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One Dimensional Treatment of Polyatomic Crystals by the Laplace Transform Method

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The one dimensional periodic potential problem is solved using the Laplace transform method and a condensed expression for the relation $E \times k$ and effective mass for one electron in a polyatomic structure is determined. Applications related to the effect of the asymmetry of the potential upon the one dimensional band structure are discussed.

Resolve-se o problema do potencial periódico, a uma dimensão, fazendo uso do método da Transformada de Laplace. Obtem-se uma expressão compacta para a relação E × k e massa efetiva, para um eletron em estrutura poliatômica. Discutem-se aplicações relacionadas aos efeitos da assimetria do potencial sobre a estrutura de banda unidirnensional.

1. INTRODUCTION

In a one dimensional Kronig-Penney model[1], the crystal potential is represented by an array of Dirac delta functions located at the lattice sites. With this simple model, it was possible to explain and under-

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stand important properties of the real three dimensional crystals, and to have an exact solution to tbe Schrödinger equation. Several methods have been used to solve the one electron Schrödinger equation, exactly, with a periodic potential represented by Dirac delta functions [2]. None of them, however, makes use of the Laplace Transform Method, and allows such an easy generalization of the dispersion relation, for several atoms per cell, as this method does.

Let us consider a polyatomic, one dimensional, crystal made up of p distinct atoms per cell. Let a be the length of the unit cell, and let us represent the potential energy, due to atom i, by a Dirac delta function of strenght P_i, located at the position $\beta_i a$, where β_i is a fraction of a, that is, $0 \leq \beta_i \leq 1$. The one electron Schrödinger equation, for the whole lattice, is

$$\left[-\frac{h^2}{8\pi^2 m}\frac{d^2}{dx^2} - eV(x) \right]\psi(x) = E\,\psi(x) \ , \tag{1}$$

$$\left[\frac{d^2}{dx^2} + \frac{2}{a^2}U(x) \right]\psi(x) = -K^2\psi(x) \ , \tag{2}$$

where

$$K^2 \equiv \frac{8\pi^2 m}{h^2}E \ , \tag{3}$$

$$U(x) \equiv \frac{4\pi^2 a^2}{h^2}eV(x) \ , \tag{4}$$

$$U(x) = a\sum_{n=-\infty}^{\infty}\sum_{i=1}^{p} P_i\,\delta\left[x-(n+\beta_i)a\right], \tag{5}$$

for $0 < \beta_i < 1$ and $n = 0, \pm 1, 12, \pm 3, \ldots$ Expression (5) is our model of the potential energy for the whole lattice. In Fig. 1, we show the potential function $U(x)$ for one cell only, that is, for $0 \leq x \leq a$, which is the cell nearest to the origin and which corresponds to the second

summation only, in Eq. (5). This potential $U(x)$ is periodic, with period a, or $U(x+a) = U(x)$.

The Schrödinger equation, for the whole lattice with p distinct atoms per cell, is, in this model,

$$\frac{d^2}{dx^2}\psi_p(x) + \frac{2}{a} \sum_{n=-\infty}^{\infty} \sum_{i=1}^{p} P_i \delta\left[x-(n+\beta_i)a\right]\psi_p(x) = -K^2\psi_p(x), \tag{6}$$

where the subscript on the wave function denotes the number of peaks per cell.

Let us define the Laplace Transform, of the wave function $\psi_p(x)$, by $y_p(s)$:

$$y_p(x) = L\{\psi_p(x)\} \equiv \int_0^\infty e^{-sx}\, \psi_p(x)dx \ . \tag{7}$$

The inverse Laplace Transform of $y_p(s)$ is the wave function $\psi_p(x)$, i.e.,

$$L^{-1}\{y_p(s)\} = \psi_p(s) \ . \tag{8}$$

If we multiply both sides of Eq.6 by $\exp(-sx)$, and integrate from zero to infinity, we'obtain

$$\int_0^\infty e^{-sx}\frac{d^2}{dx^2}\psi_p(x)dx + \frac{2}{a}\int_0^\infty dx\ e^{-sx} \sum_{n=-\infty}^{\infty} \cdot \sum_{i=1}^{p} P_i\delta\left[x-(n+\beta_i)a\right]\psi_p(x) \tag{9}$$

$$= -K^2 y_p(s) \ .$$

The Laplace transform of the second derivative of $\psi_p(x)$ is given by

$$L\{\psi_p''(x)\} = s^2 L\{\psi_p(x)\} - s\psi_p(0) - \psi_p'(0) \ . \tag{10}$$

The integral that appears in Eq. (9) can be easily performed because P_i is a constant, and proceeding in this way we can write

$$\frac{2}{a}\int_0^\infty dx\; e^{-sx}\;\psi_p(x)\;\sum_{n=-\infty}^{\infty}\;\sum_{i=1}^{p}\;P_i\delta\left[x-(n+\beta_i)a\right] = \tag{11}$$

$$= \frac{2}{a}\sum_{n=0}^{\infty}\;\sum_{i=1}^{p}\;P_i\;e^{-s(n+\beta_i)a}\psi_p(na+\beta_i a)\;.$$

