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Investigation of bound states and transmission across orderly arranged pairs of attractive and repulsive delta potentials

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ABSTRACT

The pattern of bands generated by the transmission coefficient T for transmission across N ionic molecules in one dimension simulated by N alternating pairs of attractive and repulsive delta potential is studied by exploring its relation with the conditions for the occurence of threshold bound state. The number of peaks in the first band of T is found to be the difference between N and the number of negative energy bound states generated by this potential. Further we systematically study the nature of distribution of peaks in higher bands as a function of potential strength and distance parameters and compare it with the results obtained in our earlier works.

1. Introduction

Bound states, band structures and properties of the transmission coefficient T generated by uniformly spaced Dirac potentials having same strength parameter has been a subject of considerable interest in view of their potential application in modern technology and also in the conceptual understanding of the underlying physical phenomena [1–27]. We refer such potentials as Dirac comb potentials. A given Dirac comb potential may contain only attractive or repulsive delta potential terms. In addition one may construct Dirac comb potential with alternating attractive and repulsive delta terms. Physically speaking an attractive Dirac comb can approximately represent the potential experienced by an electron as it traverses uniformly placed positive ions. Similarly repulsive Dirac comb can approximate the potential between an electron and evenly spaced negative ions. On the other hand the Dirac comb potential having alternating attractive and repulsive delta terms can simulate an ionic crystal in one dimension(1D). Electronic devices also can be constructed to approximately simulate various types of Dirac comb potentials to explore their potential applications.

In recent years we have explored systematically different aspects of physics that can be obtained by solving the Schroedinger equation in 1D for various types of Dirac comb potentials [28–31]. In particular we find that any type of Dirac comb potential having N_a=N attractive terms can generate a maximum of N_a bound states irrespective of the potential strength and spacing between two adjacent delta terms. This prompted us to explore the possibility of determining specific value of potential strength V and a such that a Dirac comb potential generates a specified number of $n \leq N$ bound states. We found that in the case of the above types of Dirac comb potentials having N number of delta terms it is possible to construct Nth order polynomial $D_1(N, g)$ in the dimensionless parameter $g = \lambda Va$ having positive roots g_n, n=1,2,..,N and when $g = g_n$ n bound states get generated and the highest bound state is a threshold bound state. Here λ is a parameter having dimension L introduced to compensate the dimensionality of delta term. Formally the polynomial [28] $D_1(N, g)$ can be expressed as

$$D_1(N, g) = \sum_{n=0}^{N} c_n(N) g^n,$$

We developed a reliable inductive heuristic recursive procedure to determine the coefficients $c_n(N)$ for any N [29]. Subsequently this procedure was suitably generalized in the case of Dirac comb potentials containing alternating attractive and repulsive delta terms. These studies were used to explore the properties of band structure of positive energy states when the delta terms are confined symmetrically inside a 1D box. Further interesting properties of the bands generated by the peaks of T across Dirac comb potentials were also explored. Refs. [28–31] contain an exhaustive description of these results.

In the light of the above it is natural to explore a somewhat more complicated version of the Dirac comb potential which can be expressed as

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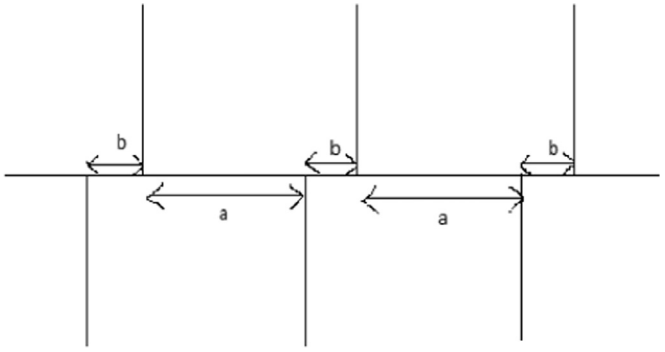

Fig. 1. N=3 alternating pairs of attractive and repulsive delta potentials with distance parameters b and a.

