

On the number of states bound by one-dimensional finite periodic potentials

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Bound states and zero-energy resonances of one-dimensional finite periodic potentials are investigated, by means of Levinson's theorem. For finite range potentials supporting no bound states, a lower bound for the (reduced) time delay at threshold is derived. © 1995 American Institute of Physics.

I. INTRODUCTION

In this paper we consider the one-dimensional potential function

$$V_N(x) = \sum_{i=0}^{N-1} v(x-id) \quad (1.1)$$

forming a finite periodic chain of N nonoverlapping potentials of general shape. The single potential $v(x)$ has its support in the interval $[-a/2, a/2]$ and $d \geq a$ (nonoverlapping condition). The system is of practical interest, for instance for the physics of superlattice electronic devices¹ and optical properties of multiquantum wells.² As the number N increases, it also constitutes a simple model exhibiting a solid-state-like behavior, i.e., energy bands and gaps.^{3,4} Recently, a complete analytical solution of the scattering problem for $V_N(x)$ has been presented,^{3,4} yielding closed compact expressions for the transmission and reflection coefficients in terms of those for the single potential $v(x)$.

The present work completes the analysis of this system by providing a general description of the bound state structure of $V_N(x)$, in terms of certain quantities characterizing the single scatterer. More precisely, using Levinson's theorem and the factorization property of the scattering matrix, we generalize the analysis of Ref. 5, for the double-potential system, and show that $V_N(x)$ admits at most $N-1$ resonance distances d_j , $j=1, \dots, N-1$, for which the reflection coefficient vanishes at threshold and which correspond to a bound state level turning into a resonance. As a consequence, we find that, by lowering the spacing d between the potentials, $V_N(x)$ can lose at most $N-1$ bound state solutions.

For a potential supporting no bound states, the method also allows us to derive a lower bound for the (reduced) time delay at threshold which improves one recently obtained in Ref. 5.

The work is organized as follows. In Sec. II we review some basic facts of the one-dimensional scattering. In Sec. III we discuss the two-potential system, as a preparative for Sec. IV, where we state and prove our main result on the finite periodic potential. Finally, in Sec. V, the lower bound for the zero-energy time-delay, in absence of bound states, is derived.

II. PRELIMINARIES

In this section we present some well-known results of the one-dimensional scattering problem, to establish notation and some needed facts.

The S-matrix. Let $V(x)$, $x \in \mathbb{R}$, be a finite range potential that we shall assume bounded everywhere. The associated scattering matrix is the 2×2 unitary matrix

$$S(k) = \begin{pmatrix} T(k) & R(k) \\ L(k) & T(k) \end{pmatrix}, \quad (2.1)$$

where $T(k) = |T(k)|e^{i\alpha_T(k)}$, $R(k) = |R(k)|e^{i\alpha_R(k)}$, and $L(k) = |L(k)|e^{i\alpha_L(k)}$ are the transmission and reflection coefficients, from the right and left, respectively, at energy $E = k^2/2m$ (m is the mass of the particle and we have set $\hbar = 1$). In addition of being unitary, $S(k)$ has also the property^{6,7}

$$S(-k) = S^*(k). \quad (2.2)$$

For our choice of potential, it is a smooth function of $k \geq 0$, behaving like^{6,7}

$$S(k) = I + O(1/k), \quad (2.3)$$

as $k \rightarrow \infty$. On the other hand, for the low energy limit, the following dichotomy is known to hold⁵⁻⁷

$$|T(k)|^2 = Ck^2 + O(k^4), \quad C > 0, \quad (2.4)$$

for the generic case, and

$$|T(k)|^2 = C' + O(k^2), \quad 0 < C' \leq 1, \quad (2.5)$$

for the exceptional case where the potential supports a zero-energy solution. Notice that $C' = 1$ if $v(x)$ is parity invariant.^{5,8} In the following, we shall speak of a zero-energy resonance whenever $|T(0)| = 1$.

