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Band structures in transmission coefficients generated by Dirac comb potentials

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ABSTRACT

Using the threshold conditions and bound state energies investigated earlier by us as a critical input we systematically study the nature of band formation in the transmission coefficient generated by Dirac comb potentials having equispaced (i) attractive, (ii) repulsive and (iii) alternating attractive and repulsive delta terms having same strength and confined within a fixed range. We find that positions of the peaks of transmission coefficient generated by a combination of one attractive and one repulsive delta terms having same strength and separated by gap a is independent of the potential strength and coincide with the energy eigenvalues of 1D box of range a. We further study analytically and numerically the transmission across Dirac comb potentials containing two or three delta terms and these results are useful in the analysis of the transmission in the general case. In the case of Dirac comb potentials containing N_a attractive delta terms we find that the nature of the first band and higher bands of the transmission coefficient are different, and if such a potential generates N_b number of bound states, the first band in the transmission coefficient generated by the potential has $N_{T1} = N_a - N_b$ peaks. In the case of higher bands generated by delta comb potential having N delta terms each band has $N-1$ peaks. Further we systematically study the behavior of band gaps and band spread as a function of potential strength and number of terms in the Dirac comb. The results obtained by us provide a relation between bound state spectrum, number of delta terms in the Dirac comb and the band pattern which can be explored for potential applications.

1. Introduction

The study of Schrodinger equation governed by an array of delta function potential provides a simple basis to initiate the investigation of several problems in solid state physics. The well-known Kronig–Penney model using delta function potentials provides a simple picture for band formation in solids [1]. Locally periodic one dimensional array of potentials is useful in the study of lattices in the crystal and localization of different types of disorders in lattices [2–5]. They are useful to explore the effect of impurities in solids [6–10]. The study of transmission across these potentials is of considerable interest because it is helpful in the calculation of transport of electrons through nanostructures [11], conducting polymers [12], metals, semiconductors [13] and quantum wires [14,15]. Tsu and Esaki [16] being pioneers in this field studied the transport in terms of resonant transmission in a finite superlattice. Transmission properties of delta potentials also find application in the field of acoustics [17] and optics [18]. As a consequence there is a continued interest in the spectral and transmission properties generated by an array of delta potentials [19–26]. In this paper we focus on some novel features generated in the transmission coefficient for different types of arrays of locally periodic delta potentials. Our work has potential applications in the study of periodic structures like quantum wires with serial stubs and even disordered structure with defective stubs, tunneling of Bose–Einstein condensates [28] and different kinds of lattices [27]. Various mesoscopic structures, heterostructures and ballistic transport of electrons through carbon nanotubes can also be studied.

The present work is in a sense, a continuation of our systematic quantum mechanical study of threshold conditions, bound states, spectral properties and band structure generated by the array of delta potentials [29–31]. The types of Dirac comb potentials that we use to investigate transmission properties are:

$$U_{+}(N, a_N, x) = \lambda V \sum_{n=1}^{N} \delta(x - na_N), \quad V > 0, \quad a_N = a/(N-1), \quad N \geq 2, \tag{1}$$

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$$U_{-}(N, a_N, x) = -\lambda V \sum_{n=1}^{N} \delta(x - na_N), \quad V > 0, \quad a_N = a/(N-1), \quad N \geq 2, \tag{2}$$

$$U_{\mp}(N, a_N, x) = \lambda V \sum_{n=1}^{N} (-1)^n \delta(x - na_N), \quad V > 0, \quad a_N = a/(N-1), \quad N \geq 2, \tag{3}$$

$$U_{\pm}(N, a_N, x) = -U_{\mp}(N, a_N, x). \tag{4}$$

Clearly the parameter a represents the spread of the Dirac comb potentials listed above. $U_{+}(N, a_N, x)$ and $U_{-}(N, a_N, x)$ represent repulsive and attractive Dirac comb potentials containing N terms respectively. Similarly, when N is even $U_{\mp}(N, a_N, x)$ and $U_{\pm}(N, a_N, x)$ represent the Dirac comb potentials having $N/2$ pairs of delta function terms with alternating signs. On the other hand, when N is odd, unpaired last term in $U_{\mp}(N, a_N, x)$ and $U_{\pm}(N, a_N, x)$ is an attractive or repulsive delta term potential respectively. The parameter λ used above has the dimensionality of length. In the present paper we use the system of units in which $\hbar = 1$ and $2m=1$. Hence the potential strength parameter V and energy E has the dimensionality of L^{-2}. As a consequence the numerical results reported in this paper for V and E are in L^{-2} unit. They can be converted to more convenient units when mass m is specified. For example, in the case of electron $E(\text{eV}) = 0.03816\,(\text{nm}^{-2})$. In our earlier work [29,30] we have comprehensively studied the bound state spectrum, threshold conditions and density of states generated by the above potentials and in [31] we have further examined systematically the band formation in the positive energy region generated by the above defined potentials when they are confined within a box. Our approach unearths a set of new interesting features present in the transmission coefficient generated by the above potentials and these are complementary to the results reported in earlier works [19–26] in the same broad area.

