Tunneling through a one-dimensional piecewise constant potential barrier—Illustrated with a non-uniform multi-barrier system and the genesis of the `Alias Effect`

Siddhant Das
Electronics and Communication Engineering, National Institute of Technology, Tiruchirappalli, TN, India.
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In this paper we look at transmission through one-dimensional potential barriers that are piecewise constant. The Transfer Matrix approach is adopted and a new formula is derived for multiplying long matrix sequences that not only leads to an elegant representation of the wave function, but also results in much faster computation than earlier methods. The proposed method covers a broad spectrum of potentials of which multi-barrier systems are special cases. The paradigm is exemplified with a finite lattice of non-uniform rectangular barriers—non-uniformity being crucial, as the uniform case has been solved exactly by Griffiths and Steinke. For the non-uniform multi-barrier problem, the intervening wells strongly influence the transmission probability. Surprisingly, we find that the wells act ‘individually’, i.e. their influence is only a function of their width and is independent of their exact ‘location’ in a multi-barrier system. This leads to a startling observation, which we have termed as the ‘Alias Effect’. The exact solutions are supported with asymptotic formulas.

Keywords: Piecewise Constant Potential, Resonant Multi-Barrier Tunneling, Transfer Matrix, Transmission Coefficient, Alias Effect

I. INTRODUCTION

Tunneling of particles is a ubiquitous quantum phenomenon that gained lot of interest since its conception (by Hund) and is a subject of intense study even today. Many queer properties of matter can be understood based on the tunneling characteristics of charge carriers—for instance the emergence of band structure in solids. Moreover, tunneling in scanning tunneling microscopy, tunneling magnetic resistance, Josephson tunneling and many other physical phenomena rest directly on the transmission of particles through quantum barriers. It is rather difficult to obtain exact solutions of the Schrödinger equation for arbitrary potentials which are of general interest. Thus one must consider the problems on a case by case basis. In this paper we look at a wide class of potential barriers that are piecewise constant. A piecewise constant potential barrier is discontinuous at one or more points. We will make the potential geometry more precise later.

The motivation for this study is twofold. First of all some potentials that arise in applications in condensed matter theory are special cases of this problem. For instance the analysis of semi-conductor super lattices by Tsu and Esaki was founded on a uniform multiple rectangular barrier model. A finite lattice of rectangular barriers is one of the simplest examples of a piecewise constant potential barrier. Although this problem was taken up by many researchers who presented analytic solutions that analytic solutions can seldom be found. However the continuous potential can always be approximated to any level of accuracy as a sequence of flat steps. The resulting potential falls under the purview of the present class of problems, which can be solved exactly. The accuracy of these ‘step solutions’ can be made arbitrarily good by choosing finer and finer partitions. Thus it is worthwhile to consider a piecewise constant potential barrier.

In the following section we formulate the problem precisely. By adopting the transfer matrix approach an explicit formula for multiplication of arbitrarily long matrix sequences is derived, thus obtaining the transmission characteristics of the potential exactly. This forms the central part of the paper. In Section III the uniform multi-barrier is revisited and the role of asymmetry is demonstrated. The multi-barrier Alias Effect is introduced and illustrated with examples in Section III A. We conclude the analysis in Section IV, outlining prospects of further study.

II. PROBLEM FORMULATION

Figure 1 depicts a schematic piecewise constant potential barrier that requires the specification of two real valued sequences for its definition. These are denoted by \(\{x_j\}_{j=0}^{N+1}\) and \(\{V_j\}_{j=0}^{N+1}\), where \(N\) is the number of jump discontinuities of the potential barrier. \(\{x_j\}\) must be an increasing sequence. In the following discussion \(j\) runs from 1 to \(N+1\) unless otherwise stated.

For consistency of notation we choose \(x_j\) on the extended real line and require \(x_0 = -\infty\) and \(x_{N+1} = +\infty\). For a localized barrier we let \(V_j = V_{N+1} = 0\). The potential \(V(x)\) can be written as,

\[
V(x) = V_j, \quad x_{j-1} < x < x_j, \quad (1)
\]

...
These amplitudes are collected in the ket $|\theta_j \rangle$.

$$|\theta_j \rangle \equiv \left( \begin{array}{c} A_j \\ B_j \end{array} \right).$$  

(5)

For the problem under consideration there exist $N + 1$ tessellations of the real axis given by the intervals $x_{j-1} < x < x_j$, $j = 1, 2, \ldots, N + 1$. In each region $\psi$ is defined by equation (4) up to two undetermined constants—a total of $2N + 2$ constants. We are essentially looking at the transmission problem. Hence we assume that the particle is incident from left. This input fixes one of the constants by requiring $B_{N+1} = 0$ (since there is no reflector at $+\infty$).