Levinson's theorem. Levinson's theorem establishes the relationship between the low energy behavior of the phase $\alpha_T(k) = \arg T(k)$ and the total number M of bound states of $V(x)$ (see Ref. 5 and references therein). If $\alpha_T(k)$ is defined to be continuous and such that $\alpha_T(\infty) = 0$, then one has [when $k = 0$ we drop it from the notation, i.e., $\alpha_T \equiv \alpha_T(0)$, $T \equiv T(0)$, and so on]

$$\alpha_T = (M - \frac{1}{2})\pi, \quad L = R = -1 \quad (2.6)$$

for the generic case, and

$$\alpha_T = M\pi, \quad T \neq 0 \quad (2.7)$$

for the exceptional case with a zero-energy solution. A zero-energy solution is usually called "half bound state" because of the additional term $1/2$ in Eq. (2.7).

Factorization formula. Write the potential $V(x)$ as the sum $V(x) = V_1(x) + V_2(x)$, where we have defined ($y \in \mathbb{R}$)

$$V_1(x) \equiv V(x)\chi_{(-\infty, y)}(x), \quad V_2(x) \equiv V(x)\chi_{(y, \infty)}(x), \quad (2.8)$$

with $\chi_I(x)$ being the characteristic function of the interval I . Let

$$S_i(k) = \begin{pmatrix} T_i(k) & R_i(k) \\ L_i(k) & T_i(k) \end{pmatrix} \quad (2.9)$$

be the scattering matrix for the potential $V_i(x)$, $i=1,2$. Then, we have the factorization formula⁹

$$\begin{pmatrix} \frac{1}{T(k)} & -\frac{R(k)}{T(k)} \\ \frac{L(k)}{T(k)} & \frac{1}{T(k)^*} \end{pmatrix} = \begin{pmatrix} \frac{1}{T_1(k)} & -\frac{R_1(k)}{T_1(k)} \\ \frac{L_1(k)}{T_1(k)} & \frac{1}{T_1(k)^*} \end{pmatrix} \begin{pmatrix} \frac{1}{T_2(k)} & -\frac{R_2(k)}{T_2(k)} \\ \frac{L_2(k)}{T_2(k)} & \frac{1}{T_2(k)^*} \end{pmatrix}. \tag{2.10}$$

Time delay. Since $S(k)$ is unitary, it can be written $S(k) = e^{i\Delta(k)}$, where $\Delta(k) = -i \log S(k)$ is called the phase shift operator. Taking one half of the trace of $\Delta(k)$ and differentiating with respect to energy [$d/dE = (m/k)d/dk$] yields the averaged (total) time delay¹⁰

$$\tau(k) = \frac{1}{2} \frac{m}{k} \text{Tr} \Delta'(k) = \frac{1}{2} \frac{m}{k} \text{Tr}(-iS^\dagger(k)S'(k)) = \frac{m}{k} \alpha_T'(k) = \frac{1}{2} \frac{m}{k} (\alpha_R'(k) + \alpha_L'(k)), \tag{2.11}$$

where the prime denotes the derivative with respect to k . Notice that $\alpha_T'(k) = \alpha_R'(k) = \alpha_L'(k)$ for a parity invariant potential.⁵ In the same way, we also define the spatial shift, $H(k)$, caused by the time delay $\tau(k)$, by

$$H(k) = \frac{k}{m} \tau(k) = \alpha_T'(k) = \frac{1}{2} (\alpha_R'(k) + \alpha_L'(k)). \tag{2.12}$$

III. THE TWO-POTENTIAL SYSTEM

Consider the potential

$$V(x) = v_1(x) + v_2(x-d), \tag{3.1}$$

where $v_1(x)$ and $v_2(x)$ have their supports in the intervals $[-a_1/2, a_1/2]$ and $[-a_2/2, a_2/2]$, respectively, and $d \geq (a_1 + a_2)/2$. Let

$$s_i(k) = \begin{pmatrix} t_i(k) & r_i(k) \\ l_i(k) & t_i(k) \end{pmatrix} \tag{3.2}$$

be the scattering matrix for the potential $v_i(x)$, $i=1,2$. When the coordinate axis is shifted by $-d$, the scattering matrix $s_2(k)$ is transformed as $l_2(k) \rightarrow l_2(k)e^{i2kd}$, $r_2(k) \rightarrow r_2(k)e^{-i2kd}$, $t_2(k) \rightarrow t_2(k)$. Therefore, according to the factorization formula (2.10), we find for the transmission coefficient

