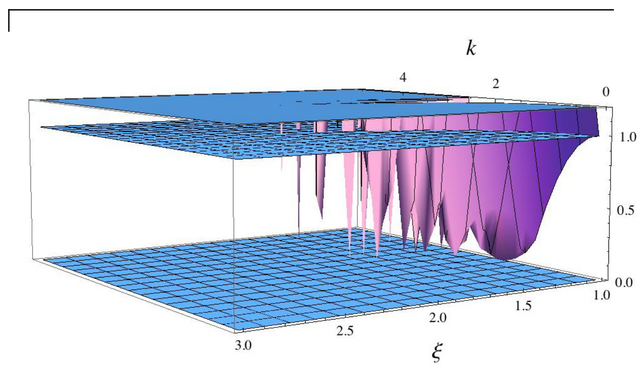

FIGURE 4. 3D plot of the energy bands for $\xi = 1$ to $\xi = 3$ with $\gamma = 2$. Atractive case.

In the attractive case with constant mass, Fig. 2, we have only one band. It is noteworthy to remark that, in the mass jumps case, the longer is $\xi^2 = m_2/m_1$, *i.e.*, the bigger is the ratio between masses, the narrower is the energy band width. This effect is shown in Figs. 5 and 6, where we depict the band for the values $\xi = 1.5$ in Fig. 5 and $\xi = 2.5$ in Fig. 6. In both cases, the width is shown by the distance between the two blue lines measured over the k axis. This can be compared to the energy band width for the equal masses case, $\xi = 1$. This latter case has been already studied by Cerveró and coworkers [16].

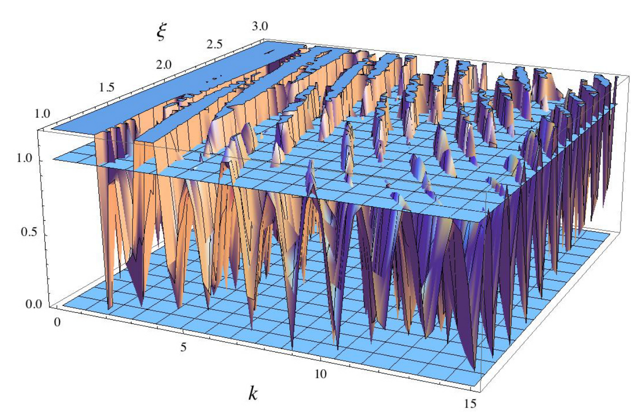

FIGURE 3. 3D plot of the energy bands for $\xi = 1$ to $\xi = 3$ with $\gamma = 2$. Repulsive case.

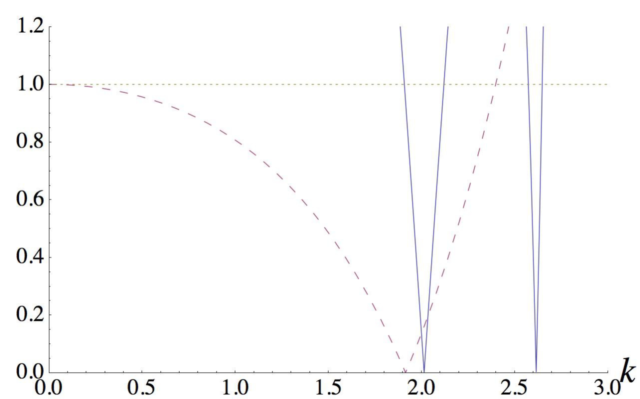

FIGURE 5. Energy bands for the attractive case with $\gamma = 2$, $\xi = 1.5$.

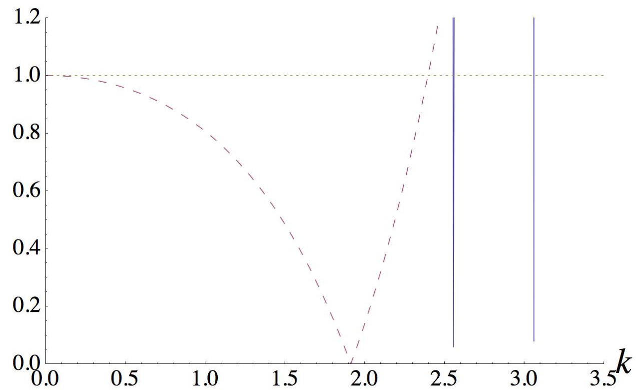

FIGURE 6. Energy bands for the attractive case with $\gamma = 2$, $\xi = 2.5$.

