

From the above relations, we easily obtain

$$\overline{C_k}(\mathbf{r}_0) = \exp\{-i(\mathbf{k}, \mathbf{r}_0)\} \cdot C_k(\mathbf{r}_0). \quad (48)$$

In case the scalar product  $(\mathbf{k}, \mathbf{r}_0)$  is an integral multiple of  $2\pi$ , then the operators  $C_k(\mathbf{r}_0)$  and  $C_k(\mathbf{r}_0)$  are equal and hence the operators  $\exp\{-i(\mathbf{k}, \mathbf{r})\}$  and  $T_{\mathbf{r}_0}$  commute.

The scalar product  $(\mathbf{k}, \mathbf{r})$  vanishes when the wave vector  $\mathbf{k}$  is the inverse of the vector  $\mathbf{r}_0$  or when the  $\mathbf{k}$  is given by the relation

$$\mathbf{k} = \frac{1}{2} |\mathbf{H} \times \mathbf{r}_1| = \frac{1}{c} \mathbf{A}(\mathbf{r}_1) \quad (49)$$

and the vectors  $\mathbf{r}_0$ ,  $\mathbf{r}_1$  and  $\mathbf{H}$  are coplanar.

In the case  $\mathbf{r}_1 = \mathbf{r}_0$  we obtain the Harper's operator (40).

An analytic study of the condition (49) with the three vectors  $\mathbf{r}_0$ ,  $\mathbf{r}_1$  and  $\mathbf{H}$  coplanar, has been made by FISHBECK<sup>12</sup> and is just the condition for the Harper's operator to form an Abelian group. It can be shown that the operators (46) and (47) form a group and do not commute.

## Solution of the Dirac Equation for the Rectilinear Periodic Motion of an Electron

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In this paper the Dirac equation for a rectilinear onedimensional periodic potential is treated. It is shown that the energy eigenvalues are periodic functions of the wave number  $K_x$  and the continuous spectrum is split into energy bands. The end points of the energy bands are the points where the Bragg reflection takes place.

These results are obtained by perturbation theory, as well as by the method of determinants, since the resulting eigenvalue equation has the form of a determinant which is similar to the Hill determinant.

### 1. Introduction

We consider the motion of an electron parallel to the  $x$ -axis in a field that is a function of  $x$  only. We suppose that the vector potential  $A$  is zero everywhere and that  $e\varphi = -V(x)$ . The Dirac wave function may be written in the form:

$$\psi = f(x) \exp\left\{\frac{i}{\hbar} (P_2 y + P_3 z - W t)\right\}. \quad (1)$$

Substituting this expression into the Dirac equation we obtain:

$$\left[ -i\hbar \alpha_1 \frac{d}{dx} + \frac{W - V(x)}{c} + \alpha_2 P_2 + \alpha_3 P_3 + \alpha_4 m c \right] f(x) = 0 \quad (2)$$

where  $\alpha_i$ ,  $i = 1, 2, 3, 4$  are the Dirac matrices and they satisfy the relations

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 2 \delta_{ij}. \quad (3)$$

The Eq. (2) in scalar function  $f_i(x)$  has the form:

<sup>1</sup> N. MOTT and I. SNEDDON, Wave Mechanics and its Applications, § 56, Clarendon Press, Oxford 1948.

$$\begin{aligned} -i\hbar \frac{df_1}{dx} + \frac{W - V(x)}{c} f_4 + i P_2 f_1 - P_3 f_3 - m c f_4 &= 0, \\ -i\hbar \frac{df_2}{dx} + \frac{W - V(x)}{c} f_3 - i P_2 f_2 + P_3 f_1 - m c f_3 &= 0, \\ -i\hbar \frac{df_3}{dx} + \frac{W - V(x)}{c} f_2 + i P_2 f_3 - P_3 f_4 + m c f_2 &= 0, \\ -i\hbar \frac{df_4}{dx} + \frac{W - V(x)}{c} f_1 - i P_2 f_4 + P_3 f_3 + m c f_1 &= 0. \end{aligned} \quad (4)$$