It now remains to determine the $2N + 1$ constants. Any $2N$ of these can be uniquely expressed in terms of the other amplitude by necessitating that the wave function and its derivative be continuous at the discontinuities of $V(x)$. This also satisfies the equation of continuity. For illustrating the solution we choose $A_{N+1}$ to be the independent amplitude (in terms of which others are expressed) and this must be specified through an initial condition $\Psi(x, 0) = \psi(x)e^{-i\mathcal{H}t}|_{t=0}$, for instance).

The required smoothness of the wave function is guaranteed by

$$\frac{d\psi_j}{dx} = \frac{d\psi_{j+1}}{dx} \bigg|_{x=x_j}, \quad j = 1, 2, \ldots, N. \quad (6)$$

Equation (6) translates into

$$|\theta_j \rangle = M_j |\theta_{j+1} \rangle, \quad (7)$$

where

$$M_j = \frac{1}{2\kappa_j} \begin{pmatrix} (k_j + k_{j+1})e^{(k_j+k_{j+1})x_j} & (\kappa_j - k_{j+1})e^{i(k_j+k_{j+1})x_j} \\ (k_j - k_{j+1})e^{-(k_j+k_{j+1})x_j} & (\kappa_j + k_{j+1})e^{-i(k_j+k_{j+1})x_j} \end{pmatrix}. \quad (8)$$

Figure 1 labels the regions of constant potential by Roman numerals. In these regions the Time Independent Schrödinger Equation has to be solved independently to yield the wave function $\psi(x)$, which is defined piecewise,

$$\psi(x) = \psi_j(x), \quad x_{j-1} < x < x_j, \quad (2)$$

where the $\psi_j$s satisfy

$$\psi_j^{''} + \kappa_j^2 \psi_j = 0, \quad \kappa_j^2 = \frac{2\Re(E - V_j)}{\hbar^2}, \quad (3)$$

$\Re$ is the mass of the particle with energy $E$. Equation (3) admits general solutions of the form

$$\psi_j = A_j e^{i\kappa_j x} + B_j e^{-i\kappa_j x}. \quad (4)$$

$A_j$ and $B_j$ are the probability amplitudes for the forward and backward travelling wave components respectively.

$M_j$s are known as the transfer matrices.\textsuperscript{5,10} Note that $M_j$ is nonsingular for all $j$ (except when $E = V_{j+1}$) with a determinant $\Delta_j = 2\kappa_j$. Moreover for $E = V_j$ (possibly for more than one $j$), $\kappa_j = 0$ and $M_j$ becomes indeterminate. We handle this case separately at the end of the section. The transfer matrices are rather special and are endowed with strong algebraic properties which are ramifications of the continuity equation. We will return to this point later. By iterating equation (7), we express $|\theta_j \rangle$ in terms of $|\theta_{N+1} \rangle = \left( \begin{array}{c} A_{N+1} \\ 0 \end{array} \right)$.

$$|\theta_j \rangle = M_j M_{j+1} \cdots M_N |\theta_{N+1} \rangle. \quad (9)$$

Computation of the matrix product sequence in equation (9) poses a formidable challenge, especially when $N$ is large. If all the $M_j$s were identical (which is the case for a uniform multi-barrier system), the product in equation (9) reduces to a power, which can be calculated using well defined prescriptions. Griffiths and Steinke have exploited this advantage of the uniform multi-barrier problem. However (in general) all $M_j$s would be different and a unified method must be outlined to efficiently handle long matrix product sequences. We overcome this problem by using an alternative representation for the $M_j$s and then deriving a formula for the matrix product.

Any $2 \times 2$ complex valued matrix can be uniquely expressed as a linear combination of the three Pauli matrices and the identity matrix, which collectively span $\mathbb{C}^{2 \times 2}$. They are listed below.

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (10)$$

FIG. 1. $V(x)$ for an arbitrary piecewise constant potential barrier with $N$ jump discontinuities.
The collection \( \{ \sigma_p \} \) is the Pauli basis. Now,

\[
M_j = \sum_p c^p_j \sigma_p, \quad c^p_j = \frac{1}{2} \text{trace } (M_j \sigma_p). \tag{11}
\]

In this form \( M_j \) is identified as a Pauli Vector. The subscript \( j \) in the scalar \( c^p_j \) denotes the order of the transfer matrix while the superscript is identified with the index of the basis element it is multiplied with. In all the summations that follow the index runs over 0, 1, 2, 3 unless otherwise stated. It can be shown that the product of two transfer matrices,

\[
M_j M_k = \left( \sum_p c^p_j \sigma_p \right) \left( \sum_q c^q_k \sigma_q \right) = \sum_p \sum_q c^p_j c^q_k \phi(p,q) (i)^{\kappa_{pq}\phi(p,q)} \tag{12}
\]

where,

\[
\phi(a,b) = (a + b (1)^{a+b-1}) \mod 4 \tag{13}
\]

\[
\varepsilon_{abc} = \frac{1}{2} (a - b) (b - c) (c - a). \tag{14}
\]