$$T(k) = \frac{t_1(k)t_2(k)}{1 - r_1(k)l_2(k)e^{2ikd}}. \tag{3.3}$$

For sake of simplicity, we assume in the following that $v_1(x)$ and $v_2(x)$ are parity invariant, i.e., $l_i(k) = r_i(k)$, $i=1,2$. Then, we may also write

$$|T(k)|^2 = \frac{|t_1(k)t_2(k)|^2}{1 - 2|l_1(k)l_2(k)|\cos(\alpha_{l_1}(k) + \alpha_{l_2}(k) + 2kd) + |l_1(k)l_2(k)|^2} \tag{3.4}$$

and

$$\alpha_T(k) = \alpha_{t_1}(k) + \alpha_{t_2}(k) + A(k), \tag{3.5}$$

where we have defined

$$A(k) = \arctan \left(\frac{|l_1(k)l_2(k)| \sin(\alpha_{l_1}(k) + \alpha_{l_2}(k) + 2kd)}{1 - |l_1(k)l_2(k)| \cos(\alpha_{l_1}(k) + \alpha_{l_2}(k) + 2kd)} \right). \quad (3.6)$$

Denoting by $h_i = \lim_{k \rightarrow 0} \alpha'_{l_i}(k)$, $i=1,2$, the zero-energy limit of the spatial shifts for $v_1(x)$ and $v_2(x)$, respectively, we have the following.

Proposition 1:

(A) Assume that $v_1(x)$ and $v_2(x)$ have n_1 and n_2 bound states, respectively. If one can find a distance $d \geq (a_1 + a_2)/2$, such that

- (i) $h_1 + h_2 + 2d > 0$, then $V(x)$ has $n_1 + n_2$ bound states;
- (ii) $h_1 + h_2 + 2d = 0$, then $V(x)$ has $n_1 + n_2 - 1$ bound states and a “half bound state;”
- (iii) $h_1 + h_2 + 2d < 0$, then $V(x)$ has $n_1 + n_2 - 1$ bound states.

(B) If $v_1(x)$ [or $v_2(x)$] has in addition a “half bound state,” then $V(x)$ has $n_1 + n_2$ bound states for all $d \geq (a_1 + a_2)/2$.

(C) If $v_1(x)$ and $v_2(x)$ have both in addition a “half bound state,” then $V(x)$ has $n_1 + n_2$ bound states and a “half bound state” for all $d \geq (a_1 + a_2)/2$.

Proof: The proof follows essentially the one given in Ref. 5, for the special case of two identical potentials. We apply Levinson's theorem to Eqs. (3.5), (3.6). We define $\alpha_T(\infty) = \alpha_{l_1}(\infty) = \alpha_{l_2}(\infty) = 0$, implying $A(\infty) = \arctan(0) = 0$ [$l_i(\infty) = 0$, $i=1,2$, by Eq. (2.3)]. Since $|l_1(k)l_2(k)| \neq 1$, for all $k \neq 0$, the denominator in Eq. (3.6) never vanishes for $k \neq 0$, so that $A(k)$ is a continuous function of k .

(A) According to Eqs. (2.4), (2.6), we have

$$|l_i(k)|^2 = 1 - |t_i(k)|^2 = 1 - c_i k^2 + O(k^4), \quad c_i > 0, \quad i=1,2 \quad (3.7)$$

and (dropping the $k=0$ argument)

$$\alpha_{l_i} = (n_i - 1/2)\pi, \quad i=1,2. \quad (3.8)$$

Using Eq. (3.7), the fact that the $\alpha_{l_i}(k)$ are odd functions of k [by Eq. (2.2)], and that $l_1(k)l_2(k) \rightarrow 1$ as $k \rightarrow 0$, implying $\alpha_{l_1} + \alpha_{l_2} = 0 \pmod{\pi}$, we find

$$A = \lim_{k \rightarrow 0} A(k) = \lim_{k \rightarrow 0} \arctan \left(\frac{2(h_1 + h_2 + 2d)k + O(k^3)}{(h_1 + h_2 + 2d)^2 k^2 + (c_1 + c_2)k^2 + O(k^4)} \right). \quad (3.9)$$

Thus, $A = \pi/2$, 0 , $-\pi/2$ if $h_1 + h_2 + 2d$ is positive, zero and negative, respectively. Introducing Eqs. (3.8) and (3.9) into Eq. (3.5), we obtain the desired result, according to Levinson's theorem (2.6),(2.7).

