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A generalised Dirac–Kronig–Penney model

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Abstract. In the present work, a generalisation of the Dirac–Kronig–Penney model for polyatomic crystals has been developed. The crystal potential is taken as a periodic array of δ-function potentials, with several δ-functions of different strength in each unit cell. The dispersion law of Dirac electrons in such a potential is found in a closed form.

In a recent paper (Eldib *et al* 1987), the well known Kronig–Penney model has been generalised to be applicable for polyatomic crystals, containing M different atoms in the unit cell. Nevertheless, relativistic effects in the band structure have not been considered in the above-mentioned model. These effects can be important at high energies on the electrons in solids consisting of heavy atoms (for a review on relativistic electrons in one-dimensional systems, see Roy (1986)). Relativistic electronic states in diatomic (equally spaced atoms) crystals have been discussed in an earlier paper by Sen Gupta (1974). The aim of the present work is to generalise the Dirac–Kronig–Penney model for polyatomic crystals, taking into account relativistic effects.

A number of researchers have treated δ-function potentials with the Dirac equation (Sutherland and Mattis (1981) and McKellar and Stephenson (1987), and references therein). It has also been noted that the solution obtained by solving the Dirac equation for a δ-function potential, and the expression attained when considering the limiting case of a square well (or barrier) are different. Fairbairn *et al* (1973) argued that this disagreement is related to the Klein paradox. In the above-mentioned work, McKellar and Stephenson have shown a reasonable way to use δ-function potentials with the one-dimensional Dirac equation. For electrostatic-type potentials which approach a δ-function limit (located at x_0), they found the following boundary condition for the two-component electron wavefunction (in the standard representation):

$$\psi(x_0^+) = \begin{bmatrix} \cos(A/\hbar c) & -i\sin(A/\hbar c) \\ -i\sin(A/\hbar c) & \cos(A/\hbar c) \end{bmatrix} \psi(x_0^-) \tag{1}$$

A being the strength of the potential.

We shall use the boundary condition (1) to find the dispersion law of Dirac electrons under the action of the crystal potential

$$V_c(x) = \sum_{\mu=1}^{M} \sum_{n=-\infty}^{\infty} V_\mu(x - R_\mu - nL) \tag{2}$$

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where the 'atomic' potentials are taken as $V_\mu(x) \to A_\mu \delta(x)$, with $A_\mu > 0$. The position of each ion in the unit cell is denoted by R_μ and L is the lattice parameter. The Bloch theorem is as follows:

$$\psi(x) = \exp(\mathrm{i}\kappa x)\varphi(x) \tag{3}$$

$\varphi(x)$ being a two-component periodic function, with the same period as the crystal lattice. Therefore, it suffices to find $\varphi(x)$ within the unit cell $[0, L]$. The function $\varphi(x)$ satisfies the equation (Domínguez-Adame 1987)

$$[-\mathrm{i}\hbar c\sigma_x(\partial_x + \mathrm{i}\kappa) + \sigma_z mc^2 + V_c(x) - E(\kappa)]\varphi(x) = 0 \tag{4}$$

σ_x and σ_z being the usual 2×2 Pauli matrices. The solution of this equation is readily found

$$\varphi_\mu(x) = \exp(-\mathrm{i}\kappa x)\begin{bmatrix} \exp(\mathrm{i}\eta x) & \exp(-\mathrm{i}\eta x) \\ \xi^{-1}\exp(\mathrm{i}\eta x) & -\xi^{-1}\exp(-\mathrm{i}\eta x) \end{bmatrix} P_\mu$$
$$R_\mu < x < R_{\mu+1} \qquad \mu = 0, 1, \ldots, M \tag{5}$$

with $R_0 \equiv 0$ and $R_{M+1} = L$. For simplicity, we have introduced the notation $\eta\hbar c = (E^2 - m^2c^4)^{1/2}$ and $\xi^2 = (E + mc^2)/(E - mc^2)$. P_μ denotes here a two-component constant vector. After applying the boundary condition (1) at each R_μ, we obtain

$$P_{\mu+1} = \mathbf{D}_\mu(\eta)P_\mu \qquad \mu = 1, 2, \ldots, M \tag{6}$$

where

$$\mathbf{D}_\mu(\eta) = \begin{bmatrix} \alpha_\mu(\eta) & \beta_\mu(\eta) \\ \beta_\mu^*(\eta) & \alpha_\mu^*(\eta) \end{bmatrix} \tag{7}$$

with

$$\alpha_\mu(\eta) = \cos(A_\mu/\hbar c) - \mathrm{i}(E/\eta\hbar c)\sin(A_\mu/\hbar c)$$
$$\beta_\mu(\eta) = -\mathrm{i}(mc^2/\eta\hbar c)\sin(A_\mu/\hbar c)\exp(-2\mathrm{i}\eta R_\mu). \tag{8}$$