The only contribution comes from positive values of n because the range of integration, of the delta function, is for positive values of x. Substituting results (11) and (10) into (9), we areable to write

$$L\{\psi_p(x)\} = y_p(x) = \frac{s}{s^2+K^2}\psi_p(0) + \frac{1}{s^2+K^2}\psi'_p(0)$$

$$- \frac{2}{a}\sum_{n=0}^{\infty}\;\sum_{i=1}^{p}\;\frac{P_i\psi_p(na+\beta_i a)}{s^2+K^2}\;e^{-s(n+\beta_i)a}\;, \tag{12}$$

where $\psi_p(0)$ and $\psi'_p(0)$ are the values of the wave function $\psi_p(x)$, and its derivative $\psi'_p(x)$, calculated at the origin. Taking the inverse Laplace Transform of both sides of Eq.12, we obtain

$$\psi_p(x) = \psi_p(0)\cos Kx + \psi'_p(0)\;\frac{\sin Kx}{K} -$$

$$- \frac{2}{a}\sum_{n=0}^{\infty}\;\sum_{i=1}^{p}\;P_i\psi_p(na+\beta_i a)\frac{\sin K\left[x-(n+\beta_i)a\right]}{K}\;\cdot\;u(x-na-\beta_i a), \tag{13}$$

where was used the fact that

$$L^{-1}\{e^{-sb}\left[\frac{1}{s^2+K^2}\right]\} = \frac{\sin K(x-b)}{K}\;u(x-b), \tag{14}$$

and $u(x-a)$ is a step function which has the value one, for positive values of the argument, and zero otherwise. It is easy to see that ,

for x limited to the first unit cell, Eq.13 reduces to

$$\psi_p(x) = \psi_p(0)\cos Kx + \psi_p'(0)\frac{\sin Kx}{K} -$$

$$- \frac{2}{aK}\sum_{i=1}^{p} P_i\psi_p(\beta_i a)\sin K(x-\beta_i a)u(x-\beta_i a), \qquad (15)$$

where $0 \leq x \leq a$.

2. THE DISPERSION EQUATION

Equation (14) is the formal solution of the Schrödinger equation, for the model (6), for $0 \leq x \leq a$, but since the potential energy is a periodic function, as expressed by (7), the solutions $\psi_p(x)$ have to satisfy the boundary conditions

$$\psi_p(x+na) = \exp(ikna)\psi_p(x), \qquad (16)$$

$$\psi_p'(x+na) = \exp(ikna)\psi_p' x, \qquad (17)$$

where k is a real number, and n an integer. These conditions, also known as Bloch's theorem, lead to eigenstates of the Schrödinger equation which are travelling waves, the wave (states) being differentiated from one another by the number k, or the way the phase changes, from cell to cell, in the crystal. Imaginary values of k do not give travelling waves, and so they represent forbidden states for the electrons. Once k is given, the value of the wave function and its derivative, at all points in the crystal, can be obtained, from their values in the first cell, just by applying Eqs.16 and 17. In particular, we have

$$\psi_p(a) = \exp(ika)\psi_p(0), \qquad (18)$$

$$\psi_p'(a) = \exp(ika)\psi_p'(0). \qquad (19)$$

These expressions allow us to relate each accessible state (travelling wave) to the energy (frequency of the wave) of the state. This can be achieved by considering $\psi_p(x)$ in Eq.15, taking its derivative with respect to x, and then imposing the conditions (18) and (19). Proceeding in this way, we arrive at

$$e^{ika}\psi_p(0) = \psi_p(0)\cos Ka + \psi_p'(0)\frac{\sin Ka}{K} - \frac{2}{Ka}\sum_{i=1}^{p} P_i\psi_p(\beta_i a)\sin K(a-\beta_i a).u(a-\beta_i a), \quad (20)$$

$$e^{ika}\psi_p'(0) = -K\psi_p(0)\sin Ka + \psi_p'(0)\cos Ka - \frac{2}{a}\sum_{i=1}^{p} P_i\psi_p(\beta_i a).$$

$$.\ \cos K(a-\beta_i a).u(a-\beta_i a) - \frac{2}{Ka}\sum_{i=1}^{p} P_i\psi_p(\beta_i a)\sin K(a-\beta_i a)\cdot\delta(a-\beta_i a). \quad (21)$$

Equations (20) and (21) can be simplified because the step function is always 1, since $0<\beta_i<1$, and the product of the sine by the delta function is always zero. We can, therefore, write

$$\psi_p(0)\left[\cos Ka - e^{ika}\right] + \psi_p'(0)\frac{\sin Ka}{K} - \frac{2}{aK}\sum_{i=1}^{p} P_i\psi_p(\beta_i a)\sin K(a-\beta_i a) = 0, \quad (22)$$

$$\psi_p(0)\left[-Ke^{-ika}\sin Ka\right] + \psi_p'(0)\left[e^{-ika}\cos Ka - 1\right] - \frac{2}{aK}e^{-ika}\sum_{i=1}^{p} P_i\psi_p(\beta_i a).$$

$$.\ \cos K(a-\beta_i a) = 0 \quad (23)$$

It is necessary to know the value of the wave function, at the position $\beta_i a$ of each atom inside the unit cell, before imposing the condition for the system of Eqs.22 and 23 to have a nontrivial solution. In Ref.3, the set of equations above was solved for the simple cases of $p=1$ and $p=2$, that is, mnoatomic and diatomic lattices. In general, we need the relation between $\psi_p(\beta_i a)$ and $\psi_p(0)$, for $i = 1, 2, 3, \ldots p$.