(B) If, say, $v_2(x)$ has a “half bound state,” but not $v_1(x)$, then $\alpha_{l_2} = n_2\pi$ and $\alpha_{l_1} = (n_1 - 1/2)\pi$. Furthermore, according to Eq. (3.6), $l_2=0$ implies $A=0$ for all $d \geq (a_1 + a_2)/2$, and Eq. (3.5) yields $\alpha_T = (n_1 + n_2 - \frac{1}{2})\pi$ for all $d \geq (a_1 + a_2)/2$. We conclude by Eq. (2.6).

(C) We have $\alpha_{l_i} = n_i\pi$, $i=1,2$ and, seemingly to point (B), $A=0$ for all $d \geq (a_1 + a_2)/2$, implying $\alpha_T = (n_1 + n_2)\pi$ for all $d \geq (a_1 + a_2)/2$. We conclude by Eq. (2.7).

The Proposition is readily generalized to the case where $v_1(x)$ and $v_2(x)$ are nonsymmetric. In that case, one can easily check that $h_1 + h_2$ is to be replaced by $\alpha'_{r_1} + \alpha'_{l_2}$. For point (B), the only modification is that, as $k \rightarrow 0$, $l_2(k) \rightarrow l_2 \in \mathbb{R}$ (see the Appendix of Ref. 8) instead of $l_2(k) \rightarrow 0$. Then, $\alpha_{r_1} + \alpha_{l_2} = 0 \pmod{\pi}$, and now $A=0$ because of the vanishing of the sine [the same remark holds for point (C)].

In the nonresonant case $h_1 + h_2 + 2d \neq 0$, the transmission probability $|T(k)|^2$ has the form (2.4). A straightforward calculation from Eq. (3.4) yields, for the constant C ,

$$C = \frac{c_1 c_2}{(h_1 + h_2 + 2d)^2}. \quad (3.10)$$

From Eqs. (3.5), (3.6), we also find for the spatial shift at threshold,

$$H = h_1 + h_2 - \frac{1}{2} \frac{(h_1 + h_2 + 2d)^2 + c_1 + c_2}{h_1 + h_2 + 2d}. \quad (3.11)$$

In the special case $v_1(x) = v_2(x) = v(x)$ [i.e., $V(x) = V_2(x)$ with the notation of Eq. (1.1)], we recover Proposition 1 of Ref. 5. The resonant condition (ii) becomes $h + d = 0$, where $h = h_1 = h_2$, and corresponds to a transmission probability which is unity at threshold (zero-energy resonance).

IV. THE FINITE PERIODIC POTENTIAL SYSTEM

Let

$$V_N(x) = \sum_{i=0}^{N-1} v(x - id) \quad (4.1)$$

be a finite periodic chain of N nonoverlapping potentials. The single potential $v(x)$ has its support in the interval $[-a/2, a/2]$ and $d \geq a$. We denote by

$$S_N(k) = \begin{pmatrix} T_N(k) & R_N(k) \\ L_N(k) & T_N(k) \end{pmatrix}, \quad s(k) = \begin{pmatrix} t(k) & r(k) \\ l(k) & t(k) \end{pmatrix} \quad (4.2)$$

the scattering matrices for $V_N(x)$ and $v(x)$, respectively. Using the factorization formula (2.10) and the Cayley-Hamilton theorem, one can write the transmission probability $|T_N(k)|^2$ in the compact form^{3,4}

$$|T_N(k)|^2 = \frac{1}{1 + U_{N-1}^2(z) [1 - |t(k)|^2] / |t(k)|^2}, \quad (4.3)$$