$$U_{\mp}(N, b, a, x) = -\lambda V \sum_{1}^{N} [\delta(x - na - nb + a + b) - \delta(x - nb - na + a))]; V > 0 \quad (1)$$

In Fig. 1 we illustrate this potential for N=3, that is, three pairs of attractive and repulsive delta potentials having same strength parameter. The above defined potential contains N pairs of attractive and repulsive potentials. The parameter b defines the spacing between attractive and repulsive delta terms in the pair and the parameter a represents the spacing between two adjacent pairs. Clearly when a=b, we have the Dirac comb potential explored earlier [28,29]. The present case is interesting because it can simulate in 1D the potential experienced by an electron as it traverses a linear chain of ionic molecules. Unlike the Dirac comb potential explored earlier, the present potential is governed by five parameters namely N, V, λ, a and b. It is natural to expect that in this case also maximum number of negative energy bound states will be N. However the specification of condition for the generation of $n \leq N$ number of bound states is more complicated and is investigated in the present paper. We explore whether it is possible to construct polynomial $D_{\mp}(N, f)$ of a suitably defined dimensionless parameter f such that its roots f_n can provide condition for the occurence of threshold bound state. We show that it is indeed possible to analytically construct polynomials $D_{\mp}(N, f)$ where $f = \lambda^2 V^2 ab$. This is an interesting generalization of the results obtained in reference [28,29] and hence can be used as a starting point for the systematic exploration of band pattern and properties of T generated by $U_{\mp}(N, b, a, x)$.

In Section 2 we obtain the polynomials $D_{\mp}(N, f)$ governing the conditions for the occurence of threshold energy bound state for the potential $U_{\mp}(N, b, a, x)$ in addition to some specific analytical results related to the bound state of $U_{\mp}(2, b, a, x)$ and $U_{\mp}(3, b, a, x)$. In Section 3 we explore the band structure generated by T. Section 4 contains summary and discussions.

2. Condition for the occurence of threshold energy bound state for the potential $U_{\mp}(N, b, a, x)$

Our method starts with the solution of the Schroedinger equation given by

$$-\frac{d^2\phi(x)}{dx^2} + U_{\mp}(N, b, a, x)\phi(x) = E\phi(x), -\infty < x < \infty. \quad (2)$$

to obtain the bound states generated by the potential $U_{\mp}(N, b, a, x)$. For all our calculations we set $\hbar$=2m=1 and as a result V and E have dimensionality L^{-2}. In all our numerical calculations we have set $\lambda = 1$. In general $U_{\mp}(N, b, a, x)$ can have no more than N bound states. However the exact number of bound states that are generated critically depend on parameter λ, V, a and b. In this section we systematically obtain the relations connecting the number of bound states N_b and the potential parameters. In the case of $U_{\mp}(1, b, a, x)$ the solution of the Schroedinger equation for bound state leads to the following equation [28] satisfying the eigenvalue

$$(2z + g)(2z - g) = -exp(-2z)g^2 \quad (3)$$

where $g = \lambda V a$, $z = \alpha a$ and $E = -\alpha^2$. In the limit $z \to 0$ we obtain

$$g^2 = z(2 + g^2) + terms\ with\ higher\ powers\ of\ z.$$

This implies g=0 is the critical value for the occurence of the threshold or zero energy bound state. This means there will be one bound state no matter how small g is. Having obtained this initial result we now explore analytically the threshold condition for bound states systematically for N=2–8. The procedure becomes prohibitively complicated and lengthy as N increases and therefore we give the details of the procedure for N=2 and N=3 only.