In order to have this relation, we may proceed in the following way. For a fixed value of x, say $x = \beta_j a$, the summation in i, in Eq. 15, can be divided into two parts, $i<j$ and $i>j$. The sum is zero for this last case, since, for $i>j$, the step function is zero, and for $i=j$ the sine vanishes. It then follows:

$$\psi_p(\beta_j a) = \psi_p(0)\cos(K\beta_j a) + \psi_p'(0)\frac{\sin(K\beta j a)}{K} - \frac{2}{aK}\sum_{i=1}^{j-1} P_i \psi_p(\beta_i a)\sin|K(\beta_j-\beta_i)a|, \tag{24}$$

$$\psi_p(\beta_j a) = \psi_0(\beta_j a) - \frac{2}{aK}\sum_{i=1}^{j-1} P_i \psi_p(\beta_i a)\sin K(\beta_j-\beta_i)a, \tag{25}$$

and this is valid for any $j=1, 2, 3, \ldots$, where $\psi_0(x)$ is the wave function corresponding to the case of zero peaks per cell, i.e., the free electron case. The wave function, in the summation above, is always calculated at points situated on the left of the point we are interested in. With this, we can obtain, starting with $j = 1,2,3,\ldots$, all $\psi_p(\beta_j a)$ in terms of $\psi_0(\beta_3 a)$, $\psi_0(\beta_{j-1} a)$, $\psi_0(\beta_{j-2} a)$, etc., where $\psi_0(\beta_j a)$ is given in Eq.15 in terms of $\psi_0(0)$ and $\psi_0'(0)$. Replacing the values of $\psi_p(\beta_i a)$, that appear in the summations of Eqs. 22 and 23, by the corresponding expressions in terms of $\psi_p(0)$ and $\psi_p'(0)$, obtained as explained above, we go to a system of two equations in the unknowns $\psi_p(0)$ and $\psi_p'(0)$. In order to have a nontrivial solution, the following relation between energy and wave number must hold:

$$\cos(ka) = \cos(ka) + \sum_{\ell=1}^{p} (-1)^{\ell} 2^{(\ell-1)} \sum_{i \subset C_{p,\ell}} \prod_{t=1}^{\ell} P_{f_i(t)} \cdot \frac{1}{Ka}\sin K\left[\beta_{f_i(t+1)} - \beta_{f_i(t)}\right]a, \tag{26}$$

(see Appendix). For a given crystalline structure, this equation is a relation between wave number k and energy K^2, where the number k enumerates the accessible quantum states, when k is real, and when k is imaginar~, it characterizes the forbbiden quantum states. So, through Eq. 26, we can calculate the energy associated with each accessible k-state.

The allowed energy levels for the electron, in this model, are those values of K for which the righthand side of Eq.26 is limited by ± 1. Outside this range, the values of K correspond to forbbiden energy states, since they make the left-hand side of the equation outside the interval $[+1,-1]$, and this is only possible when k is imaginary.

If we plot, the righthand side of Eq.26, on a vertical axis, and $(Ka)^2$ on a horizontal axis, we observe the following typical results: for $(Ka)^2<0$, that is, K imaginary and negative energies, the righthand side of Eq. 26 contains hyperbolic functions, instead of trigonometric ones, and this means that once it crosses the +1 line, at $(Ka)^2 = E_1$, in Fig.2, it will never cross this line again for decreasing values of $(Ka)^2$. Consequently, there are no available states for the electron with energy below E_1, in Fig.2. When $(Ka)^2$ increases, from the value E_1 towards zero, the righthand side of Eq.26 crosses the line -1, at $(Ka)^2 = E_2$, and then crosses it again, at $(Ka)^2 = E_3$, etc. The set of values of $(Ka)^2$, from E_1 to E_2, constitute a band of allowed energy, and it is the only negative band that this model presents. This comes from the fact that we are representing the potential energy by Dirac delta functions, and we know that an isolated Dirac delta function potential permits only one bound state (state with negative energy). When we place several Dirac delta functions together, in a array, the isolated bound state apreads due to the overlap of the wave functions, centered on different lattice points.

The only negative band the model allows of is called the valence band. In Fig.2, E_1 is the bottom of the valence band, E_2 the top of it, and (E_2-E_1) is the width of this band. The set of values of $(Ka)^2$, for which the righthand side of Eq.26 varies from E_3 to E_4, is called the conduction band. E_3 is the bottom of the conduction band, and (E_3-E_2) is the gap.

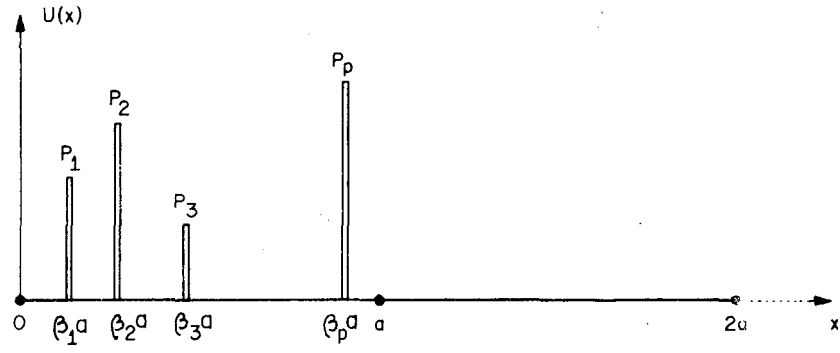

Fig.1 - One dimensional representation of the potential for polyatomic crystal.

