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Mathematical Solution of Kronig-Penney Model Determinant

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Abstract: Kronig Penny model is an excellent approximation of crystal potential in the band theory of solids. The only problem students face in this topic is the solving of determinant. Of course, it was solved by originators after tedious calculations and they dropped it in publications. The same route is followed in earlier works. But a systematic way of solving it may develop an interest in students and might be helpful in scholarly article. In this paper it is solved in an appealing way never found elsewhere in literature, rather it was left as declared much tedious. This paper is endowed with full mathematical solution.
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I. INTRODUCTION

The great academician Pro L. D. Landau always emphasized on self-consistent and complete solution of a problem. With this inspiration I worked out this problem. The Kronig–Penney model played a significant and unique role in the deep understanding of the electronic states in one-dimensional crystals [1]. The one-dimensional Kronig–Penney (KP) potential is approximated as a periodic array of square-well shape. Exactly, the model has also been playing an important role in various problems in solid state physics [2]. The SchrÖdinger equation for an electron in this potential has a solution in the form of the Kronig–Penney equation (KPE), which illustrates the formation of electronic energy bands. The KPE is routinely found from the determinant of a 4 ×4 matrix resulting from four boundary conditions on the wavefunction and its derivative [3]. An interesting point of the Kronig–Penney model is that not only the band structure of a Kronig–Penney crystal can be analytically obtained as well known in the solid state physics community, but also the function formalisms of all solutions, both in the permitted and forbidden energy ranges, can be analytically obtained and explicitly expressed.

In almost all standard textbooks [4],[5],[6], the problem is handled without exploring route of solution. Rather it is mentioned that the solution is tedious enough. Somewhere an effort is done [6] but procedure is not so good looking from reading point of view. In this paper it is done in more interesting way.

The rest of the paper is organized as follows. Proposed embedding and method involved is elucidated in section II. Concluding remarks are given in section III. References are given in section IV.

II. THE KP MODEL DETERMINANT

A pictorial representation of the periodic potential in the Kronig-Penney model, illustrating wells of depth ‘V0’ and width ‘a’ separated from one another by barriers of width ‘b’, L = a+b is the unit cell length.

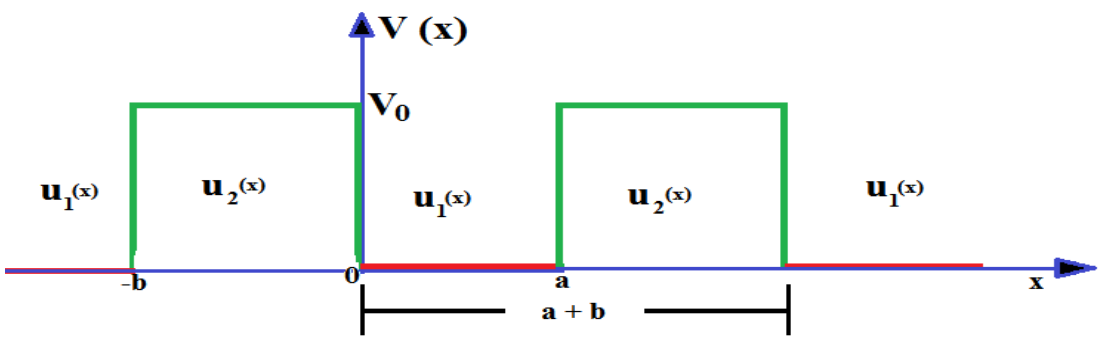

Figure 1. Model Potential

SchrÖdinger equation for an electron in periodic potential, of spatial period L=a+b, can be written as

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{2m}{\hbar^2}\left\{E-V\left(x\right)\right\}\Psi=0 \qquad \ldots(1)$$

The periodic potential can be represented as

$$V(x)=\begin{cases}0, & 0<x<a\\ V_0, & -b<x<0\end{cases}$$

$$V(x)=V(x+L);\; L=a+b \qquad \text{...(2)}$$

We can introduce the following parameters for sake of convenience

$$\frac{2mE}{\hbar^2}=\alpha^2>0<\beta^2=\frac{2m(V_0-E)}{\hbar^2}, \quad \forall E: 0<E<V_0 \qquad \text{...(3)}$$

Periodicity of potential enables us to express wave function as BlÖch functions

$$\Psi_k(x)=e^{ikx}u_k(x)$$

$$u_k(x)=\begin{cases}u_1, & V(x)=0\\ u_2, & V(x)=V_0\end{cases} \qquad \text{...(4)}$$

SchrÖdinger equation yields

$$u_1''+2iku_1'+(\alpha^2-k^2)u_1=0$$

$$u_2''+2iku_2'-(\beta^2+k^2)u_2=0 \qquad \text{...(5)}$$

The periodic boundary conditions obeyed by BlÖch functions are

$$u_1(0)=u_2(0); \quad u_1(a)=u_2(-b)$$

$$u_1'(0)=u_2'(0); \quad u_1'(a)=u_2'(-b) \qquad \text{...(6)}$$

The non trivial solution requires following determinant to be zero.