In order to understand the pattern of bands generated in the transmission coefficient generated by the above potential for general N, it is useful to fully explore analytically and numerically the transmission coefficient generated by these potentials when they contain 2 or 3 delta terms. Hence, in Section 2 we explore analytically and numerically several features of the transmission co-efficient across two delta function potentials, both of which may be attractive, repulsive or a combination of attractive and repulsive delta potentials. In Section 3 we similarly explore transmission across three delta function potentials. Using the results obtained in these cases the pattern of behavior of transmission coefficient for general $N > 3$ is studied in Section 4. Section 5 contains a comprehensive summary of main results and conclusions.

2. Transmission across two delta function potentials

Let us first consider transmission in one dimension across a sum of two delta function potentials given by

$$U(x) = \lambda_1 V_1 \delta(x - a) + \lambda_2 V_2 \delta(x - 2a) \tag{5}$$

Here λ_1 and λ_2 are parameters having dimension of length to compensate the dimensionality of delta terms. In this paper we choose $\lambda_1 = \lambda_2 = \lambda = 1$. V_1 and V_2 are potential strength parameters, but our main focus is when $|V_1| = |V_2| = |V|$. Using the symbols $k^2 = E$ and the time independent Schrödinger equation governed by $U(x)$ takes the form

$$\left[\frac{d^2}{dx^2} + k^2 - \lambda_1 V_1 \delta(x - a) - \lambda_2 V_2 \delta(x - 2a)\right]\phi(x) = 0 \tag{6}$$

In the case of transmission, the solution of (6) has the general form given by

$$\varphi = \varphi_1 = A_1 e^{ikx} + B_1 e^{-ikx}, \quad x < a, \tag{7}$$

$$\varphi = \varphi_2 = A_2 e^{ikx} + B_2 e^{-ikx}, \quad a < x < 2a, \tag{8}$$

$$\varphi = \varphi_3 = A_3 e^{ikx} + B_3 e^{-ikx}, \quad x > 2a. \tag{9}$$

The terms $T = |A_3/A_1|^2$ and $R = |B_1/A_1|^2 = |B_1/A_3|^2 \times T$ define the transmission and reflection coefficients respectively and $B_3 = 0$.

The wave function is continuous at $x = a$ and at $x = 2a$, but their derivatives are discontinuous due to the delta potential terms [29]. We solve the Schrödinger equation taking this in to account as described in Refs. [29,30] and obtain the following expression for T and R.

$$T = 16k^4[(\lambda^2 V_1^2 + 4k^2)(\lambda^2 V_2^2 + 4k^2) + \lambda^4 V_1^2 V_2^2 + 2\lambda^2 V_1 V_2 \cos(2ka)(4k^2 - \lambda^2 V_1 V_2) + 4k\lambda^3 V_1 V_2 (V_1 + V_2)\sin(2ka)]^{-1} \tag{10}$$

$$R = [(\lambda^2 V_1^2(\lambda^2 V_2^2 + 4k^2)) + \lambda^2 V_1^2(\lambda^2 V_2^2 + 4k^2) + \lambda^4 V_1^2 V_2^2 + 2\lambda^2 V_1 V_2 \cos(2ka)((4k^2 - \lambda^2 V_1 V_2) + 4k\lambda^4 V_1^2 V_2^2 \sin(2ka))/16k^4] \times T = 1 - T \tag{11}$$

Now let us explore the nature of variation of T as a function of $E = k^2$ in three different cases:

i. when both delta terms are repulsive, i.e., $V_1 = V_2 = V > 0$;
ii. when both delta terms are attractive $V_1 = V_2 = -V < 0$;
iii. when first delta term is attractive and second one is repulsive, i.e., $-V_1 = V_2 = V > 0$.

The case (iii) indicated above is more interesting. In this case the explicit expression for T and R are:

$$T = 16k^4[(\lambda^2 V^2 + 4k^2)^2 + \lambda^4 V^4 - 2\lambda^2 V^2 \cos(2ka)(4k^2 + \lambda^2 V^2)]^{-1} \tag{12}$$

$$R = [(2\lambda^2 V^2(\lambda^2 V^2 + 4k^2) - 2\lambda^2 V^2 \cos(2ka)(4k^2 + \lambda^2 V^2))/16k^4] \times T = 1 - T \tag{13}$$

In Fig. 1 we depict the variation of T as a function of $E = k^2$ in all the above three cases when $|V| = 30$. It is clear that at the peak positions $T=1$ in all cases, indicating that reflectionless transmission occurs at energies where transmission peaks. Interestingly in case (iii) when $-V_1 = V_2 = |V|$, the positions of the transmission peaks k_n^2 are given by

$$k_n^2 = n^2\pi^2/a^2, \quad n = 1, 2\ldots \tag{14}$$

and these are independent of potential strength $|V|$. One can analytically verify the validity of this result by noting that in Eq. (11) when $-V_1 = V_2 = |V|$ and $ka = n\pi$ we get $R=0$. The energies k_n^2 are nothing but the energy eigenvalues of one dimensional box of range a. This feature does not hold true in cases (i) and (ii) referred above. However, one expects that in between two peaks, the variation of transmission coefficient is $|V|$ dependent. In Fig. 2 we illustrate this by choosing two different values of $|V|$, having magnitudes $|V|=30$ and $|V|=5$. When we choose a lesser value of $|V|$, expectedly, transmission coefficient is closer to unity over the entire energy range.

In Figs. 3 and 4 we show the variation of the transmission peak energy E_p as a function of sequence number p of the transmission