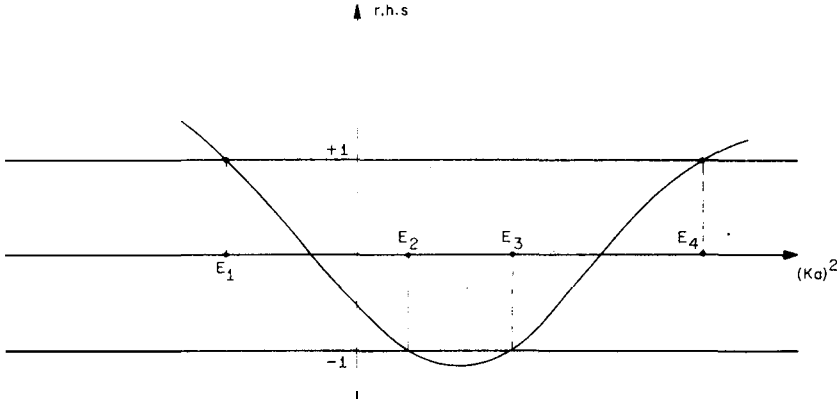

Fig.2 - Typical plot of the righthand side (rhs) of Eq.26, as discussed in the text, versus the energy K^2.

3. THE EFFECTIVE MASS

Electrons in a crystal respond, to applied external fields, as though they had an effective mass m^*, different from the mass, m_0, in vacuum. This mass can be obtained once we know the energy associated to each quantum state, i.e., the dispersion relation, since the effect of an external field is to alter the quantum state of the electron, and consequently its energy. It can be shown that the effective mass, for a one dimensional crystal is given by

$$\frac{m^*}{m_0} = \frac{\hbar^2}{m_0} \left(\frac{\partial^2 E}{\partial k^2}\right)^{-1} , \tag{27}$$

where k and E are related by Eq.26 or, having in mind Eq.3, by

$$\frac{m^*}{m_0} = 2\left[\frac{\partial^2}{\partial x^2}(Z^2)\right]^{-1} = \left[Z\frac{\partial^2 Z}{\partial x^2} + \left(\frac{\partial Z}{\partial x}\right)^2\right]^{-1} , \tag{28}$$

where $x \equiv ka$ and $Z \equiv Ka$.

The relation that we have between x and Z is the one obtained through Eq.(26), so it is convenient to rewrite Eq.28 in terms of the derivative of $\cos(x)$ with respect to x:

$$\frac{d}{dx}(\cos x) = \frac{d}{dZ}(\cos x)\,\frac{dZ}{dx} , \tag{29}$$

$$\frac{d^2}{dx^2}(\cos x) = \frac{d^2}{dx dZ}(\cos x)\frac{dZ}{dx} + \frac{d}{dZ}(\cos x)\frac{d^2 Z}{dx^2} . \tag{30}$$

In the band edges, the only place where expression (27) has a meaning, we have $x = 0$ or $x = \pi$. Then, from Eq.29, we obtain

$$\frac{d}{dZ}(\cos x)\,\frac{dZ}{dx} = 0 , \qquad \text{at the band edges.} \tag{31}$$

The righthand side of Eq.(26) contains hyperbolic functions, for $Z<0$, and trigonometric ones, for $Z>0$, and the only value of Z for which this equation could have an inflexion point would be at $Z = 0$. So for $Z \neq 0$ and at the band edges we can take $\frac{dZ}{dx} = 0$ and then from Eq. (30)

$$\frac{d^2Z}{dx^2} = \pm \left[\frac{d}{dZ}(\cos x)\right]^{-1} \tag{32}$$

where the plus sign is for $x = \pi$ and the minus sign is for $x = 0$. So, the effective mass at the band edges is

$$\frac{m^*}{m_0} = \frac{1}{Z}\frac{d}{dZ}(\cos x), \tag{33}$$

and, finally, using Eq.26, we obtain

$$\begin{aligned}
s\frac{m^*}{m} &= -\frac{\sin Z}{Z} \\
&+ \sum_{\ell=1}^{p} (-1)^{\ell} 2^{(\ell-1)} \frac{1}{Z^{\ell+1}} \sum_{i} C_{p,\ell} \left\{-\frac{\ell}{Z} \prod_{t=1}^{\ell} P_{f_i(t)} \sin\left[\left(\beta_{f_i(t+1)} - \beta_{f_i(t)}\right)Z\right]\right. \\
&+ \sum_{h=1}^{\ell}\left[\beta_{f_i(h+1)} - \beta_{f_i(h)}\right] P_{f_i(h)} \cos\left[\left(\beta_{f_i(h+1)} - \beta_{f_i(h)}\right)Z\right] \sum_{\substack{q=1 \\ q\neq h}}^{\ell} P_{f_i(q)} \cdot \\
&\left. \cdot \sin\left[\left(\beta_{f_i(q+1)} - \beta_{f_i(q)}\right)Z\right]\right\},
\end{aligned} \tag{34}$$

where $s = 1$, if $x = \pi$, and $s = -1$ if $x = 0$.

4. APPLICATIONS

There are several applications of Eq.26 and 34, especially to those problems related to polyatomic one dimensional crystals. These equations allow us to calculate the band structure and effective mass, for a one dimensional structure, with as many atoms per cell as we want. We can also verify the way the effective mass and the band structure change, when one changes the regularity of the distribution of the potential peaks, inside the unit cell. This change can be accomplished either by changing the strength of the potential corresponding to some points inside the cell, or by displacing the location of the potential inside the cell.