$$\Delta=\begin{vmatrix} 1 & 1 & 1 & 1\\ i(\alpha-k) & -i(\alpha+k) & (\beta-ik) & -(\beta+ik)\\ e^{i(\alpha-k)a} & e^{-i(\alpha+k)a} & e^{-(\beta-ik)b} & e^{(\beta+ik)b}\\ i(\alpha-k)e^{i(\alpha-k)a} & -i(\alpha+k)e^{-i(\alpha+k)a} & (\beta-ik)e^{-(\beta-ik)b} & -(\beta+ik)e^{(\beta+ik)b}\end{vmatrix}=0 \qquad \text{...(7)}$$

This Eq. (7) is very fundamental mathematical problem of KrÖnig Penny model. Many solid state physicists say it tedious and leaves the methodology untouched. But according to the Great Russian scientist and academician Lev Landau one can never be a theoretical physicist without knowing the mathematics inherent in the physical theory. That is why I worked to find non-tedious solution of this determinant. Earlier to this work in literature one could find complicated and boring algebra regarding this problem. Random way of applying mathematical operations leads to uninteresting and unnecessary complications. Such complications are hurdles in research methodology. Here I shall introduce each operation with sound logic and deep reasoning.

Up to this level all the things are visible in existing literature, now my original task starts:

1) Little observation shows that in second and fourth rows '-ik' appears in each terms. So we should remove it. First and third rows bear rather simple structures. In any determinant following operations with above requirement can be done.

$$R_2 \to R_2+ikR_1; \quad R_4 \to R_4+ikR_3 \qquad \text{...(8)}$$

This immediately leads to one simplification

$$\Delta=\begin{vmatrix} 1 & 1 & 1 & 1\\ i\alpha & -i\alpha & \beta & -\beta\\ e^{i(\alpha-k)a} & e^{-i(\alpha+k)a} & e^{-(\beta-ik)b} & e^{(\beta+ik)b}\\ i\alpha e^{i(\alpha-k)a} & -i\alpha e^{-i(\alpha+k)a} & \beta e^{-(\beta-ik)b} & -\beta e^{(\beta+ik)b}\end{vmatrix}=0 \qquad \text{...(9)}$$

2) Now we have '-ik' with exponents only. It will be beneficial to merge it with spatial period of the potential. The value of the determinant is zero, therefore any row or any column can be multiplied by nonzero finite numbers. We exploit this fact and apply

$$R_3 \to e^{-ikb} R_3; \quad R_4 \to e^{-ikb} R_4 \qquad \ldots(10)$$

We can introduce the below parameter for brevity only

$$\varpi = e^{ik(a+b)}, \qquad \varpi^* = e^{-ik(a+b)}; \qquad \varpi\varpi^* = 1 \qquad \ldots(11)$$

This consideration converts the above determinant into below one

$$\Delta = \begin{vmatrix} 1 & 1 & 1 & 1 \\ i\alpha & -i\alpha & \beta & -\beta \\ \varpi^* e^{i\alpha a} & \varpi^* e^{-i\alpha a} & e^{-\beta b} & e^{\beta b} \\ i\alpha\varpi^* e^{i\alpha a} & -i\alpha\varpi^* e^{-i\alpha a} & \beta e^{-\beta b} & -\beta e^{\beta b} \end{vmatrix} = 0 \qquad \ldots(12)$$

3) Next observation is that last two columns look simpler than first two columns. We try to remove ϖ* from last rows in these columns.

$$C_1 \to \varpi C_1; \quad C_2 \to \varpi C_2 \qquad \ldots(13)$$

As Δ=0 this operation will not affect it.

$$\begin{vmatrix} \varpi & \varpi & 1 & 1 \\ i\alpha\,\varpi & -i\alpha\,\varpi & \beta & -\beta \\ e^{i\alpha a} & e^{-i\alpha a} & e^{-\beta b} & e^{\beta b} \\ i\alpha\, e^{i\alpha a} & -i\alpha\, e^{-i\alpha a} & \beta e^{-\beta b} & -\beta e^{\beta b} \end{vmatrix} = 0 \qquad \ldots(14)$$

4) Before further calculation we substitute

$$\alpha\, a = x, \qquad \beta\, b = y \qquad \ldots(15)$$

$$\begin{vmatrix} \varpi & \varpi & 1 & 1 \\ i\alpha\,\varpi & -i\alpha\,\varpi & \beta & -\beta \\ e^{ix} & e^{-ix} & e^{-y} & e^{y} \\ i\alpha\, e^{ix} & -i\alpha\, e^{-ix} & \beta e^{-y} & -\beta e^{y} \end{vmatrix} = 0 \qquad \ldots(16)$$

5) Determinant will be easily treatable if its elements become zero in any way

$$C_2 \to (C_2 + C_1)/2; \qquad C_3 \to (C_3 + C_4)/2 \qquad \ldots(17)$$

In this way negative exponents will be removed and zeros are created.

