ON THE INFLUENCE OF THE UNIT CELL TYPE ON THE WAVE FUNCTION IN ONE-DIMENSIONAL KRONIG-PENNEY MODELS

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\textbf{Abstract.}- We study the influence of the different choice of unit cells on the Bloch solutions of Schrödinger equation for one-dimensional periodic Kronig-Penney models with rectangular potential barriers or potential wells and partially constant effective mass. We obtain generalized Kronig-Penney relations for bulk states and exact expressions for the corresponding periodic parts of the Bloch wave functions for the two possible choices of the matching conditions in an unit cell. We show also that our analytic expressions reduce to the well known expressions for the Kronig-Penney relations and Bloch waves under constant effective mass and appropriate matching conditions

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The superlattice (SL) electronic structure is of primary importance and interest in both fundamental and applied aspects, and it has been extensively studied recently [1-10]. Theoretical studies of the electronic properties of SLs may be carried out in the framework of one-dimensional Kronig-Penney (KP) models [4,11], in particular, calculating the electronic surface states [2,4-6], the electronic interface states [3,7-9] and the electronic bulk states [10] in the semiconductor superlattices. The basic point in these considerations is to determine the general solution to the corresponding one-dimensional Schrödinger equation together with the conditions for existence of surface and interface states, which conditions depend strongly on the corresponding wave functions [2-9]. It has been noted by several authors [12-14] that the kind of the wave function depends on the choice of the unit cell, therefore, it seems very important to have a more detailed knowledge of this dependence between the choice of the unit cell and the wave function.

The aim of this letter is to consider some aspects of this problem, in particular, how the periodic parts of the Bloch solutions to the corresponding Schrödinger equation with periodic potential and partially constant effective mass depend on the choice of the unit cell, more precisely, on the matching points for the wave functions and their derivatives in this unit cell.

We are going to consider two cases of infinite one-dimensional KP-models: with rectangular potential barriers given on Fig.1, and with rectangular potential wells given on Fig.2. In the first case (potential barriers) the potential $V(x)$, determined by the conditions:

$$V(x) = \begin{cases} V = \text{const}, & \Omega^1(x) : nb + (n+1)a \leq x \leq (n+1)(a+b), \\ 0, & \Omega^2(x) : n(a+b) \leq x \leq nb + (n+1)a, \quad (n = 0, \pm 1, \pm 2, \ldots) \end{cases}$$

(1)

is periodic with respect to $x$ with a period equal to the lattice constant $(a+b)$, i.e. $V(x) = V(x + (a+b))$. For an electron with a partially constant effective mass $m(x)$

$$m(x) = \begin{cases} m_1 = \text{const}, & \Omega^1(x) : nb + (n+1)a \leq x \leq (n+1)(a+b) \\ m_2 = \text{const}, & \Omega^2(x) : n(a+b) \leq x \leq nb + (n+1)a, \quad (n = 0, \pm 1, \pm 2, \ldots) \end{cases}$$

(2)

moving in the periodic potential field (1), the one-dimensional stationary Schrödinger equation

$$\frac{d^2\Psi(x)}{dx^2} + \frac{2m(x)}{\hbar^2} [E - V(x)] \Psi(x) = 0$$

(3)

has, according to the Bloch-Floquet theorem [4,11], the following periodic in $x$ solutions with period $(a+b)$:

$$\psi_I(x) = A \exp \left[(-i\alpha + \gamma)x\right] + B \exp \left[(-i\alpha - \gamma)x\right]$$

(4)

in "regions I": $\Omega^1(x) : nb + (n+1)a \leq x \leq (n+1)(a+b)$, and of the form

$$\psi_{II}(x) = C \exp \left[i(-\alpha + \beta)x\right] + D \exp \left[i(-\alpha - \beta)x\right]$$

(5)

in "regions II": $\Omega^2(x) : n(a+b) \leq x \leq nb + (n+1)a$. Further in our consideration we assume the quantities $\beta$ and $\gamma$, introduced by (4) and (5), to be real and positive and their explicit dependences on the electron energy $E, (0 < E < V)$, are given by

$$\beta = \sqrt{\frac{2m_2}{\hbar^2}E}, \quad \gamma = \sqrt{\frac{2m_1}{\hbar^2}(V-E)}$$