Let us consider a periodic one dimensional structure with period a, and p atoms per cell. The potential of each atom is represented by a Dirac delta function, of strength P_i, located at $\beta_i a$ with $0<\beta_i<1$. According to Eqs.4 and 5, the potential is given by

$$V(x) = \frac{\hbar^2}{me}\frac{1}{a^2}\sum_{i=1}^{p} P_i\,\delta(x-na-\beta_i a)\ , \quad na \le x \le (n-1)a, \tag{35}$$

and the average potential, per cell, is

$$\langle eV\rangle = \frac{1}{a}\int_{na}^{(n+1)a} eV(x)\,dx = \frac{\hbar^2}{ma^2}\sum_{i=1}^{p} P_i\ . \tag{36}$$

We know that the dispersion relation, Eq.26, gives the same band structure for the following two lattices: one of them has period a, one atom per cell located at βa, and represented by a Dirac delta function of strength P. The other has period pa (p integer), p identical atoms per cell, located at $\beta_j a = (j-1)a + \beta a$, with $1 \le j \le p$, and each atom represented by a Dirac delta function of magnitude pP. Both lattices have the same average potential per cell, and they are really identical since, in the second one, we took a period of repetition which is a multiple of the minimum one, a. So they have identical band structures.

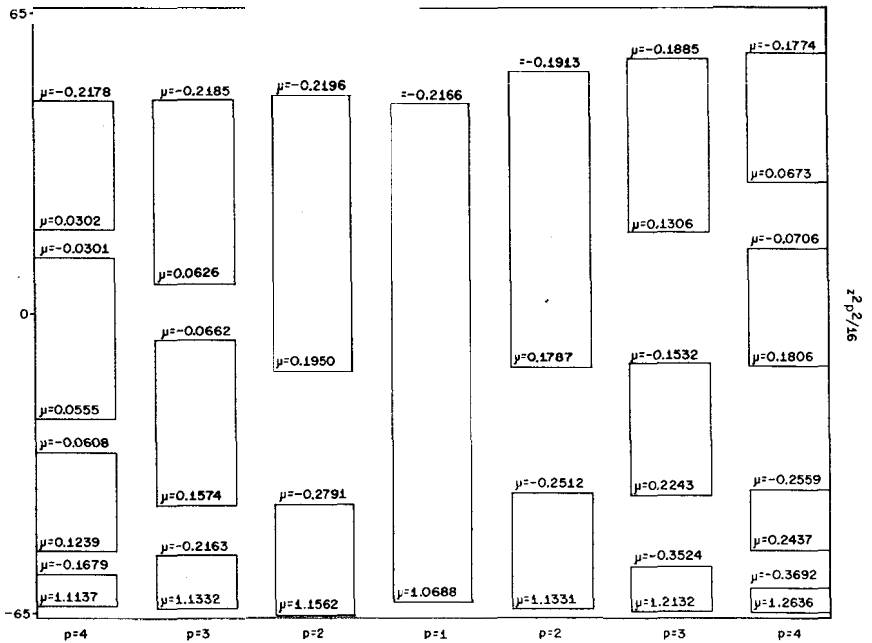

Fig.3 - Energy bands corresponding to polyatomic structures, with the same average potential per cell. The various bands are obtained by introducing an asymmetry into the monoatomic structure. Here, p is the number of atoms per cell, and μ is the relation m^*/m_0 at the band edges.

However, if we change the location of any peak, inside the cell of the second lattice, i.e., if we consider a displacement $(\Delta\beta)a$ in a particular atom k such that its new position is $\beta_k a = (k-1)a+\beta a+(\Delta\beta)a$, or if we change the magnitude of any potential inside the cell, then the lattice is not equivalent to a monoatomic one anymore, but becomes a lattice with p peaks per cell, that is, it becomes a polyatomic lattice.

If we perform either one of the asymmetries mentioned above, each energy band of the monoatomic lattice will break up in $(p-1)$ bands. The separation of these bands, as well as the variation of the effective mass, is due only to the asymmetry introduced, since the average potential per cell' is kept constant in all cases.

Fig.3 shows the splitting of the first energy band of a monoatomic lattice (central portion of the figure), corresponding to the case $P=1.5$, $p = 1$ and $\beta = 0$. If we consider two or three peaks per cell, characterized, respectively, by $P_1 = P_2 = 3$, $\beta_1 = 0$, and $\beta_2 = 1/2$ or $P_1 = P_2 = P_3 = 4.5$, with $\beta_1 = 0$, $\beta_2 = 1/3$ and $\beta_3 = 2/3$, etc., we would obtain the same results as those obtained for the monoatomic case. But considering the cases

$$p = 2,\ \beta_1 = 0,\ \beta_2 = .4\ ,\ P_1 = P_2 = 3,$$

$$p = 3,\ \beta_1 = 0,\ \beta_2 = .25,\ \beta_3 = 2/3,\ P_1 = P_2 = P_3 = 4.5\ ,$$

$$p = 4,\ \beta_1 = 0,\ \beta_2 = .2\ ,\ \beta_3 = .55,\ \beta_4 = .75,\ P_1=\ldots=P_4= 6\ ,$$

we get the right side of Fig.3.

