Relativistic and nonrelativistic Kronig–Penney models

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The wavefunction and the Kronig–Penney dispersion relation of an electron moving in a one-dimensional periodic array of delta potentials are found, in the relativistic as well as in the nonrelativistic case. The Green's function method and Bloch's theorem are used in a simple form.

I. INTRODUCTION

The Kronig–Penney model[1] has been widely used to introduce some important concepts of electron dynamics in a periodic potential, namely, Bloch functions and the occurrence of energy bands. This model assumes a single electron moving in one-dimensional periodic square well potentials. However, this potential is frequently replaced by a

one-dimensional periodic array of delta functions, the area of the barriers and the lattice parameter remaining unchanged. To obtain the wavefunction and the electron energy, one must solve the appropriate nonrelativistic Schrödinger equation or the relativistic Dirac equation with suitable boundary conditions. Boundary conditions for the electron wavefunction in the delta potential do not correspond to any real physical situation[2]: nonrelativistic wavefunction derivative and relativistic wavefunction are not continuous.

In the present article, we find the wavefunction and the energy of an electron moving in an infinite one-dimensional array of delta potentials. In order to solve the problem, Green's function method and Bloch's theorem[3] are applied in a simple and pedagogic way. Fairbairn *et al.*[4] employed analogous techniques to analyze the relativistic effects on surface states. The procedure is based on the expansion of Bloch waves in terms of a complete and orthogonal set of plane waves, i.e., we take the Fourier transform. This procedure does not need any previous knowledge of Green's function method[5] and it can be used in both nonrelativistic and relativistic equations (Secs. II and III, respectively). Furthermore, "strange" boundary conditions are avoided; we only require the periodicity of Bloch functions. In turn, we need a cumbersome, although straightforward, algebra. Also, we calculate the relativistic corrections at low energy, with the aid of the dispersion relation (Sec. IV).

II. NONRELATIVISTIC ELECTRON IN THE PERIODIC POTENTIAL

Let us suppose a nonrelativistic electron with mass m is moving under the action of the one-dimensional potential

$$V(x) = A \sum_{n=-\infty}^{\infty} \delta(x - nL), \tag{1}$$

where L is the lattice parameter and A is the area of the barriers. According to Bloch's theorem, the wavefunction of such an electron in the periodic potential is expressed as

$$\psi(x) = \exp(ikx)\,U(x), \tag{2}$$

$\hbar k$ being the crystal momentum. Here, $U(x)$ is periodic with period L, i.e.,

$$U(x + nL) = U(x), \quad n = 0, \pm 1, \pm 2, \ldots \tag{3}$$

and satisfies the following equation[6]:

$$[-(\hbar^2/2m)(\partial + ik)^2 + V(x)]\,U(x) = \epsilon_0(k)\,U(x), \tag{4}$$

where ∂ denotes differentiation with respect to x and $\epsilon_0(k)$ is the nonrelativistic electron energy.

We must solve this equation to find the electron energy $\epsilon_0(k)$. For this purpose, we expand $U(x)$ in terms of plane waves $\phi(l,x) = (2\pi)^{-1/2}\exp(ilx)$ so we can write

$$U(x) = \int_{-\infty}^{\infty} dl'\,\phi(l',x)a(l'). \tag{5}$$

Inserting expansion (5) in Eq. (4), multiplying the result by $\phi^*(l,x)$, and integrating over all x values, one obtains

$$a(l) = \left(\frac{2mA}{\hbar^2}\right)[\alpha_0^2 - (l+k)^2]^{-1} \times \sum_{n=-\infty}^{\infty} \phi^*(l,nL)\,U(nL), \tag{6}$$

where $\alpha_0 = \alpha_0(k) = [2m\epsilon_0(k)/\hbar^2]^{1/2}$. Thus beginning with expansion (5), the solution for Eq. (4) is

$$U(x) = \left(\frac{mA}{\pi\hbar^2}\right) \sum_{n=-\infty}^{\infty} U(nL) \int_{-\infty}^{\infty} dl \times \exp[il(x - nL)]\,[\alpha_0^2 - (l+k)^2]^{-1}.$$