Equation (12) results from expanding the bracketed pair and injecting the product identities of the Pauli matrices. \( \varepsilon_{abc} \) is the Levi-Civita Symbol (or permutation symbol) which along with \( \phi(a,b) \) preserves the non-commutativity of matrix multiplication. Equation (12) expresses \( M_j M_k \) in the form of equation (11), which is a distinctive advantage since matrix products get expressed as linear combinations of simple matrices. We use induction to obtain a Pauli Vector representation for the matrix product sequence appearing in equation (9). In the following discussion the summation indices are augmented with an additional subscript for the sake of clarity. The recipe holds good for multiplying arbitrary \( 2 \times 2 \) matrices (not necessarily transfer matrices). We illustrate the inductive construction by multiplying \( m \) matrices \( \{ T_j \in \mathbb{C}^{2 \times 2} \}_{j=1}^m \) beginning with \( T_1 \),

\[
T_1 = \sum_{p_1} \sigma_{p_1} c^p_{11}
\]

\[
T_1 T_2 = \sum_{p_2} \sigma_{p_2} c^p_{12} = \sum_{p_2} \sigma_{p_2} \sum_{q_1} c^q_{12} \phi(p_2,q_1) (i)^{\kappa_{12}\phi(p_2,q_1)}
\]

\[
(T_1 T_2) T_3 = \sum_{p_3} \sigma_{p_3} c^p_{13} = \sum_{p_3} \sigma_{p_3} \sum_{q_2} c^q_{13} \phi(p_3,q_2) (i)^{\kappa_{13}\phi(p_3,q_2)}
\]

\[
= \sum_{p_3} \sum_{q_2} \sum_{q_1} c^q_{12} \phi(q_1,q_2) (i)^{\kappa_{12}\phi(q_1,q_2)} + \sum_{p_3} \sum_{q_2} \sum_{q_1} \phi(p,q_1) (i)^{\kappa_{12}\phi(p,q_1)}
\]

setting \( q_0 \overset{\text{def}}{=} 0 \) and noting that \( q_1 = \phi(q_1,0) = \phi(q_1, q_0) \), the general formula can be written as

\[
T_1 T_2 \cdots T_{m-1} T_m = \sum_{p_m} \sum_{q_{m-1}} \sum_{q_{m-2}} \cdots \sum_{q_3} \sum_{q_2} \sum_{q_1} \prod_{j=1}^{m-1} \left( c^p_{j} \phi(q_j,q_{j-1}) (i)^{\kappa_{j,q_{j-1}+\phi(q_j,q_{j-1})}} \right) c^p_{m} (i)^{\kappa_{m,q_{m-1}+\phi(q_{m},q_{m-1})}}. \tag{15}
\]

It must be stated that the representation depicted above is not unique. For instance, in calculating the product of four matrices one can use associativity to multiply two of these in two pairs and use equation (12) to compose the resulting pair—in which case a different form would result involving higher compositions of \( \varepsilon_{abc} \) and \( \phi(a,b) \). Naturally, these are equivalent representations. However we chose the form given in equation (15) for its compact representability and ease of computation. Note that in equation (15) except for the outer most summation, the inner multiple summations are scalars. Although the computational power of equation (15) is not readily apparent, it can be used to solve the problem for any \( N \) in a reasonable time. It will also turn out to be a useful
At this point we address a problem that arises when injecting equation (17) in equation (2) gives equation (18). These are defined as

\[ M_j M_{j+1} M_{j+2} \ldots M_{N-1} M_N = \sum_p \mu_p^j \sigma_p, \quad (16) \]

where the \( \mu_p^j \)'s can be readily obtained using the above prescription. The set of transfer matrices \( \{ M_j \}_{j=1}^N \) is independent of initial conditions, and is completely specified by the barrier parameters and particle energy, through equation (8). Thus we have uniquely expressed every \( |\theta_j \rangle \) in terms of \( |\theta_{N+1} \rangle = A_{N+1} |+ \rangle \), where \( |+ \rangle = \left( \begin{array}{c} 1 \\ 0 \end{array} \right) \) and \( |- \rangle = \left( \begin{array}{c} 0 \\ 1 \end{array} \right) \). With equation (9), (16) and an initial condition, \( \psi(x) \) is pinned down uniquely. And equation (4) can be rewritten as

\[
\psi_j(x) = (-|\sigma_p \rangle e^{i\kappa_j x} + |\sigma_p \rangle e^{-i\kappa_j x}) \left( \prod_{l=j}^N M_l \right) |\theta_{N+1} \rangle e^{i\kappa_j x} \\
= (+ |\sigma_p \rangle e^{i\kappa_j x} - |\sigma_p \rangle e^{-i\kappa_j x}) \left( \sum_p \mu_p^j \sigma_p \right) |\theta_{N+1} \rangle e^{i\kappa_j x} + (-|\sigma_p \rangle e^{i\kappa_j x} + |\sigma_p \rangle e^{-i\kappa_j x}) \left( \sum_p \mu_p^j \sigma_p \right) |\theta_{N+1} \rangle e^{i\kappa_j x} \\
= A_{N+1} \sum_p \mu_p^j \left( (+ |\sigma_p \rangle e^{i\kappa_j x} + (+ |\sigma_p \rangle e^{-i\kappa_j x}) \right) \\
= (\mu_j^0 + \mu_j^3) A_{N+1} e^{i\kappa_j x} + (\mu_j^3 + i\mu_j^2) A_{N+1} e^{-i\kappa_j x}. \quad (17)
\]