3.2. Limit cases for ξ

In this section we will study the limits for the "strong coupling" ($m_1 >> m_2$) and "weak coupling" ($m_1 \sim m_2$). Here, we use $a = 1$ and $m = m_1 = 1$ for simplicity. In the first case, the limit of $\xi \to 0$ on the Eq. (20) gives:

$$| \cos(k-\alpha) | \leq \frac{1}{\sqrt{1+\left(\frac{k}{2}-\frac{2\gamma}{k}\right)^2}}\,, \qquad (21)$$

with $\tan\alpha = (2\gamma/k) - (k/2)$. The behavior of (21) is shown in Figs. 7 and 8. It is clear that the band width goes to zero if we start at the point $k_m = 2\sqrt{\gamma}$ and we take both limits $k \to 0$ and $k \to +\infty$. At this starting point, the equation on the right term in (21) gets its maximum. We observe a perturbation on the permitted energy band closest to the point k_m which doubles this band. This effect depends on the parameter γ. This splitting is periodic in γ and occurs at the values $\gamma_n = n^2(\pi^2/4)$, with $n \in \mathbb{N}$. This comes from the values of γ that minimize condition (21).

In the weak coupling case ($m_1 \sim m_2$):

$$\left| \left(1-\left(\frac{\gamma}{k}\right)^2\right)\cos 2k + \frac{2\gamma}{k}\sin 2k + \left(\frac{\gamma}{k}\right)^2 \right| \leq 1 \qquad (22)$$

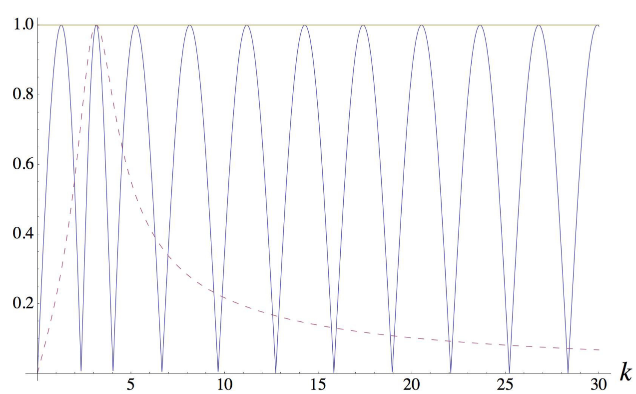

FIGURE 7. Energy bands for the repulsive case and the strong coupling limit, $\gamma_{n=1} = \frac{\pi^2}{4}$.

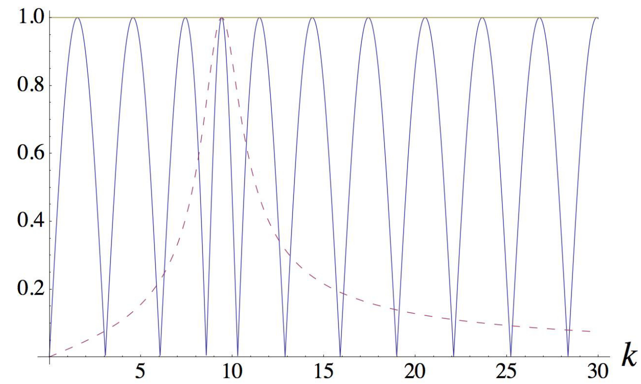

FIGURE 8. Energy bands for the repulsive case and the strong coupling limit, $\gamma_{n=3} = \frac{9\pi^2}{4}$.

we observe, in the case $k \gg \gamma$, the same band structure as observed for equal masses, which is shown in Fig. 1.

For low energies, the condition:

$$\gamma(\gamma+2) \leq k^2 \qquad (23)$$

is easily derived. In this case, it appears one permitted energy band only, which gets narrower as γ grows, up to saturate the inequality (23). This is depicted in Figs. 9 and 10.