When N=2 the potential $U_{\mp}(2, b, a, x)$ assumes the form given by

$$U_{\mp}(2, b, a, x) = -\lambda V\delta(x) + \lambda V\delta(x - b) - \lambda V\delta(x - a - b) + \lambda V\delta(x - a - 2b). \quad (4)$$

The solution of the Schroedinger equation for the above potential in five regions of interest are

$$\varphi = \varphi_1 = A_1 e^{\alpha x}, \quad x \leq 0, \quad (5)$$

$$\varphi = \varphi_2 = A_2 e^{\alpha x} + B_2 e^{-\alpha x}, \quad 0 \leq x \leq b, \quad (6)$$

$$\varphi = \varphi_3 = A_3 e^{\alpha x} + B_3 e^{-\alpha x}, \quad b \leq x \leq a + b, \quad (7)$$

$$\varphi = \varphi_4 = A_4 e^{\alpha x} + B_4 e^{-\alpha x}, \quad a + b \leq x \leq a + 2b, \quad (8)$$

$$\varphi = \varphi_5 = B_5 e^{-\alpha x}, \quad x > a + 2b, \quad (9)$$

At the position of every delta potential term the wave functions and their derivatives have to satisfy the required boundary conditions [28]. For example at x=b

$$\varphi_2|_{b-0} = \varphi_3|_{b+0}$$
$$\frac{d}{dx}\varphi_3|_{x=b+0} - \frac{d}{dx}\varphi_2|_{x=b-0} = \int_{b-0}^{b+0} U_{\mp}(N, b, a, x)\varphi(x)dx = \lambda V\phi_2(b) = \lambda V\phi_3(b)$$

and similar conditions are to be imposed at the position of every delta terms at x=0, b, $a + b$ and $a + 2b$. Imposition of these conditions lead to the following set of 8 homogenous linear algebraic equations satisfied by the unknown coefficients A_i,i=1,2,3,4 and B_i, i=2,3,4,5.

$$A_1 = A_2 + B_2 \quad (10)$$

$$\alpha(A_2 - B_2) - \alpha A_1 = -\lambda V A_1 \quad (11)$$

$$A_2 e^{\alpha b} + B_2 e^{-\alpha b} = A_3 e^{\alpha b} + B_3 e^{-\alpha b} \quad (12)$$

$$\alpha[A_3 e^{\alpha b} - B_3 e^{-\alpha b}] - \alpha[A_2 e^{\alpha b} - B_2 e^{-\alpha b}] = \lambda V[A_2 e^{\alpha b} + B_2 e^{-\alpha b}] \quad (13)$$

$$A_3 e^{\alpha(a+b)} + B_3 e^{-\alpha(a+b)} = A_4 e^{\alpha(a+b)} + B_4 e^{-\alpha(a+b)} \quad (14)$$

$$\alpha[A_4 e^{\alpha(a+b)} - B_4 e^{-\alpha(a+b)}] - \alpha[A_3 e^{\alpha(a+b)} - B_3 e^{-\alpha(a+b)}] = -\lambda V[A_3 e^{\alpha(a+b)} + B_3 e^{-\alpha(a+b)}] \quad (15)$$

$$A_4 e^{\alpha(a+2b)} + B_4 e^{-\alpha(a+2b)} = B_5 e^{-\alpha(a+2b)} \quad (16)$$

$$-\alpha[A_4 e^{\alpha(a+2b)} - B_4 e^{-\alpha(a+2b)}] - \alpha B_5 e^{-\alpha(a+2b)} = \lambda V B_5 e^{-\alpha(a+2b)} \quad (17)$$

The admissible values of α for which non trivial solution of the above equations is possible are obtained by equating the appropriate determinant formed by the coefficients A_i and B_i to be equal to zero. Careful simplification of the determinant leads to the following equation:

$$[16b(\lambda V)^2 - 8ab^2(\lambda V)^4] + terms\ containing\ powers\ of\ \alpha^m, m \geq 1. \quad (18)$$

This implies that in order to have threshold energy bound state($\alpha \to 0$) following condition is to be satisfied:

$$16b(\lambda V)^2 - 8ab^2(\lambda V)^4 = 0. \quad (19)$$

In terms of the parameter $g = \lambda V a$ and $\eta = b/a$, the above equation

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