Injecting equation (17) in equation (2) gives

\[
\psi(x) = (\mu_j^0 + \mu_j^3) A_{N+1} e^{i\kappa_j x} + (\mu_j^3 + i\mu_j^2) A_{N+1} e^{-i\kappa_j x}, \quad x_{j-1} < x < x_j, \quad j = 1, 2, \ldots, N+1. \quad (18)
\]

At this point we address a problem that arises when \( \kappa_j = 0 \) in equation (8). Note that this occurs when \( E = V_j \) and equation (3) leads to solutions of the form \( \psi_j = A_j x + B_j \) (not exponentials). Using these in equation (6) gives the correct transfer matrices and the subsequent procedure is same as before. The transmission and reflection coefficients can be readily calculated from equation (18). These are defined as

\[
T = \left| \frac{A_{N+1}}{A_1} \right|^2, \quad R = \left| \frac{B_1}{A_1} \right|^2. \quad (19)
\]

The choice of letting \( A_{N+1} \) be the independent undetermined constant was made considering the form of equation (19). Also note that these coefficients are independent of the initial condition \( A_{N+1} \). Thus the complete set of transfer matrices uniquely determines the transmissibility of the potential barrier. Quite independent of the barrier geometry, an important identity follows from the equation of continuity for the probability current density:

\[
T + R = 1. \quad (12)
\]

The satisfaction of this identity constrains the individual transfer matrices, inducing strong algebraic properties amidst its elements. Conversely, the matrices that satisfy these properties can only be transfer matrices for some tunneling problem. Griffiths and Steinke have derived some of these properties in their paper.\(^6\) Merzbacher also discusses these properties in his book.\(^10\) These authors discuss the properties possessed by individual transfer matrices. However, one important fact deserves appreciation. The ‘local’ algebraic constraints amidst the elements of the individual transfer matrices \( \{ M_j \} \) manifest in a similar ‘global’ identity for the transfer matrix product \( \prod_{j=1}^N M_j \) (of equation (9)). This fact has not been recognized in the papers devoted to this problem. Moreover the existence of these properties for the product matrix is independent of the order of multiplication of the transfer matrices, i.e. the induction of global product properties for \( \prod_{j=1}^N M_j \) from that of the individual transfer matrices \( M_j \)'s, overlooks the non-commutativity of matrix multiplication! Note that the product matrix can be a very complicated object, depending on how many matrices are being multiplied. Irrespective of that, the global identities hold true and can be rigorously proven. These relationships are rather profound and we reserve a thorough discussion of the same for a future paper.

We conclude this section by formulating \( T \) and \( R \) in terms of the Pauli coefficients of the transfer matrix product in equation (20).

\[
T = \frac{1}{|\mu_1| + |\mu_2|^2}, \quad R = \left| \frac{\mu_1^2 + i\mu_2^2}{\mu_1^2 + \mu_1^2} \right|^2. \quad (20)
\]

The fact that only two coefficients—\( \mu_1^0 \) and \( \mu_2^3 \)—show up in the expression for \( T \), in terms of which \( R \) can be readily expressed \( (R = 1 - T) \) implies that the \( \mu_j^3 \)'s are not independent of each other. This again is an offshoot of the special transfer matrix properties mentioned above. At any rate, this signals a computational advantage—i.e. only \( \mu_1^0 \) and \( \mu_2^3 \) have to be found for computing \( T \).

### III. DISCUSSION

We revisit the problem of tunneling through a finite collection of \textit{rectangular} barriers. This is a special case of a piecewise constant potential barrier. We are mainly interested to look at the transmission coefficient \( T \), in the situations when the barrier ceases to be uniform i.e. an asymmetric multi-barrier. The uniform barrier thus serves as a basis for comparison. In what follows, we prefer to work in units, where \( \frac{2m}{\hbar^2} = 1 \).

A collection of \( m \) rectangular barriers constitutes a \( M \)
Barrier Problem or MBP. The potential $V(x)$ for a uniform MBP is specified with the sequences $\{x_j\}$ and $\{V_j\}$,

$$\{x_j\} = \begin{cases} \frac{(j-1)}{2} (\delta + \tau) + \Theta & j = 1, 3, 5, \ldots, 2m - 1 \\ \frac{j}{2} \delta + \left(\frac{2}{2} - 1\right) \tau + \Theta & j = 2, 4, 6, \ldots, 2m \end{cases}$$

$$\{V_j\} = \begin{cases} 0 & j = 1, 3, 5, \ldots, 2m - 1 \\ V_0 & j = 2, 4, 6, \ldots, 2m \end{cases}$$