(6)
and $\alpha$ is determined by the matching conditions. To obtain the coefficients $A, B, C$ and $D$ of the wave functions (4) and (5) we make use of the matching conditions at three successive points $(x_1, x_2, x_3)$ in one unit cell such that $|x_1 - x_3| = (a + b)$, and $|x_1 - x_2| = a$, $|x_2 - x_3| = b$, or $|x_1 - x_2| = b$, $|x_2 - x_3| = a$, and we assume $x_1 \leq x_2 \leq x_3$ (Fig.1). Since there exist only two ways to choose these three points on the $x$ axis we introduce them by the following relations:

$$
\begin{align*}
    x_1 + a &= x_2, & x_2 + b &= x_3, & \text{(7)} \\
    x_1 + b &= x_2, & x_2 + a &= x_3, & \text{(8)}
\end{align*}
$$

Relations (7) and (8) specify the two types of unit cells: the unit cell of type "well-barrier" which we call $KP-1$ type cell (Fig.1a), and the unit cell of type "barrier-well", called $KP-2$ type cell (Fig.1b), respectively. Thus, if we use the matching conditions used in [1,3,15-17] and denote $y = \frac{m_2}{m_1}$, the solutions (4) and (5) for the unit cells (7) and (8) must obey the following conditions at $x = x_2$:

$$
\begin{align*}
    \psi_I(x_2) &= \psi_{II}(x_2) \\
    y \frac{d\psi_I}{dx}(x_2) &= \frac{d\psi_{II}}{dx}(x_2).
\end{align*}
$$

It follows from the periodicity of $\psi(x)$ that the solutions (4) and (5) and their first derivatives must satisfy also at the points $x = x_1$ and $x = x_3$ the conditions

$$
\begin{align*}
    \psi_I(x_3) &= \psi_{II}(x_1) \\
    y \frac{d\psi_I}{dx}(x_3) &= \frac{d\psi_{II}}{dx}(x_1)
\end{align*}
$$

for the KP-1 type unit cell defined by (7), and the boundary conditions

$$
\begin{align*}
    \psi_I(x_1) &= \psi_{II}(x_3) \\
    y \frac{d\psi_I}{dx}(x_1) &= \frac{d\psi_{II}}{dx}(x_3)
\end{align*}
$$

for the KP-2 type unit cell defined by (8). From (9) and (10) and from (9) and (11) we obtain two systems of four linear homogeneous equations each, for the four constants $A, B, C$ and $D$, reflecting the differences of the two types unit cells. These two systems have nontrivial solutions only if the corresponding determinants are equal to zero, which leads to the same equation for $\beta$ and $\gamma$ given by

$$
\cos [\alpha(a + b)] = \cosh(\gamma b)\cos(\beta a) + \frac{(1 - y)^2 \alpha^2 + y^2 \gamma^2 - \beta^2}{2 y \beta \gamma} \sinh(\gamma b)\sin(\beta a). \tag{12}
$$

This equation (12) we call generalized Kronig-Penney relation.

Since only three of the four coefficients $A, B, C$ and $D$ are linearly independent we can express any three of them through the fourth. So, when $A = \mu^j B$ and $C = \lambda^j D$, where the index $j = 1, 2$ denotes the two types unit cells, the corresponding periodic wave functions (4) and (5) become

$$
\psi^j_I(x) = B \left\{ \mu^j \exp\left[-i \alpha + \gamma x\right] + \exp\left[-i \alpha - \gamma x\right]\right\}, \quad (j = 1, 2), \tag{13}
$$
\[ \psi_{II}^j(x) = D \left\{ \lambda_{II}^j \exp [i(-\alpha + \beta)x] + \exp [i(-\alpha - \beta)x] \right\}, \quad (j = 1, 2). \]  

For the KP-1 unit cell the corresponding nonhomogeneous system of equations (9) and (10) gives the following expression for \( \mu_1^I \):

\[
\mu_1^I = \frac{\cos(\beta a) - \left[ i(1 - y) \frac{a}{2} - y \frac{\beta}{2} \right] \sin(\beta a) - \exp \left[ -i\alpha(a + b) - \gamma b \right] \exp(-2\gamma x_2)}{-\cos(\beta a) + \left[ i(1 - y) \frac{a}{2} + y \frac{\beta}{2} \right] \sin(\beta a) + \exp \left[ -i\alpha(a + b) + \gamma b \right]}. 
\]  