If we substitute the expressions<sup>1</sup>

$$\begin{aligned} f_2 &= \frac{i P_3}{K} \varphi_2, & f_1 &= \varphi_1 - \frac{P_2 + i m c}{K} \varphi_2, \\ f_3 &= -\frac{i P_3}{K} \varphi_2, & f_4 &= \varphi_1 + \frac{P_2 + i m c}{K} \varphi_2 \end{aligned} \quad (5)$$

$$\text{where} \quad K^2 = P_2^2 + P_3^2 + m^2 c^2. \quad (6)$$

We obtain the following linear system of differential equations for the functions  $\varphi_1$  and  $\varphi_2$

$$\begin{aligned} \frac{d\varphi_1}{dx} + \frac{i}{\hbar} \frac{W - V(x)}{c} \varphi_1 + \frac{K}{\hbar} \varphi_2 &= 0 \\ \frac{d\varphi_2}{dx} - \frac{i}{\hbar} \frac{W - V(x)}{c} \varphi_2 + \frac{K}{\hbar} \varphi_1 &= 0 \end{aligned} \quad (7)$$



The solution of system (7) has the following form

$$\begin{aligned}\varphi_1 &= \exp \left\{ -\frac{i}{\hbar} \int \frac{W-V(x)}{c} dx \right\} \mathcal{V}(x) \\ \varphi_2 &= \exp \left\{ -\frac{i}{\hbar} \int \frac{W-V(x)}{c} dx \right\} \mathcal{U}(x)\end{aligned}\quad (8)$$

then the new functions  $\mathcal{V}(x)$  and  $\mathcal{U}(x)$  satisfy the equations

$$\begin{aligned}\frac{d\mathcal{U}}{dx} - \frac{2i}{\hbar} \frac{W-V(x)}{c} \mathcal{U} + \frac{K}{\hbar} \mathcal{V} &= 0 \\ \frac{d\mathcal{V}}{dx} + \frac{K}{\hbar} \mathcal{U} &= 0\end{aligned}\quad (9)$$

and the function  $\mathcal{V}(x)$  satisfies the second order differential equation:

$$\frac{d^2\mathcal{V}}{dx^2} - \frac{2i}{\hbar} \frac{W-V(x)}{c} \frac{d\mathcal{V}}{dx} - \frac{K^2}{\hbar^2} \mathcal{V} = 0. \quad (10)$$

The above equation equals Eq. (20) of PLESSET<sup>2</sup>.

PLESSET has studied the case in which the function  $V(x)$  is a polynomial of any degree in  $x$ , or in  $1/x$ . The case of a uniform electric field  $V(x) = ax$ , has been treated by SAUTER<sup>3</sup> and that of the simple harmonic oscillator,  $V(x) = ax^2$  by NIKOLSKI<sup>4</sup>.

By substituting (14) into Eqs. (13) the following coefficients  $A_n$  and  $B_n$

$$\begin{aligned}\frac{K}{\hbar} B_n + i \left[ \left( K_x + \frac{2\pi}{a} n \right) + \frac{W}{\hbar c} \right] A_n - i \frac{V_0}{2\hbar c} (A_{n+1} + A_{n-1}) &= 0, \\ \frac{K}{\hbar} A_n + i \left[ \left( K_x + \frac{2\pi}{a} n \right) - \frac{W}{\hbar c} \right] B_n + i \frac{V_0}{2\hbar c} (B_{n+1} + B_{n-1}) &= 0.\end{aligned}\quad (15)$$

By eliminating the coefficients  $B_n$  from the equations of the above system we get:

$$\begin{aligned}\left[ \frac{K^2}{\hbar^2} + \left( K_x + \frac{2\pi}{a} \right)^2 - \frac{V_0^2}{2\hbar^2 c^2} - \frac{W^2}{\hbar^2 c^2} \right] A_n + \frac{V_0}{\hbar c} \left[ \left( \frac{W}{\hbar c} + \frac{\pi}{a} \right) A_{n+1} \right. \\ \left. + \left( \frac{W}{\hbar c} - \frac{\pi}{a} \right) A_{n-1} \right] - \left( \frac{V_0}{2\hbar c} \right)^2 [A_{n+2} + A_{n-2}] &= 0\end{aligned}\quad (16)$$

The above equation is a fourth order recurrence equation, and some methods will be applied for its solution. At first perturbation theory will be used.