(21)

where $\delta$ is the barrier width, $\tau$ is the well width and $V_0$ is the barrier height. $\Theta$ denotes the starting point of the barrier train, which could be conveniently shifted to zero as the physical properties of the problem are invariant to translation. The jump discontinuity number $N$ equals $2m$ for a MBP. Note that the barrier length $L = m \delta + (m - 1) \tau$. With $N = 2m$ these sequences satisfy the requirements necessitated in Section II. As an example consider the case of $m = 4, V_0 = 40, \delta = 0.5, \tau = 2$. We plot $\ln(T)$ vs. $\kappa (=\sqrt{E}$ in the prescribed units) for this barrier in Fig. 2(a).\textsuperscript{13} $V(x)$ for this case is graphed in Fig. 2(b) along with the real and imaginary parts of $\psi(x)$ for a typical energy of 27.217 (in the chosen units). For plotting the wave function we have chosen $A_0$ (i.e. $A_{N+1} = 1$). $\psi$ has been scaled by a factor of $\frac{V_0}{\max(\{|\psi(x)|\})}$ to pose it along with the barrier. This also takes care of dimensions.

Note the presence of 3 ($m - 1$, in general)\textsuperscript{3,5,6,8,14} resonant peaks in Fig. 2(a), which are almost superposed on each other for $\kappa \ll \sqrt{V_0}$ and gradually resolve with increasing $\kappa$. The resonant peaks are grouped into distinct bands. Even for small $m$, the emergence of band structure is readily apparent, though this is more pronounced in the case of strictly periodic potentials.\textsuperscript{15} The resonances nearly correspond to the bound states of the infinite square well of width $\tau$. These are given by

$$\kappa \tau = n \pi, \quad n = 1, 2, 3, \ldots$$

(22)

Since the barriers are of finite height, only at low energies ($E \ll V_0$), equation (22) is a faithful estimator of the actual resonant energies. This correspondence starts to deviate as we move towards the barrier top, i.e. increase $n$. Rather unexpectedly, it will turn out that any MBP can be completely portrayed on the basis of equation (22). We compare the estimates obtained from equation (22) with the exact solution (equation (20)) in the following discussion. An interesting result that can be deduced from equation (22) is the maximum number of resonant bands (to be called as $\beta$) that occur for $\kappa < \sqrt{V_0}$. This is obtained from the condition $\frac{n \pi}{\tau} \leq \sqrt{V_0}$, which gives

$$\beta = \left\lfloor \frac{\tau \sqrt{V_0}}{\pi} \right\rfloor,$$

(23)

$[\cdot]$ is the greatest integer (floor) function. For the 4BP of Fig. 2(a), $\frac{\sqrt{V_0}}{\tau} \sim 2$ and the well width $\tau = 2$. Thus $\beta = 4$, (i.e. 4 resonant bands) which is true. We use the terms bands and peaks interchangeably at times, especially when the bands are very narrow. But it must be understood that the number of bands is $\beta$ and each band contains $m - 1$ resonant peaks.\textsuperscript{16}

Arguably, the $m - 1$ wells of a MBP, each contribute a resonant peak (thus $m - 1$ peaks) to each band below $V_0$. When the wells have the same width, the $m - 1$ states in each band are degenerate (when the barrier height is infinity). For finite barrier height these levels couple, which leads to splitting of these $m - 1$ levels. However the coupling is smallest for the lowest energy band and largest for the highest energy band (below $V_0$). Thus, the degeneracy is lifted only at higher energies.

Instead, if one takes another 4BP which has the 3 wells of different widths (i.e. an asymmetric 4BP), the resonances must be distinctly resolved at all energies. This was also observed by Rao, et al. for a 3BP.\textsuperscript{3} We illustrate this feature in Fig. 3(a), for an asymmetric four barrier of constant barrier width $\delta = 0.5$, height $V_0 = 40$, but different well widths $\tau_1 = 5, \tau_2 = 3, \tau_3 = 2$.

The barrier is also pictured as an inset. Due to the inverse relation between $\kappa$ and $\tau$ in equation (22), the
MBP of varying well widths $\tau_j$, $j = 1, 2, \ldots m - 1$ (but same barrier height $V_0$) is found:

$$\alpha = \sum_{r=1}^{R} \left[ \frac{\tau_r \sqrt{V_0}}{\pi} \right]$$, $a_r \in \{1, 2, \ldots m - 1\}$, $R \leq m - 1$.

(24)

Well widths that are repeated must be counted only once, since they give the same resonant set. $a_r$ takes care of the distinct well widths, $R$ being the total number of such widths.\(^{19}\)

For the illustrative asymmetric 4BP we have $\alpha = \sum_{j=1}^{3} \left[ \frac{\tau_j \sqrt{V_0}}{\pi} \right] = 23$. Figure 3(a) gives 20 peaks (below $V_0$) and 3 diffuse peaks around $V_0$ (vertical broken line)—a total of 23!