Similarly, the nonhomogeneous system of equations (9) and (10) gives for \( \lambda_{II}^I \):

\[
\lambda_{II}^I = \frac{\cosh(\gamma b) - i \left[ \left( \frac{1-y}{y} \right) \frac{a}{2} + \left( \frac{1}{y} \right) \frac{\beta}{2} \right] \sinh(\gamma b) - \exp \left\{ i [\alpha(a + b) + \beta a] \right\} \exp(-i2\beta x_2)}{-\cosh(\gamma b) + i \left[ \left( \frac{1-y}{y} \right) \frac{a}{2} - \left( \frac{1}{y} \right) \frac{\beta}{2} \right] \sinh(\gamma b) + \exp \left\{ i [\alpha(a + b) - \beta a] \right\}}.
\]  

Hence, for the both types of unit cells (7) and (8) it is seen from (15) and (17) that the wave functions (13) in the "region I" are different: \( \psi_1^I \neq \psi_1^I \); and from (16) and (18) we see that the wave functions (14) in the "region II" are also different: \( \psi_{II}^I \neq \psi_{II}^I \). Consequently, the choice of matching points inside the unit cell through relations (7)-(11) determines the form of the periodic parts (13) and (14) of Bloch solutions for the model under consideration.

Let’s consider the case \( y = 1 \), i.e. when the electron effective mass (2) is constant: \( m_1 = m_2 = m_o \). In this case \( \beta \) and \( \gamma \) in (6) become

\[
\beta_o = \sqrt{\frac{2m_o}{h^2}E}, \quad \gamma_o = \sqrt{\frac{2m_o}{h^2}(V - E)} \]  

and equation (12) is reduced to the well-known Kronig-Penney equation [11]. If for the KP-1 model (Fig.1a) we set \( x_2 = a \) in relation (7), and then, making use of (16) and (19), we find for the coefficient \( \lambda_{II}^I \equiv (\lambda_{II}^I)^B \) the following value:

\[
(\lambda_{II}^I)^B = \frac{\cosh(\gamma o b) - i \frac{\beta_o}{\gamma_o} \sinh(\gamma o b) - \exp \left\{ i [\alpha(a + b) + \beta o a] \right\} \exp(-i2\beta o a)}{-\cosh(\gamma o b) + i \frac{\beta_o}{\gamma_o} \sinh(\gamma o b) + \exp \left\{ i [\alpha(a + b) - \beta o a] \right\}}.
\]  

which coincides with the corresponding "expression (17)" in Bloss’ paper [2]. For the KP-2 model (Fig.1b) if \( x_2 = 0 \) in (8) we have the classical KP-model [11]. In this case from (17) and
(19) and from (18) and (19) we find the following expressions for the corresponding coefficients 
\( \mu_I^2 \equiv (\mu_I^2)^{KP} \) and \( \lambda_{II}^2 \equiv (\lambda_{II}^2)^{KP} \):

\[
(\mu_I^2)^{KP} = \frac{\cos(\beta_o a) - \frac{2\mu}{\hbar^2} \sin(\beta_o a) - \exp[i\alpha(a + b) + \gamma_o b]}{-\cos(\beta_o a) - \frac{2\mu}{\hbar^2} \sin(\beta_o a) + \exp[i\alpha(a + b) - \gamma_o b]} \tag{21}
\]

\[
(\lambda_{II}^2)^{KP} = \frac{\chi(\gamma_o b) + i \frac{\beta_o}{\hbar^2} \sinh(\gamma_o b) - \exp \{-i[\alpha(a + b) + \beta_o a]\}}{-\chi(\gamma_o b) + i \frac{\beta_o}{\hbar^2} \sinh(\gamma_o b) + \exp \{-i[\alpha(a + b) - \beta_o a]\}} \tag{22}
\]