Before studying (16) it is useful to write it in its normal form:

$$\left[ \frac{W^2}{\hbar^2 c^2} - \frac{K_0^2}{\hbar^2} - \left( K_x + \frac{2\pi}{a} n \right)^2 \right] A_n - \frac{V_0}{\hbar c} \left[ \left( \frac{W}{\hbar c} + \frac{\pi}{a} \right) A_{n+1} + \left( \frac{W}{\hbar c} - \frac{\pi}{a} \right) A_{n-1} \right] + \left( \frac{V_0}{2\hbar c} \right)^2 [A_{n+2} + A_{n-2}] = 0 \quad (17)$$

$$\text{where} \quad K_0^2 = K^2 - \frac{V_0^2}{2\hbar^2 c^2}. \quad (18)$$

The Eq. (17) is very similar to the recurrence equation of the Hill type and can be treated in the same way<sup>6</sup>. This procedure is followed in § 4.

## 2. Periodic Potential Field

Now we consider the case that the function  $V(x)$  is a periodic function of  $x$ ; also

$$V(x) = V(x+a). \quad (11)$$

For the determination of the Energy eigenvalues  $W$  it is more convenient to use the system of Eq. (7); then for the very simple case where

$$V(x) = V_0 \cos \frac{2\pi}{a} x \quad (12)$$

we have to solve the following system

$$\begin{aligned}\frac{d\varphi_1}{dx} + \frac{i}{\hbar} \frac{W - V_0 \cos(2\pi/a)x}{c} \varphi_1 + \frac{K}{\hbar} \varphi_2 &= 0, \\ \frac{d\varphi_2}{dx} - \frac{i}{\hbar} \frac{W - V_0 \cos(2\pi/a)x}{c} \varphi_2 + \frac{K}{\hbar} \varphi_1 &= 0.\end{aligned}\quad (13)$$

By taking into account the BLOCH<sup>5</sup> theorem we conclude that the solution of (13) will be of the form

$$\begin{aligned}\varphi_1 &= \sum_{n=-\infty}^{\infty} A_n \exp\{i(K_x + (2\pi/a)n)x\}, \\ \varphi_2 &= \sum_{n=-\infty}^{\infty} B_n \exp\{i(K_x + (2\pi/a)n)x\}.\end{aligned}\quad (14)$$

recurrence equations are obtained which connect the

<sup>2</sup> M. PLESSET, Phs. Rev. (2) **41**, 278 [1932].

<sup>3</sup> F. SAUTER, Z. Phys. **69**, 742 [1931].

<sup>4</sup> K. NIKOLSKI, Z. Phys. **62**, 677 [1930].

<sup>5</sup> F. BLOCH, Z. Phys. **55**, 555 [1928].

<sup>6</sup> E. WHITTAKER and G. WATSON, A Course of Modern Analysis, The University Press, Cambridge 1927.

### 3. Perturbation Theory

We consider the case in which the parameter  $V_0$  is small; then by perturbation theory it is possible to expand the solution and the energy eigenvalues in the form of a series, i. e.

$$A_n = \sum_{l=0}^{\infty} A_{n,l} V_0^l, \quad \frac{W}{\hbar c} = \sum_{l=0}^{\infty} W_l V_0^l \quad (19)$$

with the condition  $A_0 = 1$ . — In addition we have

$$(W/\hbar c)^2 = W_0^2 + 2 V_0 W_0 W_1 + V_0^2 [2 W_0 W_2 + W_1^2] \\ + V_0^3 [2 W_0 W_3 + 2 W_1 W_2] + V_0^4 [2 W_0 W_4 + 2 W_1 W_3 + W_2^2] + \dots \quad (20)$$