If we keep the regularity of the positions of the peaks, but change the strength of the potential, then we get again the splitting of the bands.' This is shown on the left side of Fig.3, and corresponds to the cases:

$$p = 2,\ \beta_1 = 0,\ \beta_2 = 1/2,\ \ P_1 = 2.5,\ P_2 = 3.5\ ,$$

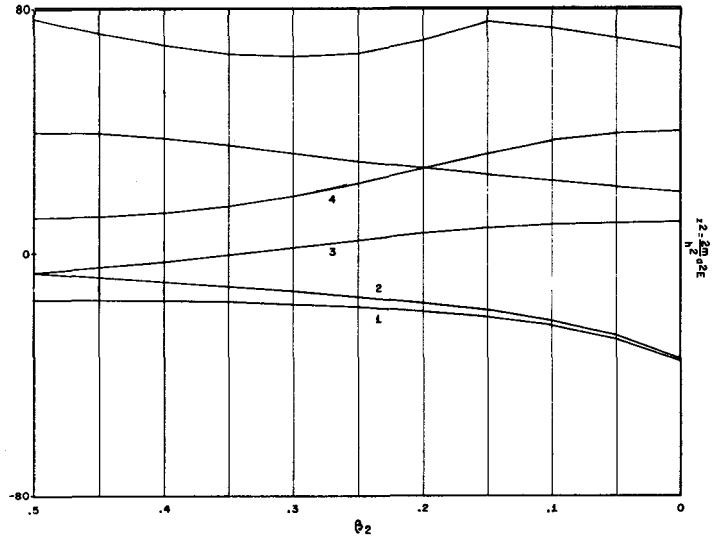

Fig.4 - Band structure for the diatomic lattice, in terms of the position, β_2, of the second atom in the cell. Here, β_1=0 and P_1=P_2= 3.

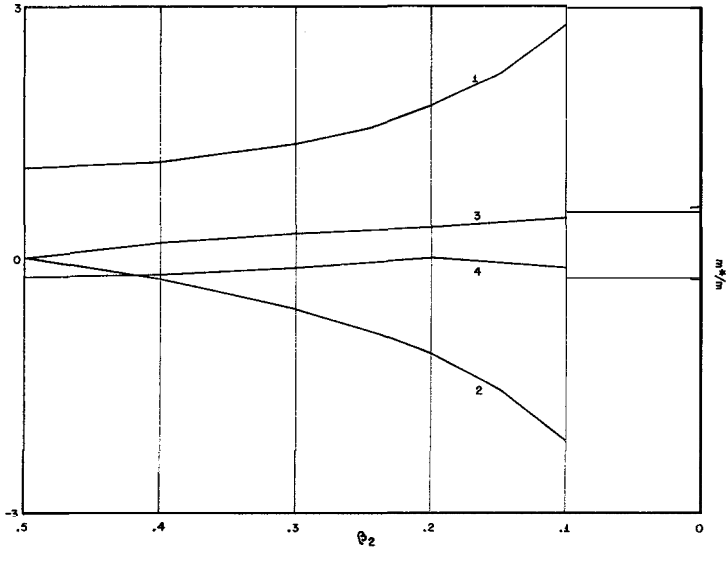

Fig.5 - Electron effective mass, at the oand edges shown in Fig.4.

$p = 3$, $\beta_1 = 0$, $\beta_2 = 1/3$, $\beta_3 = 1/3$, $P_1 = 4$, $P_2 = 5$, $P_3 = 4.5$,

$p=4$, $\beta_1=0$, $\beta_2=1/4$, $\beta_3=2/4$, $\beta_4=3/4$, $P_1=P_4=6$, $P_2=6.5$, $P_3=5.5$.

Also plotted, in Fig.3, is the relation $\mu=m^*/m_0$ on the band edges, according to Eq.34.

The model also allows us to verify the way the band structure, and the effective mass, vary with respect to a continuum variation of the position of one of the peaks, inside the cell. Figure 4 shows the dependence of the first energy bands on the position β_2 of the second peak for a diatomic lattice with fixed strength $P_1 = P_2 = 3$ and $\beta_1=0$. The negative band tends to higher negative values, when β_2 approaches zero, since at this position the lattice is a monoatomic one, with a peak $P = 6$ per cell, and this corresponds to a maximum binding potential. The gap, which appears when $\beta_2 \neq 1/2$, and is the result of the splitting of the first band, can be considered as the energy difference between the bottom of the positive energy band and the top of the negative one. The gap also increases with β_2, even though the bottom of the positive band does not vary much with β_2. In Fig.5, we plot the effective mass corresponding to the bands showed in Fig.4.

Similar results are obtained for a triatomic lattice, when we consider $P_1 = P_2 = P_3 = 4.5$, $\beta_1 = 0$, $\beta_3 = 2/3$, and β_2 taking values from 1/3 to zero. The results, for the first bands, are shown in Fig. 6, and Fig.7 shows the corresponding effective mass.

In Fig.8, we plot the splitting of the bands with respect to an asymmetry, ΔP, in the potential, for a lattice with four peaks per cell, where each peak is held in a fixed position inside the cell, that is, $\beta_1 = 0$, $\beta_2 = 1/4$, $\beta_3 = 2/4$, and $\beta_4 = 3/4$, but each peak with a variable strength given by $P_1 = P_4 = 6 + \Delta P$, and $P_2 = P_3 = 6 - \Delta P$. The average potential per cell is kept constant, in this way, for each value of AP, and the splitting of the band is due only to the asymmetry introduced. Figure 9 shows the corresponding effective mass.