These values (21) of \( (\mu_I^2)^{KP} \) and (22) of \( (\lambda_{II}^2)^{KP} \) have been implicitly used in [11]. However, choosing \( x_2 = \frac{1}{2}b \) in (8), from (17) and (19) and from (18) and (19) we find that the corresponding coefficients 
\( \mu_I^2 \equiv (\mu_I^2)^G \) and \( \lambda_{II}^2 \equiv (\lambda_{II}^2)^G \), given by

\[
(\mu_I^2)^G = \frac{\cos(\beta_o a) - \frac{2\mu}{\hbar^2} \sin(\beta_o a) - \exp[i\alpha(a + b) + \gamma_o b]}{-\cos(\beta_o a) - \frac{2\mu}{\hbar^2} \sin(\beta_o a) + \exp[i\alpha(a + b) - \gamma_o b]} \tag{23}
\]

\[
(\lambda_{II}^2)^G = \frac{\chi(\gamma_o b) + i \frac{\beta_o}{\hbar^2} \sinh(\gamma_o b) - \exp \{-i[\alpha(a + b) + \beta_o a]\}}{-\chi(\gamma_o b) + i \frac{\beta_o}{\hbar^2} \sinh(\gamma_o b) + \exp \{-i[\alpha(a + b) - \beta_o a]\}} \tag{24}
\]

are identical to Gubanov’s results [12]. Comparing (21) with (23), and (22) with (24), we immediately obtain the following relations between them:

\[
(\mu_I^2)^G = (\mu_I^2)^{KP} \exp(-\gamma_o b), \quad (\lambda_{II}^2)^G = (\lambda_{II}^2)^{KP} \exp(-i\beta_o b).
\]

Note that the exponential factors in (23) and (24) is due only to the different choice of the coordinate origin in the unit cell.

The case of the Kronig-Penney models with rectangular potential wells and partially constant effective mass (2) we treat in the same way, and the corresponding results are obtained taking into account the periodic potential \( V(x) \) (Fig.2):

\[
V(x) = \begin{cases} 
0, & \text{if } 0 \leq x < nb + (n+1)a \\
-\Omega, & \Omega_1(x) : n(a + b) \leq x \leq nb + (n + 1)a \\
-\Omega, & \Omega_2(x) : nb + (n + 1)a \leq x \leq nb + (n + 1)(a + b), \quad (n = 0, \pm 1, \pm 2, \ldots)
\end{cases} \tag{25}
\]

where \( V > 0 \). Relations (7) and (8) again specify two types of unit cells: the unit cell of the type "well-barrier" called \( KP-1a \) type cell (Fig.2a), and the unit cell of the type "barrier-well" called \( KP-2a \) type cell (Fig.2b). In the regions with constant potentials the quantities \( \theta \) and \( \phi \), which now play the roles of \( \gamma \) and \( \beta \) in (4) and (5), are related to the electron energy \( E \) by means of the equations

\[
\theta^2 = \frac{2m_1}{h^2} E, \quad \phi^2 = \frac{2m_2}{h^2} (E + V).
\]

In the case \( \theta^2 > 0, \ \phi^2 > 0 \) the Schrödinger equation (3) for an electron with effective mass (2), moving in the potential field (25), for the both types of unit cells has nontrivial solutions only if the quantities \( \theta \) and \( \phi \) satisfy the corresponding generalized Kronig-Penney relation

\[
\cos[\alpha(a + b)] = \cos(\theta a) \cos(\phi b) + \frac{(1 - y^2)\alpha^2 - (y^2\theta^2 + \phi^2)}{2y\theta\phi} \sin(\theta a) \sin(\phi b), \tag{26}
\]
where \( y = \frac{m_2}{m_1} \). Now the periodic part \( \phi(x) \) of the Bloch wave function is of the form

\[
\phi^j_I(x) = B \left\{ \nu^j_1 \exp[i(-\alpha + \theta)x] + \exp[i(-\alpha - \theta)x] \right\}, \quad (j = 1, 2),
\]

in "regions I" (barriers): \( \Omega^1(x) : n(a + b) \leq x \leq nb + (n + 1)a, \) and of the form

\[
\phi^j_{II}(x) = D \left\{ \chi^j_{II} \exp[i(-\alpha + \varphi)x] + \exp[i(-\alpha - \varphi)x] \right\}, \quad (j = 1, 2)
\]