Clearly, the well widths of a MBP play a very special role in positioning the resonant peaks. This is explored further in Fig. 4, which takes $\tau$ (the well width of a uniform MBP) as an independent parameter and plots $\ln(T(\kappa, \tau))$ on the $\kappa - \tau$ plane for $m = 4$, $V_0 = 40$, and $\delta = 1$. The color scale gives the value of $\ln(T)$. The horizontal axis is $\kappa$ and $\tau$ ranges from 1 to 10 on the vertical axis. The broken vertical line (white) is $\kappa = \sqrt{V_0}$. Resonant peaks project out as red dots, defining distinct tracks on the $\kappa - \tau$ plane. These tracks begin as isolated curves at low energies, gradually branch into 3 tracks, at middle energies, entering the region $\kappa > \sqrt{V_0}$. (Fig. 4 inset gives a magnified view of these branches) In general we expect $m - 1$ tracks for a uniform MBP. The branching of the resonant tracks is a consequence of the resolution of the $m - 1$ peaks in each band with increasing energy observed earlier.

Consider the horizontal broken line (black) at $\tau = 7$. This corresponds to a uniform 4BP of well width 7 and other parameters are same as above. (The transmission characteristics of this 4BP is provided in the top of Fig. 4). Note that the intersections of the horizontal line with the resonant tracks (for $\kappa < \sqrt{V_0}$) is consistent with the resonant peaks of the top figure (mapped by means of vertical arrows). From a mathematical standpoint the red regions display a smooth continuation from the discrete bound states of the infinite square well (in the left) to the continuum states of the free particle (right), where the resonant tracks coalesce into a continuous ‘band’ for $\kappa > \sqrt{V_0}$. Superposed on Fig. 4 are rectangular hyperbolas (black continuous curves) defined in equation (22) for $n = 1, 2, 3, \ldots$ which approximate the resonant tracks (for small $\kappa$) and later deviate as $\kappa$ becomes comparable to $\sqrt{V_0}$. In fact, this picture sets the regime of energies for which asymptotic analysis using the results of the infinite square well problem are valid. The number of intersections of a horizontal line (at a given $\tau$) with the resonant tracks below $\kappa = \sqrt{V_0}$ gives the number of resonant bands ($= \beta$). The direct proportionality between $\beta$ and $\tau$ (equation (23)) is captured in Fig. 4 i.e. horizontal lines at smaller $\tau$ have lesser number of intersections with the resonant tracks compared to those at

resonant peaks are ordered in a specific manner, i.e. the well with the maximum width contributes to the initial resonant peaks.

The resonant peaks above $\kappa = \sqrt{V_0}$ have broadened. This is expected from the classical tunneling characteristics\(^{17}\) (which sets in as the large energy limit of the quantum mechanical transmission coefficient). In Fig. 3(b) we plot $\ln(T)$ vs. $\kappa$ for the asymmetric 4BP (same as Fig. 3(a)) along with that of uniform 4BPs of same barrier height $V_0 = 40$, barrier width $\delta = 1$\(^{18}\) and well widths $\tau = 5$ (red), $\tau = 3$ (green) and $\tau = 1$ (blue).

The most striking feature is that there is a one to one correspondence between the resonant peaks of the uniform barrier plots and those of the asymmetric barrier. This is a reaffirmation of our previous remark—every well contributes its resonant energies independently, in accordance with equation (22). In Fig. 3(b) the resonances are labeled by quantum numbers $m$, $n$ and $l$ for the three different wells. Note, in Fig. 2(b) the wave function corresponded to an energy of 27.217, at which the first resonant peak of the fourth band arises. The wave function for this case becomes nearly sinusoidal at the site of the wells and has 3 well defined nodes in each well, which is an attribute of the fourth bound state wave function of a particle in a box of width $\tau$.

A natural way to extend equation (23) for a generic
FIG. 4. (top) \( \ln(T) \) vs. \( \kappa \) for 4BP of \( V_0 = 40 \), \( \delta = 1 \) and \( \tau = 7 \). (middle) Color plot of \( \ln(T(\kappa, \tau)) \) on the \( \kappa-\tau \) plane. Color legend gives the value of \( \ln(T) \). Broken vertical line (white) denotes \( \kappa = \sqrt{V_0} \) while solid horizontal line (black) denotes \( \tau = 7 \). Note that \( T \) along this line (\( T(\kappa, 7) \)) pertains to the barrier geometry of the top figure. Hence there is a one to one correspondence between the resonant peaks (some are mapped by vertical arrows). Black solid curves show rectangular hyperbolas \( \kappa \tau = n\pi \) for \( n = 1, 2, 3, \ldots \). These curves embrace the resonant tracks for \( \kappa \ll V_0 \). (bottom) Magnified view of the boxed region of the middle figure, exhibiting the trifurcation of the resonant tracks.
FIG. 5. Color plot of \( \ln(T(\kappa, \tau')) \) for an asymmetric 6BP. Color bar gives the probability scale. All barriers are of same height \( V_0 = 40 \), and width \( \delta = 1 \). All wells, except the fourth well have width \( \tau = 1 \). The fourth well has a width \( \tau' \) which is varied as a parameter along the vertical axis from 1 to 5. \( \kappa \) is taken along horizontal axis. The barrier is pictured schematically in the figure. Note that, due to alias effect (discussed later), it would not matter if any other well width was chosen as \( \tau' \) (instead of the fourth well). The picture would essentially remain intact for the energy ranges considered here. Also the bottom of the picture (\( \tau' = 1 \)) pertains to the uniform 6BP.
larger $\tau$. Analysis of the tunneling characteristics of a MBP on the $\kappa$-$\tau$ plane is very insightful. It projects the role of the well width $\tau$, in a natural way.