By introducing (19) and (20) in (16) and by equating to zero the coefficients of the various powers of the parameter  $V_0$  we obtain the following recurrence system

$$\begin{aligned} & \left( W_0^2 - \frac{K_0^2}{\hbar^2} - T_n^2 \right) A_{n,0} = 0, \\ & \left( W_0^2 - \frac{K_0^2}{\hbar^2} - T_n^2 \right) A_{n,1} + 2 W_0 W_1 A_{n,0} - \frac{1}{\hbar c} \left[ \left( W_0 + \frac{\pi}{a} \right) A_{n+1,0} + \left( W_0 - \frac{\pi}{a} \right) A_{n-1,0} \right] = 0, \\ & \left( W_0^2 - \frac{K_0^2}{\hbar^2} - T_n^2 \right) A_{n,2} + 2 W_0 W_1 A_{n,1} + (2 W_0 W_2 + W_1^2) A_{n,0} \\ & \quad - \frac{1}{\hbar c} \left[ \left( W_0 + \frac{\pi}{a} \right) A_{n+1,1} + \left( W_0 - \frac{\pi}{a} \right) A_{n-1,1} + W_1 (A_{n+1,0} + A_{n-1,0}) \right] + \frac{1}{4 \hbar^2 c^2} (A_{n+2,0} + A_{n-2,0}) = 0, \\ & \left( W_0^2 - \frac{K_0^2}{\hbar^2} - T_n^2 \right) A_{n,3} + 2 W_0 W_1 A_{n,2} + (2 W_0 W_2 + W_1^2) A_{n,1} \\ & \quad + (2 W_0 W_3 + 2 W_1 W_2) A_{n,0} - \frac{1}{\hbar c} \left[ \left( W_0 + \frac{\pi}{a} \right) A_{n+1,2} + \left( W_0 - \frac{\pi}{a} \right) A_{n-1,2} \right. \\ & \quad \left. + W_1 (A_{n+1,1} + A_{n-1,1}) + W_2 (A_{n+1,0} + A_{n-1,0}) \right] + \frac{1}{4 \hbar^2 c^2} [A_{n+2,1} + A_{n-2,1}] = 0, \\ & \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \end{aligned} \quad (21)$$

where we have put

$$T_n = \left( K_x + \frac{2\pi}{a} n \right)$$

The above system can be easily solved in the following way.

*First equation:*

$$[W_0^2 - (K_0^2/\hbar^2) - T_n^2] A_{n,0} = 0. \quad (22)$$

Because of the condition  $A_0 = 1$  this equation has the solution

$$A_{n,0} = \delta_{n,0}. \quad (23)$$

The energy eigenvalues are

$$W_0^2 = (K_0^2 + \hbar^2 K_x^2)/\hbar^2$$

or

$$W_0 = \pm \sqrt{K_0^2 + \hbar^2 K_x^2}/\hbar. \quad (24)$$

These are exactly the energy eigenvalues of the free Dirac electron.

*Second equation:*

$$\left( W_0^2 - \frac{K_0^2}{\hbar^2} - T_n^2 \right) A_{n,1} + 2 W_0 W_1 A_{n,0} - \frac{1}{\hbar c} \left[ \left( W_0 + \frac{\pi}{a} \right) A_{n+1,0} + \left( W_0 - \frac{\pi}{a} \right) A_{n-1,0} \right] = 0. \quad (25)$$

For  $n=0$  it follows that  $W_1=0$  and for  $n=\pm 1$  we have

$$A_{1,1} = \frac{1}{\hbar c} \frac{W_0 - (\pi/a)}{T_0^2 - T_1^2}, \quad A_{-1,1} = \frac{1}{\hbar c} \frac{W_0 + (\pi/a)}{T_0^2 - T_1^2}. \quad (26)$$

In addition  $A_{0,1}=0$  and  $A_{n,1}=0$  for  $|n|>1$ .