in "regions II" (wells): \( \Omega^2(x) : nb + (n + 1)a \leq x \leq (n + 1)(a + b). \) For the KP-1a unit cell, determined by condition (7), the corresponding nonhomogeneous system of equations (9) and (10) gives the following expressions for \( \nu^1_I \) and \( \chi^1_{II} \):

\[
\nu^1_I = \frac{\cos(\varphi b) - i \left[ (1 - y)^2 \varphi - (y - \theta)^2 \right] \sin(\varphi b) - \exp \left\{ -i [\alpha(a + b) + \theta a] \right\} \exp(-i2\theta x_2)}{-\cos(\varphi b) + i \left[ (1 - y)^2 \varphi + (y - \theta)^2 \right] \sin(\varphi b) + \exp \left\{ -i [\alpha(a + b) - \theta a] \right\} \exp(-i2\varphi x_2)},
\]

\[
\chi^1_{II} = \frac{\cos(\theta a) - i \left[ \left( \frac{1 - y}{y} \right) \varphi + \left( \frac{1}{y} \right) \theta \right] \sin(\theta a) - \exp \left\{ i [\alpha(a + b) + \varphi b] \right\} \exp(-i2\varphi x_2)}{-\cos(\theta a) + i \left[ \left( \frac{1 - y}{y} \right) \varphi - \left( \frac{1}{y} \right) \theta \right] \sin(\theta a) + \exp \left\{ i [\alpha(a + b) - \varphi b] \right\} \exp(-i2\varphi x_2)},
\]

For the KP-2a unit cell, determined by (8), the coefficients \( \nu^2_I \) and \( \chi^2_{II} \) are obtained from the nonhomogeneous system of equations (9) and (11) are given by:

\[
\nu^2_I = \frac{\cos(\varphi b) + i \left[ (1 - y)^2 \varphi - (y - \theta)^2 \right] \sin(\varphi b) - \exp \left\{ i [\alpha(a + b) + \theta a] \right\} \exp(-i2\theta x_2)}{-\cos(\varphi b) - i \left[ (1 - y)^2 \varphi + (y - \theta)^2 \right] \sin(\varphi b) + \exp \left\{ i [\alpha(a + b) - \theta a] \right\} \exp(-i2\varphi x_2)},
\]

\[
\chi^2_{II} = \frac{\cos(\theta a) + i \left[ \left( \frac{1 - y}{y} \right) \varphi + \left( \frac{1}{y} \right) \theta \right] \sin(\theta a) - \exp \left\{ -i [\alpha(a + b) + \varphi b] \right\} \exp(-i2\varphi x_2)}{-\cos(\theta a) - i \left[ \left( \frac{1 - y}{y} \right) \varphi - \left( \frac{1}{y} \right) \theta \right] \sin(\theta a) + \exp \left\{ -i [\alpha(a + b) - \varphi b] \right\} \exp(-i2\varphi x_2)}.
\]

It is clearly seen that the corresponding wave functions (27) and (28) satisfy the inequalities \( \phi^1_I \neq \phi^2_I \) and \( \phi^1_{II} \neq \phi^2_{II} \).

If the electron energy is negative: \( E = -\varepsilon, \varepsilon > 0 \) and \( -V < E < 0 \), we have \( \theta^2 = -\frac{2m}{k^2} \varepsilon < 0 \) and \( \varphi^2 = \frac{2m}{k^2} (E + V) > 0 \), and denoting \( \frac{2m}{k^2} \varepsilon \equiv k^2 \), the generalized Kronig-Penney relation (26) becomes

\[
\cos [\alpha(a + b)] = \chi(h a) \cos(\varphi b) + \frac{(1 - y)^2 \alpha^2 - (y^2 k^2 + \varphi^2)}{2y \varphi k} \sin(h a) \sin(\varphi b).
\]

