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Threshold conditions, energy spectrum and bands generated by locally periodic Dirac comb potentials

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ABSTRACT

We derive expressions for polynomials governing the threshold conditions for different types of locally periodic Dirac comb potentials comprising of attractive and combination of attractive and repulsive delta potential terms confined symmetrically inside a one dimensional box of fixed length. The roots of these polynomials specify the conditions on the potential parameters in order to generate threshold energy bound states. The mathematical and numerical methods used by us were first formulated in our earlier works and it is also very briefly summarized in this paper. We report a number of mathematical results pertaining to the threshold conditions and these are useful in controlling the number of negative energy states as desired. We further demonstrate the correlation between the distribution of roots of these polynomials and negative energy eigenvalues. Using these results as basis, we investigate the energy bands in the positive energy spectrum for the above specified Dirac comb potentials and also for the corresponding repulsive case. In the case of attractive Dirac comb the base energy of the each band excluding the first band coincides with specific eigenvalue of the confining box whereas in the repulsive case it coincides with the band top. We deduce systematic correlation between band gaps, band spreads and box eigenvalues and explain the physical reason for the vanishing of band pattern at higher energies. In the case of Dirac comb comprising of orderly arranged attractive and repulsive delta potentials, specific box eigenvalues occur in the middle of each band excluding the first band. From our study we find that by controlling the number and strength parameters of delta terms in the Dirac comb and the size of confining box it is possible to generate desired types of band formations. We believe the results from our systematic analysis are useful and relevant in the study of various one dimensional systems of physical interest in areas like nanoscience.

1. Introduction

The knowledge of electronic band structure, being the signature of solid state physics is important in understanding the theory of conduction, insulation and several other properties of solids [1,2]. With the multi-faceted advances in nanosciences, in recent years there is revival of interest in exploring the properties and physical features generated by locally periodic array of finite number of atoms and molecules leading to band formation. This is useful in understanding the transition from quantal to macroscopic domain. In particular, the transition from the well separated discrete energy spectrum to band formation [3–9] with increase in the number of atoms in the array and its dependence on the potential parameters identified with the atoms shows several interesting features. Behera et al. [8] have carried out model calculations on eigenvalue spectrum and band formation in one dimension using delta function potentials [10] to represent atoms or molecules. Their numerical calculations focus on the band structures and the energy density distributions generated by locally confined delta potentials in one dimension (1D). In this paper our motivation is to systematically correlate several interesting basic features inherent in the quantum mechanics of such locally periodic delta potentials. Some of these are: exploring (i) the correlation between the number of delta potentials and the number of eigenvalues in a given positive energy band and the pattern of the band structure generated by the attractive and corresponding repulsive potential, (ii) the role played by the negative energy states and threshold conditions governing the band structure and (iii) interconnection between band gap, band spread and the size of the 1D box containing the delta potentials and to carry out a comparative study of several types of locally periodic potentials in a free 1D space and confined inside a 1D box. We believe the theory and calculations described in this paper can be useful in the study of novel 1D systems and in the exploration of

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the physics of finite number of suitably arranged atoms or molecules. Refs. [11–18] provide an additional representative list of work carried out in this area using delta potentials. In order to visualize the scope and approach taken in this paper, we provide some details of the recent results obtained by us [17,18] since they form the general frame work for the present study. In Refs. [17,18] we have investigated the spectrum and threshold conditions generated by locally periodic sum of delta function potentials $U(p, a, x)$ having same strength parameter V:

$$U(p, a, x) = \sum_{n=1}^{p} \lambda V \epsilon_n \delta(x - an), \quad a > 0. \tag{1}$$