Third equation:

$$(T_0^2 - T_n^2) A_{n,2} + 2 W_0 W_2 A_{n,0} - \frac{1}{\hbar c} \left[ \left( W_0 + \frac{\pi}{a} \right) A_{n+1,1} + \left( W_0 - \frac{\pi}{a} \right) A_{n-1,1} \right] + \frac{1}{4 \hbar^2 c^2} [A_{n+2,0} + A_{n-2,0}] = 0. \quad (27)$$

For  $n=0$  we have

$$2 W_0 W_2 = \frac{1}{\hbar c} \left[ \left( W_0 + \frac{\pi}{a} \right) A_{1,1} + \left( W_0 - \frac{\pi}{a} \right) A_{-1,1} \right]$$

or 
$$W_2 = \frac{W_0^2 - (\pi^2/a^2)}{2 \hbar c W_0} \left[ \frac{1}{T_0^2 - T_1^2} + \frac{1}{T_0^2 - T_{-1}^2} \right] = \frac{W_0^2 - (\pi^2/a^2)}{4 \hbar c W_0} \frac{1}{(K_x - (\pi/a))(K_x + (\pi/a))}. \quad (28)$$

For  $n = \pm 1$  is  $A_{\pm 1,2} = 0$  and for  $n = \pm 2$  we have

$$A_{2,2} = \frac{1}{\hbar^2 c^2} \frac{(W_0 - (\pi/a))^2 - \frac{1}{4}(T_0^2 - T_1^2)}{(T_0^2 - T_1^2)(T_0^2 - T_2^2)}, \quad A_{-2,2} = \frac{1}{\hbar^2 c^2} \frac{(W_0 + (\pi/a))^2 - \frac{1}{4}(T_0^2 - T_{-1}^2)}{(T_0^2 - T_{-1}^2)(T_0^2 - T_{-2}^2)}. \quad (29)$$

We also have  $A_{0,2} = 0$  and  $A_{n,2} = 0$  for  $|n| > 2$ .

Fourth equation:

$$(T_0^2 - T_n^2) A_{n,3} + 2 W_0 W_2 A_{n,1} + 2 W_0 W_3 A_{n,0} - \frac{1}{\hbar c} \left[ \left( W_0 + \frac{\pi}{a} \right) A_{n+1,2} + \left( W_0 - \frac{\pi}{a} \right) A_{n-1,2} + W_2 (A_{n+1,0} + A_{n-1,0}) \right] + \frac{1}{4 \hbar^2 c^2} (A_{n+2,1} + A_{n-2,1}) = 0. \quad (30)$$

For  $n=0$  it follows that  $W_3 = 0$  and for  $n = \pm 1$  we have

$$A_{1,3} = \frac{1}{T_0^2 - T_1^2} \left\{ -2 W_0 W_2 A_{1,1} + \frac{1}{\hbar c} \left[ \left( W_0 + \frac{\pi}{a} \right) A_{2,2} + W_2 \right] - \frac{1}{4 \hbar^2 c^2} A_{-1,1} \right\}, \quad (31)$$

$$A_{-1,3} = \frac{1}{T_0^2 - T_{-1}^2} \left\{ -2 W_0 W_2 A_{-1,1} + \frac{1}{\hbar c} \left[ \left( W_0 - \frac{\pi}{a} \right) A_{-2,2} + W_2 \right] - \frac{1}{4 \hbar^2 c^2} A_{1,1} \right\}.$$

For  $n = \pm 2$  is  $A_{\pm 2,3} = 0$  and for  $n = \pm 3$  we have

$$A_{3,3} = \frac{1}{\hbar c} \frac{W_0 - (\pi/a)}{T_0^2 - T_3^2} A_{2,2}, \quad A_{-3,3} = \frac{1}{\hbar c} \frac{W_0 + (\pi/a)}{T_0^2 - T_{-3}^2} A_{-2,2}. \quad (32)$$

In addition we have  $A_{0,3} = 0$  and  $A_{n,3} = 0$  for  $|n| > 3$ .

The right hand members of (31) and (32) are all known, because of (24), (26) and (29).