In this case the quantity \( \gamma^1_I \) (29) for the KP-1a model becomes

\[
(\nu^1_I) = \frac{\cos(\varphi b) - \left[ \left( \frac{1 - y}{y} \right) \varphi + \left( \frac{1}{y} \right) \theta \right] \sin(\varphi b) - \exp \left\{ -i \alpha(a + b) \right\} \exp(\pm 2k x_2)}{-\cos(\varphi b) + \left[ \left( \frac{1 - y}{y} \right) \varphi - \left( \frac{1}{y} \right) \theta \right] \sin(\varphi b) + \exp \left\{ -i \alpha(a + b) \right\} \exp(\pm 2k x_2)},
\]
and from (30) we obtain also 
\[(\chi^1_{II})^+ = (\chi^1_{II})^- = (\chi^1_{II})^\pm\]

\[\begin{align*}
(\chi^1_{II})^\pm &= \frac{ch(ka) - i \left(\frac{y}{y} \frac{\varphi}{\varphi} + \left(\frac{1}{y} \frac{\varphi}{\varphi}\right)\right) \text{sh}(ka) - \exp\{i[\alpha(a + b) + \varphi b]\} - \exp(-i2\varphi x_2)}{
-ch(ka) + i \left(\frac{y}{y} \frac{\varphi}{\varphi} - \left(\frac{1}{y} \frac{\varphi}{\varphi}\right)\right) \text{sh}(ka) + \exp\{i[\alpha(a + b) - \varphi b]\}} \exp(-i\varphi x_2). 
\end{align*}\]  

(35)

For the KP-2a model the quantity \(\nu_I^2\) (31) becomes

\[\begin{align*}
(\nu_I^2)^\pm &= \frac{\cos(\varphi b) + \left[i(1 - y) \frac{\alpha}{\varphi} \pm y \frac{k}{\varphi}\right] \sin(\varphi b) - \exp\{i[\alpha(a + b) \mp ka]\} - \exp(\pm 2kx_2)}{
-\cos(\varphi b) - \left[i(1 - y) \frac{\alpha}{\varphi} \mp y \frac{k}{\varphi}\right] \sin(\varphi b) + \exp\{i[\alpha(a + b) \pm ka]\}} 
\end{align*}\]  

(36)

and from (32) we again have 
\[(\chi^2_{II})^+ = (\chi^2_{II})^- = (\chi^2_{II})^\pm:\]

\[\begin{align*}
(\chi^2_{II})^\pm &= \frac{ch(ka) + i \left(\frac{1-y}{y} \frac{\varphi}{\varphi} + \left(\frac{1}{y} \frac{\varphi}{\varphi}\right)\right) \text{sh}(ka) - \exp\{-i[\alpha(a + b) + \varphi b]\} - \exp(-i2\varphi x_2)}{
-ch(ka) - i \left(\frac{1-y}{y} \frac{\varphi}{\varphi} - \left(\frac{1}{y} \frac{\varphi}{\varphi}\right)\right) \text{sh}(ka) + \exp\{-i[\alpha(a + b) - \varphi b]\}} \exp(-i\varphi x_2). 
\end{align*}\]  

(37)

Hence, we have the relations

\[(\phi^1_I)^+ \neq (\phi^1_I)^- \neq (\phi^2_I)^+ \neq (\phi^2_I)^-, \quad (\phi^1_{II})^+ = (\phi^1_{II})^- \neq (\phi^2_{II})^+ = (\phi^2_{II})^- .\]

When \(y = 1\) our generalized Kronig-Penney relations (26) and (33) reduce to the corresponding Kronig-Penney relations given in [18].

In conclusion we can say that the differences between the wave functions (13) and (14) and between the wave functions (27) and (28), which finally depend on the choice of unit cell and the matching conditions, should be taken into account when we compute surface and interface electronic states. In other words, varying the position of the barrier-well interface within an unit cell, we will influence the conditions for the existence of surface and interface states. For the two potentials (1) and (25) our generalized Kronig-Penney relations (12) and (26), and the particular case (33), are different, as it is in the original Kronig-Penney relations, and the corresponding Bloch wave functions for these two potentials are also different.
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Fig.1: One-dimensional Kronig-Penney model with rectangular barriers and lattice constant \((a + b)\): \(b\)-the width of the barriers, \(V\)-the height of the barriers: (a) unit cell of KP-1 type: "region II- region I" (well-barrier); (b) unit cell of KP-2 type: "region I- region II" (barrier-well).

Fig.2: One-dimensional Kronig-Penney model with rectangular wells and lattice constant \((a + b)\): \(b\)-the width of the wells, \(V\)-the depth of the wells: (a) unit cell of KP-1a type: "region II- region I" (well-barrier); (b) unit cell of KP-2a type: "region I- region II" (barrier-well).