Carrying out the integration by contour methods (we take α_0 with a small positive imaginary part so the summation converges) and taking into account the relation $U(nL) = U(0)$, we have

$$U(x) = -i\left(\frac{P}{\alpha_0 L}\right) U(0) \sum_{n=-\infty}^{\infty} \times \exp[-ik(x - nL) + i\alpha_0|x - nL|], \tag{7}$$

with $P = mAL/\hbar^2$. Note that the condition given in Eq. (3) is fulfilled for this function, i.e., $U(x)$ is periodic with the same period of the crystal lattice. Therefore, it suffices to find $U(x)$ within the unit cell $[0,L]$, so we can choose $0 \leqslant x \leqslant L$. Thus Eq. (7) becomes[7]

$$U(x) = (P/\alpha_0 L)\,U(0)e^{-ikx}[e^{ikL}\sin\alpha_0 x + \sin\alpha_0(L - x)]/(\cos kL - \cos\alpha_0 L). \tag{8}$$

Taking the limit $x \to 0$ we find the well-known Kronig–Penney dispersion relation

$$(P/\alpha_0 L)\sin\alpha_0 L + \cos\alpha_0 L = \cos kL. \tag{9}$$

Real values of $\alpha_0(k)$, obtained by the usual search methods, give us the electron energy $\epsilon_0(k)$ and consequently the band structure of the crystal.

A combination of Eqs. (2), (8), and (9) gives the electron wavefunction

$$\psi(x) = \psi(0)\,[e^{ikL}\sin\alpha_0 x + \sin\alpha_0(L - x)]/\sin\alpha_0 L, \tag{10}$$

where $\psi(0)$ is a normalization constant. Solution of the Schrödinger equation by usual methods[8] and by T matrix method[9] yields the same results.

III. RELATIVISTIC CASE

In this section, we will solve the one-dimensional Dirac equation by means of similar techniques to those used in Sec. II. Nevertheless, there is a difference with the previous situation since the relativistic wavefunction has two components.[10] This difficulty can be easily overcome if the upper and the lower components are separately expanded as a combination of plane waves. Besides that, the procedure is the same as before.

Let us consider the one-dimensional Dirac equation for an electron moving in a potential $V(x)$ given in Eq. (1). In that case, Dirac Hamiltonian is invariant under translations $x \to x + nL$, so Bloch's theorem is still valid. Thus the electron wavefunction takes the form $\psi(x) = \exp(ikx)\,U(x)$, where now the periodic function $U(x)$ has two components

$$U(x) = U_1(x)W_1 + U_2(x)W_2$$

and satisfies the first-order differential equation

$$[-i\hbar c\sigma_x(\partial + ik) + \sigma_z mc^2 + V(x)]\,U(x) = E(k)\,U(x), \tag{11}$$

σ_x and σ_z being the usual 2×2 Pauli matrices and

$$W_1 = \begin{pmatrix}1\\0\end{pmatrix}, \quad W_2 = \begin{pmatrix}0\\1\end{pmatrix}.$$

We take the Fourier transform of $U(x)$ using these spinors by writing

$$U(x)=\int_{-\infty}^{\infty} dl'\,\phi(l',x)[a_1(l')W_1+a_2(l')W_2]. \quad (12)$$

Inserting Eq. (12) in (11), multiplying the left by $\phi^*(l,x)W_r^\dagger$ ($r=1,2$ and $\dagger$ denotes the Hermitian conjugate), and integrating over all x values, we can show that

$$\hbar c(k+l)[a_1(l)+a_2(l)-a_r(l)]+(-1)^{r+1}mc^2a_r(l)+A\sum_{n=-\infty}^{\infty}\phi^*(l,nL)W_r^\dagger U(0)=E(k)a_r(l),\quad r=1,2, \quad (13)$$

where

$$U(0)=\int_{-\epsilon}^{\epsilon} dx\,U(x)\delta(x). \quad (14)$$

After some algebra, from Eqs. (12) and (13), it follows that

$$U(x)=-iB\sum_{n=-\infty}^{\infty} e^{i[\eta|x-nL|-k(x-nL)]}\{[\xi U_1(0)W_1+\xi^{-1}U_2(0)W_2]+[U_2(0)W_1+U_1(0)W_2]\times[\theta(x-nL)-\theta(-x+nL)]\}. \quad (15)$$

For the sake of simplicity, we have introduced the notation $\eta\hbar c=(E^2-m^2c^4)^{1/2}$, $\xi^2=(E+mc^2)/(E-mc^2)$, $B=A/2\hbar c$, and

$$\theta(s)=\begin{cases}1, & s\geqslant 0\\ 0, & s<0\end{cases},$$

is the Heaviside step function. We have chosen η with a small positive imaginary part to ensure the convergence of the series.