Now we consider an asymmetric 6BP of barrier specifications $V_0 = 40$, $\delta = 1$. For the plot of Fig. 5 we have taken the well widths of all the wells (except the fourth one) $\tau = 1$. The fourth well has a width $\tau'$ which is varied as a parameter on the vertical axis from 1 to 5. As in the previous figure, the color denotes the logarithm of the transmission coefficient and $\kappa$ is taken along the horizontal axis. Note that there is nothing special about the fourth well and any other well width could be chosen as $\tau'$ (without altering the picture appreciably). This freedom is attributed to the alias effect discussed later. The barrier is sketched schematically in the figure. Clearly, the dynamics of the resonant peaks in this case is extremely non-trivial and a complex structure emerges even with one well perturbation. Although, the exact details of the figure are quite perplexing, the basic frame of the resonant tracks can be reasoned in a simple manner using equation (22). The well width $\tau$ contributes resonances at $\kappa = \frac{n\pi}{\tau}$. Below the barrier top ($\kappa < V_0$) only about 2 bands can be accommodated for $\tau = 1$. (i.e. $\beta = 2$)

Thus these resonant peaks define vertical tracks in the figure. This also implies that, irrespective of the value of $\tau'$, the resonances due to the width $\tau$ will always show up. The curved resonant tracks that percolate through these vertical lines are due to the well width $\tau'$ obtained from: $\kappa \tau' = l \pi$, $l = 1, 2, 3, \ldots$ If we proceed just with the asymptotic formula (equation (22)), we would contrive a picture that looks like Fig. 6. Clearly, Fig. 6 does not describe the actual situation. This is primarily because, equation (22) is valid at energies well below the barrier top. Note that the vertical resonant tracks (red) do not show splitting (in Fig. 6) which actually occurs (in Fig. 5) due to coupling effects, discussed earlier.

A. Permutation invariance and alias effect

The transmission coefficient plots become particularly interesting for a specific class of MBPs. We have seen that the well widths have a strong bearing on the position of the resonant peaks. The role of well widths is expounded further in this sub section. Consider an asymmetric multi-barrier system of barrier height $V_0$, barrier width $\delta$, and well widths $\tau_1, \tau_2, \ldots, \tau_m$ (starting from left). If the ordering of the wells is ‘ignored’-then one can construct more asymmetric multi-barrier potentials (using the parameters of the above prototype) by permuting the position of the wells. If all the well widths are distinct, there are $(m-1)!$ possible MBPs. We refer to these barriers as permutation-equivalent MBPs. These MBPs possess the same set of well widths. Thus the transmission characteristics must always have the same number of resonant peaks in accordance with equation (24). Moreover, equation (22) guarantees that the resonances contributed by each $\tau_j$ would occur at the same location. Even if the exact position of the resonances are influenced by the barrier height and width, that influence would be the same for all the permutation-equivalent MBPs. Thus the actual position of the resonances must indeed be the same for these multi-barrier systems.

Here we have implicitly assumed that the actual ordering of the wells doesn’t influence the position of the resonant peaks. We will see that this assumption will get challenged later. Thus it seems like, the transmission coefficients of these barriers would have some sort of similarity (at least in the region where equation (22) is valid). We illustrate this pictorially in Fig. 7(a) with an asymmetric 5BP of barrier height $V_0 = 40$, width $\delta = 0.5$ with different well widths (labeled from left to right $- \tau_1, \tau_2, \tau_3, \tau_4$). We have chosen 1, 2, 3, 4 as the widths and
FIG. 7. (a) $\ln(T)$ vs. $\kappa$ for three asymmetric 5BPs with $V_0 = 40$, $\delta = 0.5$, $\tau_1, \tau_2, \tau_3, \tau_4 \in \{1, 2, 3, 4\}$. The legend gives the well widths for each plot in the specified order. Notice the aliasing of the three transmission curves for $\kappa < \sqrt{V_0}$. 
(b) $\ln(T)$ vs. $\kappa$ for three asymmetric 10BPs with same barrier parameters as Fig. 7(a). Well widths $\tau_1, \tau_2, \ldots, \tau_9 \in \{1, 0.5, 3, 0.3, 2, 5, 4, 0.8, 7\}$. Corresponding $V(x)$s are shown as insets. (inset) magnified view of 17th resonant peak.