$$\begin{vmatrix} \varpi & \varpi & 1 & 1 \\ i\alpha\,\varpi & 0 & 0 & -\beta \\ e^{ix} & \cos x & \cosh y & e^{y} \\ i\alpha\, e^{ix} & -\alpha \sin x & -\beta \sinh y & -\beta e^{y} \end{vmatrix} = 0 \qquad \ldots(18)$$

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6) Now we start treating positive exponents

$$C_1 \to (C_1 - C_2); \qquad C_4 \to (C_4 - C_3) \qquad \ldots(19)$$

$$\begin{vmatrix} 0 & \varpi & 1 & 0 \\ i\alpha\,\varpi & 0 & 0 & -\beta \\ i\sin x & \cos x & \cosh y & \sinh y \\ i\alpha\cos x & -\alpha\sin x & -\beta\sinh y & -\beta\cosh y \end{vmatrix} = 0 \qquad \ldots(20)$$

7) First column contains 'i 'as a multiplier and last row contains negative sign for most elements.

$$C_1 \to C_1 / i \qquad \ldots(21)$$

$$\begin{vmatrix} 0 & \varpi & 1 & 0 \\ \alpha\,\varpi & 0 & 0 & -\beta \\ \sin x & \cos x & \cosh y & \sinh y \\ \alpha\cos x & -\alpha\sin x & -\beta\sinh y & -\beta\cosh y \end{vmatrix} = 0 \qquad \ldots(22)$$

$$R_4 \to R_4(-1) \qquad \ldots(23)$$

$$\begin{vmatrix} 0 & \varpi & 1 & 0 \\ \alpha\,\varpi & 0 & 0 & -\beta \\ \sin x & \cos x & \cosh y & \sinh y \\ -\alpha\cos x & \alpha\sin x & \beta\sinh y & \beta\cosh y \end{vmatrix} = 0 \qquad \ldots(24)$$

8) Close observation shows more zeros can be created with middle two columns and outer two columns.

$$C_2 \to (C_2 - \varpi C_3); \qquad C_4 \to \left(C_4 + \frac{\beta}{\alpha}\varpi * C_1\right) \qquad \ldots(25)$$

$$\begin{vmatrix} 0 & 0 & 1 & 0 \\ \alpha\,\varpi & 0 & 0 & 0 \\ \sin x & \cos x - \varpi\cosh y & \cosh y & \sinh y + \dfrac{\beta}{\alpha}\varpi * \sin x \\ -\alpha\cos x & \alpha\sin x - \varpi\beta\sinh y & \beta\sinh y & \beta\cosh y - \beta\varpi * \cos x \end{vmatrix} = 0 \qquad \ldots(26)$$

9) Now we open with element R13

$$\begin{vmatrix} \alpha\,\varpi & 0 & 0 \\ \sin x & \cos x - \varpi\cosh y & \sinh y + \dfrac{\beta}{\alpha}\varpi * \sin x \\ -\alpha\cos x & \alpha\sin x - \varpi\beta\sinh y & \beta\cosh y - \beta\varpi * \cos x \end{vmatrix} = 0 \qquad \ldots(27)$$

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10) Now we open with R11

$$\begin{vmatrix} (\cos x - \varpi \cosh y) & \varpi^* \left(\dfrac{\beta}{\alpha} \sin x + \varpi \sinh y \right) \\ \alpha \sin x - \varpi\beta \sinh y & -\beta\varpi^* (\cos x - \varpi \cosh y) \end{vmatrix} = 0$$

…(28)

11) It is now easy to solve this determinant

$$R_1 \to \alpha R_1 \quad \& \quad C_2 \to C_2 / \varpi^*$$

…(29)

$$\begin{vmatrix} \alpha(\cos x - \varpi \cosh y) & (\beta \sin x + \alpha\varpi \sinh y) \\ \alpha \sin x - \beta\varpi \sinh y & -\beta(\cos x - \varpi \cosh y) \end{vmatrix} = 0$$

…(30)

12) Above determinant reduces to

$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sin x \ \sinh y + \cos x \ \cosh y = \frac{\varpi + \varpi^*}{2} = \cos k(a+b)$$

$$\boxed{\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sin \alpha a \ \sinh \beta b + \cos \alpha a \ \cosh \beta b = \cos k(a+b)}$$

…(31)

This equation KPE is the backbone of band structure formation. In the literature one feels absence of needs (1) to (12) .

III. DISCUSSION AND .CONCLUSION

Thus we have succeeded in solving KP determinant in very elegant and non tedious way. The work is of immense heuristic considerability as we cannot avoid basic mathematical route as saying mere mathematics. In theoretical physics, physics and involved mathematics are treated on equal footings. In prevailing literature I couldn't find full solution of KP model and therefore I decided to accomplish the task. After obtaining Eq. (31), the interpretation of band formation may easily be read in text books like McKelvy or Kittel. This work can also be utilized by mathematicians as a good problem for solving the determinant.

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