Inserting Eq. (15) in Eq. (14) we can obtain

$$U(0)=B(\cos kL-\cos\eta L)^{-1}\times\begin{pmatrix}\xi\sin\eta L & \sin kL\\ \sin kL & \xi^{-1}\sin\eta L\end{pmatrix}U(0).$$

The consistency of this equation leads to the relationship

$$[(PE/mc^2)\sin\eta L]/\eta L+(1-B^2)\cos\eta L=(1+B^2)\cos kL, \quad (16)$$

which is the relativistic Kronig–Penney dispersion relation.[4] Clearly, Eq. (16) reduces to (9) in the nonrelativistic limit.

Because of the periodicity of $U(x)$, we can choose $0<x<L$ (we do not include the discontinuity points at $x=0$ and $x=L$). Using Eq. (15), the evaluation of the electron wavefunction is now straightforward[7]

$$\psi(x)=B(\cos kL-\cos\eta L)^{-1}\begin{pmatrix}\xi[e^{ikL}\sin\eta x+\sin\eta(L-x)] & -i[e^{ikL}\cos\eta x-\cos\eta(L-x)]\\ -i[e^{ikL}\cos\eta x-\cos\eta(L-x)] & \xi^{-1}[e^{ikL}\sin\eta x+\sin\eta(L-x)]\end{pmatrix}\psi(0),\quad 0<x<L. \quad (17)$$

Of course, making $c\to\infty$, the upper component coincides with the nonrelativistic wavefunction (10) and the lower component vanishes.

IV. RELATIVISTIC CORRECTIONS AT LOW ENERGY

For many cases of interest, relativistic effects on electron energy are very small. Therefore, it is instructive to seek the lowest-order corrections to $\epsilon(k)=E(k)-mc^2$; we will follow a similar procedure to that given in Ref. 10.

Let γ be the following dimensionless parameter:

$$\gamma=\epsilon(k)/2mc^2.$$

Expanding the relativistic dispersion relation (16) to first order in γ we have

$$(P/\alpha L)\sin\alpha L+\cos\alpha L-\cos kL+(\gamma/2)\times[(3P/\alpha L-\alpha L)\sin\alpha L+P\cos\alpha L]\simeq B^2(\cos kL+\cos\alpha L), \quad (18)$$

being $\alpha=\alpha(k)=[2m\epsilon(k)/\hbar^2]^{1/2}$. Now we define a new parameter b by the relation $\epsilon(k)=\epsilon_0(k)(1+b\gamma)$. Carrying this expression to Eq. (18) and keeping only the first-order terms in γ we obtain

$$b\simeq -1+2A/\epsilon_0L-[(2+P)A/\epsilon_0L]/[1-\alpha_0L\cot\alpha_0L+2\epsilon_0L/A],$$

where Eq. (9) has been used. The first-order relativistic correction to the band structure is

$$\epsilon(k)\simeq\epsilon_0(k)\left[1-\frac{\epsilon_0(k)}{2mc^2}\times\left(1-\frac{2A}{\epsilon_0L}+\frac{(2+P)A/\epsilon_0L}{1+2\epsilon_0L/A-\alpha_0L\cot\alpha_0L}\right)\right]. \quad (19)$$

Relativistic corrections are caused by mass-energy effects, since there is no spin-orbit interaction in one dimension.

V. SUMMARY

Relativistic and nonrelativistic Kronig–Penney models have been solved through Green's function method and Bloch's theorem in a simple way. The electron interaction with the crystal has been taken as a one-dimensional periodic array of delta potentials. Electron wavefunction and dispersion relation are obtained in each case. Finally, first-order relativistic band structure has been derived.

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