Graph three permutations of these widths pertaining to three different asymmetric 5BPs. $V(x)$ for the corresponding curves are depicted as insets.

Quite consistent with our expectation, the curves nearly overlap! At energies below the barrier top, the curves (pertaining to the different spatial permutations of the well widths) get superposed and the differences between them surfaces only at higher energies. We refer to this phenomenon as the *Permutation-Invariant Alias Effect* (or *Alias-Effect*). Note that for a MBP there would be $\binom{m}{2}(m - 1)!$ aliased solutions.

Aliasing of the transmission coefficients is not lost even if the barrier number is increased significantly. In Fig. 7(b) we plot the case of a 10BP. The barrier parameters are same as that of Fig. 7(a), and the well widths are listed in the legend. Note that the aliasing is not perfect at the site of the resonant peaks. In fact the separation occurs on a very narrow range of energy. (Fig. 7(b) inset). This is attributed to the coupling, which might depend on the ordering of the wells. We conclude by rephrasing the Aliasing condition.

The transmission characteristics of an asymmetric MBP is ‘invariant’ to the spatial permutation of the $m-1$ wells so long as the heights and the widths of the $m$ barriers are kept same.

**IV. CONCLUSION**

In the discussion of asymmetry we focused primarily on the well widths. This doesn’t imply that the barrier widths or heights wouldn’t play a big role. If the barrier height is increased, the threshold gets shifted further, while the overall behavior is not affected appreciably. So far as barrier widths are concerned—an increase simply leads to a lowering of the over all probability, however the resonant peaks are not significantly affected. The width of the barriers have a small bearing on the extent to which the spikes (in each band) are resolved. At any rate, it is the well widths that completely dictate the transmission characteristics of a MBP. We have thus applied our formulation to study asymmetry in a multi-barrier structure. As noted earlier, these are special examples of piecewise constant potential barriers. And there are several other applications to which the methods developed in this paper can be used. We reserve a discussion of some of these for future papers. At this point we emphasize the importance of equation (12) which was a crucial ingredient in the solution.

Some of the topics that have not been considered are tunneling time and tunneling length. These are interesting parameters to look at for a MBP. Time evolution of the wave function is another aspect that requires further insight. Certainly the analysis of these problems rests directly on the discussion provided in this paper. Also, long sequence matrix products of the form presented here, call for optimal computational algorithms that reduce code and time complexities.

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This result can be derived explicitly from the continu-
ity equation. A particularly neat (and equivalent) way of
deriving the same is from the conservation of the aver-
age momentum $< p >$ associated with the wave function
$\psi$. Note: The momentum associated with the wave func-
tion(s) $A_k e^{i\omega t}$ is $\pm h_\kappa$. $A_\pm$ being the proba-

bility amplitude of finding the particle with $p = \pm h_\kappa$. Hence the aver-
age momentum associated with $\psi_j$ (equation (2)) is $< p > = (h_\kappa) A_j A_j^* + (-h_\kappa) B_j B_j^* = h_\kappa (|A_j|^2 - |B_j|^2) = \text{const} \cdot \kappa_j = \kappa N_j + 1$. Thus $|A_j|^2 - |B_j|^2 = |A_{N_j + 1}|^2 - B_{N_j + 1}|^2$. Since $B_{N_j + 1} = 0$, $|A_{N_j + 1}|^2 + |B_{N_j + 1}|^2 = 1$ or $T + R = 1$.

All the plots in this paper have been generated from pro-
grams written in MATLAB® Version—7.12.0.635
(R2011a).

By classical tunneling we refer to $T = \begin{cases} 0 & \kappa < \sqrt{V_0} \\ 1 & \kappa > \sqrt{V_0} \end{cases}$.

We choose $\delta = 1$ (instead of 0.5) for the colored plots, to
bring out the correspondence better. If one takes $\delta = 0.5$ the
curves would overlap. A higher value of delta lowers the
value of $T$ and has no effect on the position of the peaks.

Hence the correspondence between the resonant peaks of the
asymmetric MBP and the uniform MBPs is still pre-
served.

For $n\tau = \tau'$ the peaks would overlap and this must be ac-
counted for in equation (24). But resonances do not strictly
follow equation (22). Thus the formula works and this cor-
rection is not needed.

Although we have $(m - 1)!$ distinct permutation equivalent
MBPs, some of them are not aliased solutions. For instance
in a 4BP with three distinct well widths $\tau_1, \tau_2$ and $\tau_3$, con-
sider the permutations $\tau_3 \tau_1 \tau_2 \tau_3$ and $\tau_2 \tau_1 \tau_3 \tau_2$. They
would result in the same transmission coefficient, since a particle
incident from left on the first barrier is equivalent to a par-
ticle incident from right on the other. And the transmission
coefficient of the barrier must not depend on the direction
from which the particle approaches. In fact this feature is inher-
ently embedded in the structure of the transfer matrices
and can be rigorously proven.