Fifth equation:

$$(T_0^2 - T_n^2) A_{n,4} + 2 W_0 W_2 A_{n,2} + (2 W_0 W_4 + W_2^2) A_{n,0} - \frac{1}{\hbar c} \left[ \left( W_0 + \frac{\pi}{a} \right) A_{n+1,3} + \left( W_0 - \frac{\pi}{a} \right) A_{n-1,3} + W_2 (A_{n+1,1} + A_{n-1,1}) \right] + \frac{1}{4 \hbar^2 c^2} [A_{n+2,2} + A_{n-2,2}] = 0. \quad (33)$$

For  $n=0$  we obtain

$$2 W_0 W_4 + W_2^2 = \frac{1}{\hbar c} \left[ \left( W_0 + \frac{\pi}{a} \right) A_{1,3} + \left( W_0 - \frac{\pi}{a} \right) A_{-1,3} + W_2 (A_{1,1} + A_{-1,1}) \right] - \frac{1}{4 \hbar^2 c^2} [A_{2,2} + A_{-2,2}]. \quad (34)$$

By substituting the already known values of  $W_2$ ,  $A_{\pm 1,1}$  and  $A_{\pm 2,2}$ ,  $A_{\pm 1,3}$  we find the following expression for  $W_4$ :

$$W_4 = \frac{1}{2 W_0} \left\{ -W_2^2 + \frac{1}{\hbar^2 c^2} \left[ \frac{[W_0^2 + (\pi^2/a^2) - \frac{1}{4}(T_0^2 - T_1^2)]^2 - 4 W_0^2 (\pi^2/a^2)}{(T_0^2 - T_1^2)^2 (T_0^2 - T_2^2)} + \frac{[W_0^2 + (\pi^2/a^2) - \frac{1}{4}(T_0^2 - T_{-1}^2)]^2 - 4 W_0^2 (\pi^2/a^2)}{(T_0^2 - T_{-1}^2)^2 (T_0^2 - T_{-2}^2)} \right] - \frac{1}{2 \hbar^4 c^4} \frac{W_0^2 + (\pi^2/a^2)}{(T_0^2 - T_1^2)(T_0^2 - T_{-1}^2)} + \frac{W_0^2 - (\pi^2/a^2)}{\hbar^3 c^3} \left( \frac{1}{T_0^2 - T_1^2} + \frac{1}{T_0^2 - T_{-1}^2} \right) \left[ \frac{1}{T_0^2 - T_1^2} + \frac{1}{T_0^2 - T_{-1}^2} - \left( W_0^2 - \frac{\pi^2}{a^2} \right) \left( \frac{1}{(T_0^2 - T_1^2)^2} + \frac{1}{(T_0^2 - T_{-1}^2)^2} \right) \right] \right\}. \quad (35)$$

By proceeding in the same way we can calculate the coefficients  $A_{n,l}$  and  $W_l$ . So we find the following solutions:

$$\begin{aligned}
 A_0 &= 1, \\
 A_1 &= \frac{V_0}{\hbar c} \frac{W_0 - (\pi/a)}{T_0^2 - T_1^2} + \frac{V_0^3}{T_0^2 - T_1^2} \left[ -2 W_0 W_2 A_{1,1} + \frac{1}{\hbar c} \left( W_2 + \left( W_0 + \frac{\pi}{a} \right) A_{2,2} \right) - \frac{1}{4 \hbar^2 c^2} A_{-1,1} \right] + \dots, \\
 A_{-1} &= \frac{V_0}{\hbar c} \frac{W_0 + (\pi/a)}{T_0^2 - T_{-1}^2} + \frac{V_0^3}{T_0^2 - T_{-1}^2} \left[ -2 W_0 W_2 A_{-1,1} + \frac{1}{\hbar c} \left( W_2 + \left( W_0 - \frac{\pi}{a} \right) A_{-2,2} \right) - \frac{1}{4 \hbar^2 c^2} A_{1,1} \right] + \dots, \\
 A_2 &= \frac{V_0^2}{\hbar^2 c^2} \frac{(W_0 - (\pi/a))^2 - \frac{1}{4} (T_0^2 - T_1^2)}{(T_0^2 - T_1^2) (T_0^2 - T_2^2)} + O(V_0^4), \\
 A_{-2} &= \frac{V_0^2}{\hbar^2 c^2} \frac{(W_0 + (\pi/a))^2 - \frac{1}{4} (T_0^2 - T_{-1}^2)}{(T_0^2 - T_{-1}^2) (T_0^2 - T_{-2}^2)} + O(V_0^4), \\
 A_3 &= \frac{V_0^3}{\hbar^3 c^3} \frac{(W_0 - (\pi/a)) [(W_0 - (\pi/a))^2 - \frac{1}{4} (T_0^2 - T_1^2)]}{(T_0^2 - T_1^2) (T_0^2 - T_2^2) (T_0^2 - T_3^2)} + O(V_0^5), \\
 A_{-3} &= \frac{V_0^3}{\hbar^3 c^3} \frac{(W_0 + (\pi/a)) [(W_0 + (\pi/a))^2 - \frac{1}{4} (T_0^2 - T_{-1}^2)]}{(T_0^2 - T_{-1}^2) (T_0^2 - T_{-2}^2) (T_0^2 - T_{-3}^2)} + O(V_0^5), \\
 &\dots \dots \dots
 \end{aligned} \tag{36}$$

The energy  $W$  is given by the series:

$$W = \hbar c \left[ W_0 + \frac{V_0^2}{2 \hbar c W_0} \left( W_0^2 - \frac{\pi^2}{a^2} \right) \left( \frac{1}{T_0^2 - T_1^2} + \frac{1}{T_0^2 - T_{-1}^2} \right) + V_0^4 W_4 + \dots \right]. \tag{37}$$

We observe that the perturbation method adopted here is the same as that of the nonrelativistic motion of the electron, i. e. the case of the Mathieu equation<sup>7</sup>.

The calculated energy as well as the coefficients of the series diverge at the point where

$$K_x^2 = [K_x + (2 \pi/a) n]^2 \tag{38}$$

and as is well known from the quantum theory of metals, at these points the Bragg reflection<sup>8</sup> takes place. These points correspond to the ends of the energy bands.

Since the energy  $W_0$  takes positive and negative values, the same happens with  $W$ .

The energy spectrum consists of energy bands as happens in the classical case, the difference being that the positive and negative eigenvalues are symmetric.

The points at which splitting of the continuous spectrum takes place are just the points where the Bragg reflection occurs.

#### 4. The Method of Determinants

Before examining the recurrence Eq. (16) by using the method of determinants<sup>6</sup>, we shall combine it with the corresponding Klein-Gordon equation<sup>9</sup>.

The Klein-Gordon equation is of the form

$$\Delta \psi + \left( \frac{1}{\hbar c} \right)^2 (W - V(x))^2 \psi = \frac{m^2 c^2}{\hbar^2} \psi \tag{39}$$

and has the following solution

$$\psi = \exp \{ (i/\hbar) (P_3 z + P_2 y) \} \mathcal{U}(x) \tag{40}$$

when  $\mathcal{U}(x)$  satisfies the second order differential equation

$$\frac{d^2 \mathcal{U}}{dx^2} + \left( \frac{W^2}{\hbar^2 c^2} - \frac{K^2}{\hbar^2} - 2 \frac{W V(x)}{\hbar^2 c^2} + \frac{V^2(x)}{\hbar^2 c^2} \right) \mathcal{U} = 0. \tag{41}$$

<sup>7</sup> J. MEIXNER and F. SCHAEFKE, Mathieu'sche Funktionen und Sphäroid-Funktionen, Springer-Verlag, Berlin 1954.

<sup>8</sup> A. WILSON, Theory of Metals, 2nd Edit., Cambridge Univ. Press, Cambridge 1953.

<sup>9</sup> A. MESSIAH, Mécanique Quantique II, Chapitre XX, 5, Dunod, Paris 1960.