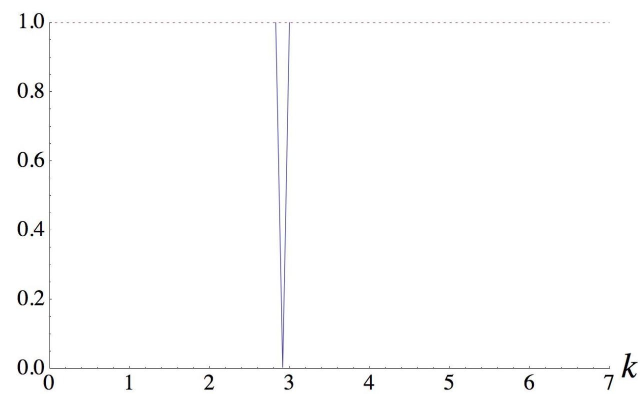

FIGURE 9. Energy bands for the repulsive case for the weak coupling. $\gamma = 2$.

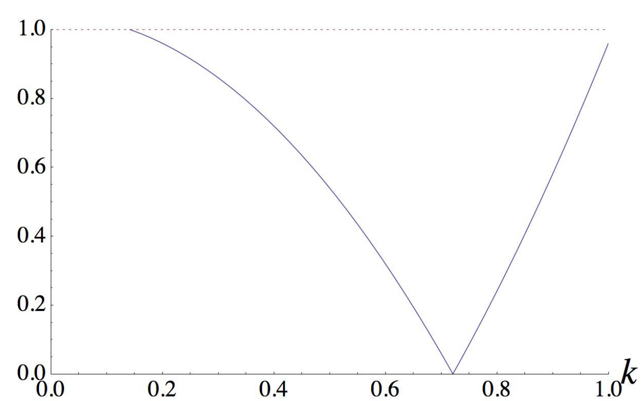

FIGURE 10. Energy bands for the repulsive case for the weak coupling. $\gamma = 0.01$.

4. Concluding remarks

We derive the spectrum of a Dirac comb with a jump of mass located at the points supporting the deltas. We analyze the simplest problem in which the mass has two values only. In addition, all the deltas are multiplied by the same coefficient γ which is either positive or negative. The result is a periodic potential which can be analyzed with the help of the Bloch theorem.

We may be tempted to generalize this model with the introduction on more different masses $m_3, m_4, \ldots, m_n$. However, this generalization does not give us anything new as it provides the same one dimensional Bravais lattice and is therefore equivalent to the situation here considered. Moreover, the introduction of more masses has the undesirable effect of complicating the situation unnecessarily. In particular, if we had n different masses, we would need to deal with an $2n \times 2n$ matrix.

The results obtained depend on the both the sign of γ and the square of the ratio between the two different masses. If $\gamma > 0$, the mass jump does not add any new effect and a band structure appears similar to the usual band structure shown in the case of constant masses. If $\gamma < 0$, *i.e.*, all deltas are attractive, the band width goes to zero as the ratio between masses goes to infinite.

It is clear that our model is equivalent to a one dimensional Bravais lattice.

The limiting cases "strong coupling" ($m_1 \gg m_2$) and "weak coupling" ($m_1 \sim m_2$) have been studied. Meanwhile for weak coupling reappears the band structure shown for equal masses, new interesting effects emerge for strong coupling.

Acknowledgements

We wish to acknowledge partial financial support by the Spanish Ministry of Science and Innovation through Project MTM2009-10751, the Junta de Castilla y León, through Project GR224.

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13. These are continuous functions (except for a finite jump at the origin) from $\mathbb{R}$ into $\mathbb{C}$ such that: (i) any $\varphi(x) \in W(\mathbb{R}/\{0\})$ admits a first continuous derivative (except at the origin), (ii) the second derivative exists almost everywhere, and (iii) both $\varphi(x) \in W(\mathbb{R}/\{0\})$ and its second derivative are a.e. square integrable, so that $\int_{-\infty}^{\infty} \{|\varphi(x)|^2 + |\varphi''(x)|^2\}\, dx < \infty$.
14. Here H is any self adjoint extension of the free Hamiltonian H_0 defined on the space of functions belonging to the Sobolev space $W(\mathbb{R})$ and such that they vanish on a neighborhood of $x = a$. Each matrix $\mathcal{T}$ defines a self adjoint extension of H_0 and eventually a singular potential, which depends on $\mathcal{T}$.
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