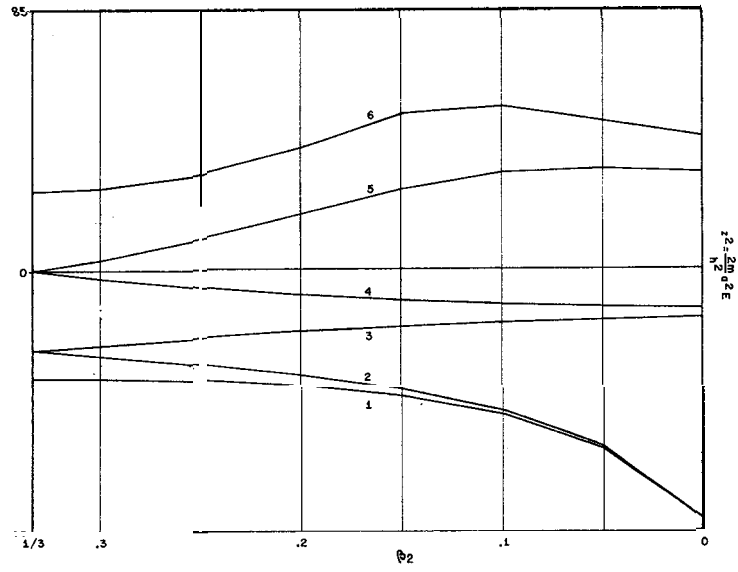

Fig.6 - Band structure for the triatomic lattice in terms of the position β_2 of the central atom. Here $\beta_1 = 0$, $\beta_3 = 2/3$, $P_1 = P_2 = P_3 = 4.5$.

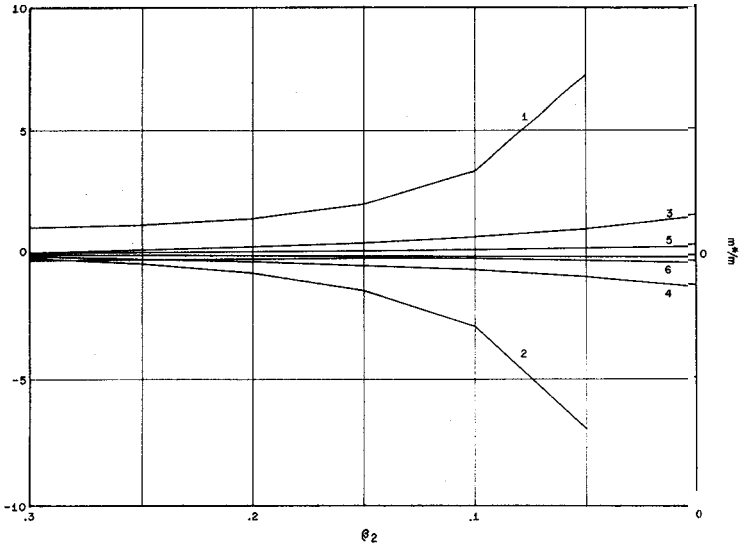

Fig.7 - Electron effective mass, at the band edges shown in Fig.6.

APPENDIX

We have shown[3] that the general expression for the dispersion relation, when we have p peaks per cell, with strengths $P_1, P_2, P_3, \ldots P_p$ and located, respectively, at $\beta_1 a$, $\beta_2 a$, $\beta_3 a \ldots \beta_p a$, with $0 \leq \beta_i \leq 1$, is of the form

$$\cos(ka) = \cos(Ka) - \sum_{i=1}^{p} \frac{P_i}{Ka} \sin Ka$$

$$+ 2 \sum_{i=j}^{p} \sum_{j>i}^{p} \frac{P_i P_j}{(Ka)^2} \sin\left[K(\beta_j - \beta_i)a\right] \sin\left[K(1-\beta_j+\beta_i)a\right]$$

$$\ldots + (-1)^p (2)^{p-1} \frac{P_1 P_2 \ldots P_p}{(Ka)p} \sin\left[K(\beta_2 - \beta_1)a\right] \ldots \sin\left[K(\beta_p - \beta_{p-1})a\right] \cdot$$

$$\cdot \sin\left[K(1-\beta_p+\beta_1)a\right] \cdot$$

This expression can be written in a condensed forrn to facilitate its handling. Let us define:

$C_{p,\ell}$ as the set of all the subsets of $1,2,3,\ldots p$, with R elements each;

f_i: $J \rightarrow I$ as a strictly increasing function defined over the set $J=\{1,2,3,\ldots \ell+1\}$, and taking values in the set $I = iU\{p+1\}$, i.e., $f_i(\ell+1)=p+1$;

$$\beta_{f_i(\ell+1)} = 1 + \beta_{f_i(1)} \cdot$$

With these definitions, we can verify that the dispersion relation above can be written as it was presented in Eq.26.