Here λ is a parameter having dimension of length introduced to compensate the dimensionality of $\delta(x - na)$. We have assumed λ to be of unit length and ϵ_n is a dimensionless parameter useful to generate different patterns of $U(p, a, x)$. We use the system of unit in which $\hbar = 1$ and $2m = 1$ such that U and energy E have dimensionality L^{-2}. The numerical data reported in this paper for eigenvalues have a dimension of L^{-2}. They can be converted to the corresponding values in more common unit when mass m and unit of length are specified. For example, in the case of electron $E(eV) = 0.03816E$ (nm^{-2}). The separation between two adjacent delta potentials is a. In Table 1 we list different types of $U(p, a, x)$ studied earlier [17,18] and identify them in this paper with appropriate symbols. In particular $U_{>-}(N, a, x)$ is defined in the half line $x > 0$ with an infinitely high wall at $x=0$. In our earlier work [17,18] this potential was indicated by the symbol $U(N, r)$ and was used to explore the s wave bound states in three dimensions (3D). For all practical purposes quantal 1D problem specified above in half line $x > 0$ and the corresponding s wave problem in 3D are equivalent. The potential $U_{\mp}(p, a, x)$ obtained by setting $\epsilon_n = (-1)^n$ is a sequence of alternating attractive and repulsive delta potentials; when p is odd the last attractive delta term is not followed by a repulsive term. One of the main results [17] is the explicit construction of polynomials $D_1(N, g)$ and $D_3(N, g)$ corresponding to $U_{-}(N, a, x)$ and $U_{>-}(N, a, x)$ in the dimensionless variable $g = \lambda Va$. The positive roots $g_1, g_2, \ldots, g_N$ of these polynomials in increasing order give the combination of potential parameters needed to generate a threshold or zero energy bound states. It was demonstrated that when N is sufficiently large the variation of these roots g_n of $D_1(N, g)$ or $D_3(N, g)$ as a function of n has a behavior similar of that of Fermi function. In the case of $D_1(N, g)$ and $D_3(N, g)$, as N becomes large the largest root $g_N \to 4$ and the smallest positive definite root tend to zero. In the case of $U_{\mp}(2N, a, x)$, $U_{\mp}(2N-1, a, x)$, the corresponding polynomials governing the threshold conditions are $D_{\mp}(2N, g)$, $D_{\mp}(2N-1, g)$ and each has N non-negative roots $g_1, g_2, \ldots, g_N$. In this case $g_N \to 2$ and the smallest positive definite root tend to 0 as N becomes large. Salient features of $U_{-}(N, a, x)$, $U_{>-}(N, a, x)$, $U_{\mp}(2N, a, x)$, $U_{\mp}(2N+1, a, x)$ and corresponding polynomials are listed in Table 1. We observe that the order of threshold polynomial is same as the number of delta potential terms in the corresponding potential. Further we find that the number of attractive delta terms in the given potential gives the upper bound for the number of bound states with $E \le 0$. When g exceeds the limiting value stated above, all N bound states get generated. When $\lambda Va = g_n$, n number of $E \le 0$ eigenvalues will be generated and highest eigenvalue $E_n=0$. This shows that using the roots g_n we can fix the potential parameters to generate a desired number of $E \le 0$ eigenvalues. As a consequence of approximate Fermi function behavior of g_n as a function of n, negative energy eigenvalue tends to group more densely at either end of the spectrum having eigenvalues $E_n \le 0$.

In the light of the results summarized above, in this paper we investigate the threshold conditions, negative energy bound states

Table 1

Different types of locally periodic sum of Dirac potentials with fixed separation parameter a investigated [17,18] using the basic expression $U(p, a, x) = \sum_{n=1}^{p} \lambda V \epsilon_n \delta(x - an)$ along with the related information needed to calculate the bound states and threshold energy conditions. The coefficient $c_n(N)$ occurring in the last column can be computed recursively as described in our earlier work [18].

Locally periodic sum of Dirac potentials	Remarks	Boundary conditions on φ for bound states (see Eqs. (4)–(6))	Polynomial governing the generation of threshold bound state
$U_{+}(N, a, x) = U(N, a, x)$ $\epsilon_n = 1$, $\lvert x \rvert < \infty$	Repulsive case	No bound states	Not applicable
$U_{-}(N, a, x) = U(N, a, x)$ $\epsilon_n = -1$, $\lvert x \rvert < \infty$	Attractive case	$\varphi(-\infty) = 0$, $\varphi(\infty) = 0$, $B_1 = 0$, $A_{N+1} = 0$ $E < 0$	$D_1(N, g) = \sum_{n=0}^{N} c_n(N) g^n$, $g = \lambda Va$ The roots g_n are within the domain (0,4)
$U_{>-}(N, a, x) = U(N, a, x)$, $x > 0$ $=\infty$, $x \le 0$	Attractive case defined in the half line $x > 0$	$\varphi(0) = 0$, $\varphi(\infty) = 0$, $B_1 = -A_1$, $A_{N+1} = 0$, $E < 0$	$D_3(N, g) = \sum_{n=0}^{N} d_n(N) g^n$, $g = \lambda Va$ The roots g_n are within the domain (0,4)
$U_{\mp}(2N, a, x) = U(2N, a, x)$ $\epsilon_n = (-1)^n$, $\lvert x \rvert < \infty$	Sequence of attractive and repulsive delta potentials	$\varphi(-\infty) = 0$, $\varphi(\infty) = 0$, $B_1 = 0$, $A_{N+1} = 0$, $E < 0$	$D_{1\mp}(2N, g) = \sum_{n=0}^{N} c_n^{\mp}(2N) g^{2n}$, $g = \lambda Va$, $c_n^{\mp}(2N) = c_n(N)$ The positive roots g_n^{+} are within the domain (0,2)
$U_{\mp}(2N+1, a, x)$ $= U(2N+1, a, x)$ $\epsilon_n = (-1)^n$, $\lvert x \rvert < \infty$	Sequence of attractive and repulsive delta potentials having last attractive term unpaired	$\varphi(-\infty) = 0$, $\varphi(\infty) = 0$, $B_1 = 0$, $A_{N+1} = 0$, $E < 0$	$D_{1\mp}(2N+1, g) = g \sum_{n=0}^{N} d_n^{\mp}(2N+1) g^{2n}$, $g = \lambda Va$, $d_n^{\mp}(2N+1) = d_n(N)$ The positive roots g_n^{+} are within the domain (0,2)