The above equation for the potential energy (12) has the form of an equation of the Hill type<sup>7</sup>, i. e.

$$\frac{d^2 \mathcal{U}}{dx^2} + \left[ \frac{W^2}{\hbar^2 c^2} - \frac{K^2}{\hbar^2} + \frac{V_0^2}{2 \hbar^2 c^2} - 2 \frac{W V_0}{\hbar^2 c^2} \cos \frac{2 \pi}{a} x + \frac{V_0^2}{2 \hbar^2 c^2} \cos \frac{4 \pi}{a} x \right] \mathcal{U} = 0 \quad (42)$$

and its solution is of the form 
$$\mathcal{U}(x) = \sum_{n=-\infty}^{\infty} C_n \exp\{i(K_x + (2 \pi/a) n) x\} \quad (43)$$

when the coefficients  $C_n$  satisfy the following recurrence equation:

$$\left( \frac{W^2}{\hbar^2 c^2} - \frac{K_0^2}{\hbar^2} - \left( K_x + \frac{2 \pi}{a} n \right)^2 \right) C_n - \frac{W V_0}{\hbar^2 c^2} (C_{n+1} + C_{n-1}) + \frac{V_0^2}{4 \hbar^2 c^2} (C_{n+2} + C_{n-2}) = 0. \quad (44)$$

The above equation is identical to (16) up to the term  $-\frac{V_0}{\hbar c} \frac{\pi}{a} (A_{n+1} - A_{n-1})$ .

The study of Eq. (44) is already known and the condition of the determination of the eigenvalues leads to the following expression:

$$\cos K_x a = 1 - 2 \Delta(0) \sin^2 a \sqrt{\frac{W^2}{\hbar^2 c^2} - \frac{K_0^2}{\hbar^2}} \quad (45)$$

where  $\Delta(0)$  is the Hill determinant<sup>6</sup> by  $K_x = 0$ .

The determinant  $\Delta(0)$  is an even function of  $W$  i. e.  $\Delta(0, W) = \Delta(0, -W)$ .

We also notice from the eigenvalue equation (45) that the energy  $W$  is a periodic function of  $K_x$  with period  $2 \pi/a$  i. e. we just have the Bloch condition i. e. the energy is an even function of the wave number  $K_x$  and in addition a periodic function with period  $2 \pi/a$ .

The above method of determinants will be applied to the recurrence Eq. (16). It is easily shown that the eigenvalue equation has the same form as (45), also

$$\cos K_x a = 1 - \Delta'(0) \sin^2 a \sqrt{\frac{W^2}{\hbar^2 c^2} - \frac{K_0^2}{\hbar^2}} \quad (46)$$

where  $\Delta'(0)$  is the following determinant

$$\Delta'(0) = \begin{vmatrix} \frac{V_0^2 a^2}{8 \hbar^2 c^2 (2n)^2 - [(W^2/\hbar^2 c^2) - (K_0^2/\hbar^2)] (a^2/\pi^2)} & 1 & -\frac{V_0^2 a^2}{2 \hbar^2 c^2 \pi^2 (2n)^2 - [(W^2/\hbar^2 c^2) - (K_0^2/\hbar^2)] (a^2/\pi^2)} & \frac{W - (\pi/a)}{1} \\ -\frac{V_0^2 a^2}{2 \hbar^2 c^2 \pi^2 (2n)^2 - [(W^2/\hbar^2 c^2) - (K_0^2/\hbar^2)] (a^2/\pi^2)} & \frac{W + (\pi/a)}{1} & \frac{V_0^2 a^2}{8 \hbar^2 c^2 (2n)^2 - [(W^2/\hbar^2 c^2) - (K_0^2/\hbar^2)] (a^2/\pi^2)} & 1 \end{vmatrix}. \quad (47)$$

This determinant is an even function of the energy  $W$  i. e.  $\Delta(0, W) = \Delta'(0, -W)$  and in addition from (46) it follows that  $W(K_x)$  is also a periodic and even function of  $K_x$  with period  $2 \pi/a$ .

From the above we notice that the relativistic motion of the electron in a onedimensional periodic potential gives an energy spectrum which consists of energy bands.