Let us consider the case that we have three peaks in the cell, P_1, P_2, and P_3, located at β_1, β_2 and β_3. The sets $C_{3,\ell}$, for $1 \leq \ell \leq 3$, are:

$$C_{3,1} = \{ \{1\}, \{2\}, \{3\} \},$$

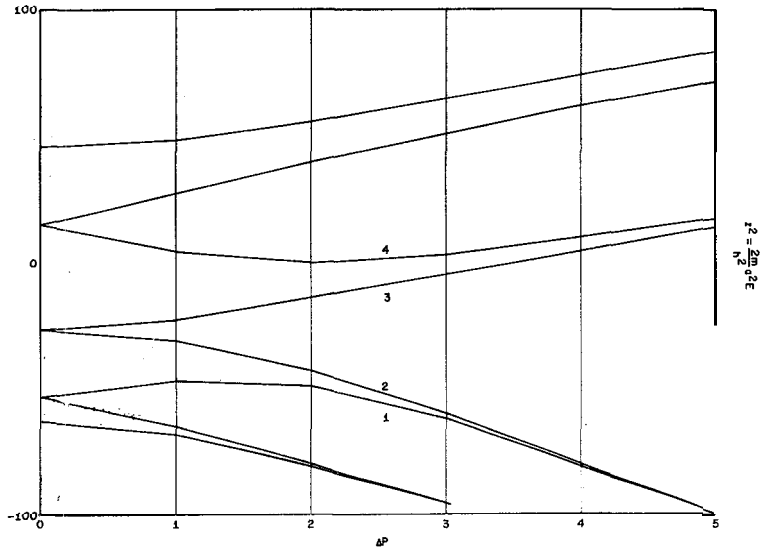

Fig.8 - Band structure for a lattice, with four atoms per cell, in terms of the asymmetry parameter, AP. Here, $\beta_1 = 0$, $\beta_2 = .25$, $\beta_3 = .50$, $\beta_4 = .75$, $P_1 = P_4 = 6 + \Delta P$, $P_2 = P_3 = 6 - AP$.

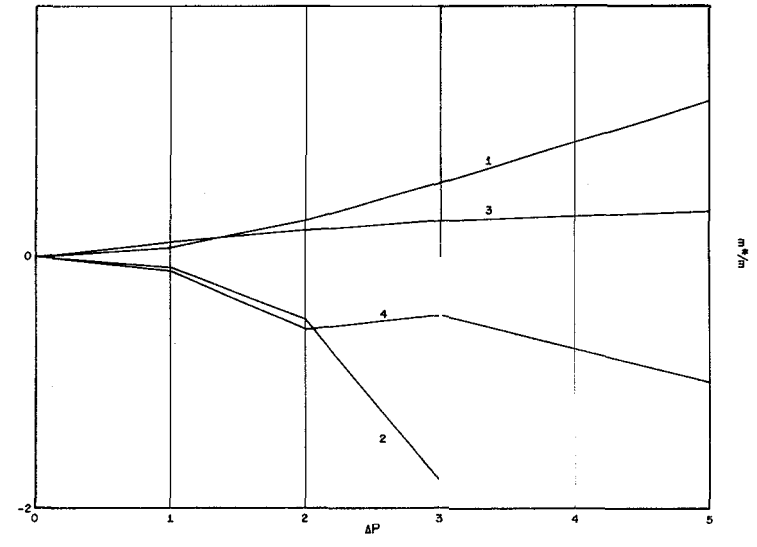

Fig.9 - Electron effective mass, at the edges of the bands, shown in Fig.8.

$$C_{3,2} = \{ \{1,2\}, \{1,3\}, \{2,3\} \},$$

$$C_{3,3} = \{ \{2,1,3\} \} .$$

For each R, the sets i are

$$i \subset C_{3,1} \Rightarrow \quad i = \{1\} \text{ or } i = \{2\} \text{ or } i = \{3\};$$

$$i \subset C_{3,2} \Rightarrow \quad i = \{1,2\} \text{ or } i = \{1,3\} \text{ or } i = \{2,3\};$$

$$i \subset C_{3,3} \Rightarrow \quad i = \{2,1,3\} .$$

For each i, the functions $f_i : J \to I$ are

$f_{\{1\}}$: $\{1,2\} \Rightarrow \{1,4\}$, for R = 1,

$f_{\{2\}}$: $\{1,2\} \Rightarrow \{2,4\}$, for ℓ = 1,

$f_{\{3\}}$: $\{1,2\} \Rightarrow \{3,4\}$, for ℓ = 1,

$f_{\{1,2\}}$: $\{1,2,3\} \Rightarrow \{1,2,4\}$, for ℓ = 2,

$f_{\{1,3\}}$: $\{1,2,3\} \Rightarrow \{1,3,4\}$, for ℓ = 2,

$f_{\{2,3\}}$: $\{1,2,3\} \Rightarrow \{2,3,4\}$, for ℓ = 2,

$f_{\{2,1,3\}}$: $\{1,2,3,4\} \Rightarrow \{1,2,3,4\}$, for ℓ = 3.

With these values, the dispersion equation becomes

$$\cos(ka) = \cos(Ka) - P_1 \frac{\sin Ka}{Ka} - P_2 \frac{\sin Ka}{Ka} - P_3 \frac{\sin Ka}{Ka} +$$

$$+ 2 \frac{P_1 P_2}{(Ka)^2} \sin\left[K(\beta_2 - \beta_1)a\right] \cdot \sin\left[K(1 - \beta_2 + \beta_1)a\right]$$

$$+ 2 \frac{P_1 P_3}{(Ka)^2} \sin\left[K(\beta_3 - \beta_1)a\right] \sin\left[K(1 - \beta_3 + \beta_1)a\right] +$$

$$+ 2\,\frac{P_2P_3}{(Ka)^2}\sin\left[K(\beta_3-\beta_2)a\right] \cdot \sin\left[K(1-\beta_3+\beta_2)a\right]$$

$$- 4\,\frac{P_1P_2P_3}{(Ka)^3}\sin\left[K(\beta_2-\beta_1)a\right]\sin\left[K(\beta_3-\beta_2)a\right]\sin\left[K(1-\beta_3+\beta_1)a\right] .$$

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