It is interesting to note that $\det\|\mathbf{D}_\mu(\eta)\| = 1$; we shall use this property below. The periodicity of $\varphi(x)$ leads to the condition

$$P_{M+1} = \exp(\mathrm{i}\kappa L)\begin{bmatrix} \exp(-\mathrm{i}\eta L) & 0 \\ 0 & \exp(\mathrm{i}\eta L) \end{bmatrix} P_1 \tag{9}$$

and by successive use of equation (6) we immediately infer that

$$\exp(\mathrm{i}\kappa L)\begin{bmatrix} \exp(-\mathrm{i}\eta L & 0 \\ 0 & \exp(\mathrm{i}\eta L) \end{bmatrix} P_1 = \mathbf{G}P_1 \tag{10}$$

where we have defined $\mathbf{G} = \mathbf{G}(\eta) = \mathbf{D}_M(\eta)\mathbf{D}_{M-1}(\eta)\ldots\mathbf{D}_1(\eta)$. This 2×2 matrix has interesting properties, namely $\det\|\mathbf{G}\| = 1$, $G_{11}^* = G_{22}$ and $G_{21}^* = G_{12}$, as can be readily verified from the properties of $\mathbf{D}_\mu(\eta)$. The consistency of equation (10) and the afore-

mentioned properties of **G** give us the required dispersion law of Dirac electrons in the crystal potential:

$$\cos(\kappa L) = \mathrm{Re}\, G_{11} \cos(\eta L) - \mathrm{Im}\, G_{11} \sin(\eta L) \tag{11}$$

where Re z and Im z indicate real and imaginary parts, respectively, of the complex number z. Note that we must evaluate only one element of the matrix **G**. The solution of the dispersion relation $E(\kappa)$ has to be found numerically, for any arbitrary value of M.

If only a few atoms are placed in the unit cell of the crystal, the dispersion law (11) can be written in a more simplified form. For monatomic crystals, we have $G_{11} = \alpha(\eta)$ so that

$$\cos(\kappa L) = \cos(\eta L) \cos(A/\hbar c) + (E/\eta\hbar c) \sin(\eta L) \sin(A/\hbar c). \tag{12}$$

This expression has formerly been proposed by McKellar and Stephenson for the Dirac–Kronig–Penney model. It should be observed that, as $c \to \infty$, equation (12) approaches the non-relativistic Kronig–Penney result.

If we now place two different atoms in each unit cell, we have $G_{11} = \alpha_1(\eta)\alpha_2(\eta) + \beta_1^*(\eta)\beta_2(\eta)$. Therefore, the relativistic dispersion law for diatomic crystals is found to be

$$\begin{aligned}\cos(\kappa L) = {} & \cos(\eta L) \cos[(A_1 + A_2)/\hbar c] + (E/\eta\hbar c) \sin(\eta L) \sin[(A_1 + A_2)/\hbar c] \\ & + 2(mc^2/\eta\hbar c)^2 \sin(A_1/\hbar c) \sin(A_2/\hbar c) \\ & \times \sin[\eta(R_2 - R_1)] \sin[\eta(L - R_2 + R_1)]\end{aligned} \tag{13}$$

which reduces to equation (12) as $A_2 = 0$. The non-relativistic limit can be written as

$$\begin{aligned}\cos(\kappa L) = {} & \cos(\eta L) + [m(A_1 + A_2)/\eta\hbar^2] \sin(\eta L) \\ & + 2A_1A_2(m/\eta\hbar^2)^2 \sin[\eta(R_2 - R_1)] \sin[\eta(L - R_2 + R_1)].\end{aligned} \tag{14}$$

This is the expression obtained by Eldib *et al* who solved directly the Schrödinger equation for the crystal potential (2).

In a similar way, the dispersion relation for triatomic crystals ($M = 3$) is found to be

$$\begin{aligned}\cos(\kappa L) = {} & \cos(\eta L) \cos[(A_1 + A_2 + A_3)/\hbar c] + (E/\eta\hbar c) \sin(\eta L) \\ & \times \sin[(A_1 + A_2 + A_3)/\hbar c] + 2(mc^2/\eta\hbar c)^2 \{\cos(A_1/\hbar c) \sin(A_2/\hbar c) \\ & \times \sin(A_3/\hbar c) \sin[\eta(R_3 - R_2)] \sin[\eta(L - R_3 + R_2)] + \sin(A_1/\hbar c) \\ & \times \cos(A_2/\hbar c) \sin(A_3/\hbar c) \sin[\eta(R_3 - R_1)] \sin[\eta(L - R_3 + R_1)] \\ & + \sin(A_1/\hbar c) \sin(A_2/\hbar c) \cos(A_3/\hbar c) \sin[\eta(R_2 - R_1)] \\ & \times \sin[\eta(L - R_2 + R_1)] + 2(E/\eta\hbar c) \sin(A_1/\hbar c) \sin(A_2/\hbar c) \\ & \times \sin(A_3/\hbar c) \sin[\eta(R_3 - R_2)] \sin[\eta(R_2 - R_1)] \\ & \times \sin[\eta(L - R_3 + R_1)]\}\end{aligned} \tag{15}$$

which reduces again to the results of Eldib *et al* in the non-relativistic limit.

In summary, we have generalised the Dirac–Kronig–Penney model for polyatomic crystals containing M atoms in each unit cell. The treatment given above may be regarded only as a simple but very instructive way to study relativistic effects in polyatomic crystals.

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