where $z = \cos(\alpha_t(k) + kd) / |t(k)|$, $\alpha_t(k) = \arg t(k)$, and the $U_N(z)$ are the Chebyshev's polynomial of the second kind, satisfying the recurrence relation¹¹

$$U_N(z) - 2zU_{N-1}(z) + U_{N-2}(z) = 0 \quad (4.4)$$

and boundary conditions $U_{-1}(z) = 0$, $U_0(z) = 1$. In the following we shall also need the identity

$$U_{N-1}^2(z) + U_{N-2}^2(z) - 2zU_{N-1}(z)U_{N-2}(z) = 1. \quad (4.5)$$

It immediately follows from Eq. (4.3) that, for a given incoming momentum k , the resonance condition $|T_N(k)|^2 = 1$ occurs when either $|t(k)|^2 = 1$ (the single potential is transparent at this energy) or $U_{N-1}(z) = 0$. In the former case, the resonance is not affected by a variation of the distance d separating the potentials. In the latter case, the resonances are determined by the zeros of $U_{N-1}(z)$, i.e.,

$$\cos(\alpha_t(k) + kd) / |t(k)| = \cos(j\pi/N), \quad j = 1, \dots, N-1, \quad (4.6)$$

and therefore, for a given $k \neq 0$, there is always an infinite number of resonance distances $d \geq a$, for which the transmission probability is unity.

Consider now the low energy behavior of the resonance conditions (4.6). In the exceptional case $|t(0)|^2 \neq 0$, it immediately follows from Eq. (4.3) that $|T_N(0)|^2 \neq 0$ [and $|T_N(0)|^2 = 1$ if $|t(0)|^2 = 1$] so that, if $v(x)$ supports a “half bound state” (or a zero-energy resonance), the same is true for $V_N(x)$, for all $d \geq a$. On the other hand, in the generic case

$$|t(k)|^2 = ck^2 + O(k^4), \quad c > 0, \tag{4.7}$$

the resonant conditions (4.6) become [use $\alpha_i(k) = -\alpha_i(-k)$, by Eq. (2.2), and Eq. (2.6)]

$$\frac{h+d}{\sqrt{c}} + O(k^2) = \cos(j\pi/N), \quad j = 1, \dots, N-1, \tag{4.8}$$

where $h = \lim_{k \rightarrow 0} \alpha'_i(k)$ is the zero-energy spatial shift for $v(x)$ and c is the positive constant appearing in Eq. (4.7). Thus, contrary to the case $k \neq 0$, as $k \rightarrow 0$, there are at most $N-1$ resonance distances

$$d_j = -h + \sqrt{c} \cos(j\pi/N), \quad j = 1, \dots, N-1, \tag{4.9}$$

for which the transmission probability is unity. Notice however that, since we must have $d \geq a$, a resonance condition, say $d = d_j$, can be realized only if $d_j \geq a$, which can be the case or not, depending on the given choice of the single potential $v(x)$.

We are now in position to state our result, which relates the zero-energy resonance conditions (4.9) to the structure of the bound state spectrum of $V_N(x)$.

Proposition 2:

- (A) Assume that $v(x)$ has n bound states. If one can find a distance $d \geq a$ such that
 - (i) $d > d_1$, then $V_N(x)$ has Nn bound states;
 - (ii) $d_{j+1} < d < d_j$, $j = 1, \dots, N-2$, then $V_N(x)$ has $Nn - j$ bound states;
 - (iii) $d < d_{N-1}$, then $V_N(x)$ has $Nn - (N-1)$ bound states;
 - (iv) $d = d_j$, $j = 1, \dots, N-1$, then $V_N(x)$ has $Nn - j$ bound states and a zero-energy resonance;
- (B) Assume that $v(x)$ has in addition a “half bound state.” Then, $V_N(x)$ has Nn bound states and a “half bound state” for all $d \geq a$.

Proof: We shall proceed by a recursion procedure. From Proposition 1, the result clearly holds for $N=2$. We assume it holds for some fixed N , $2 \leq N \leq N'$, and have to prove it for $N=N'+1$.

(A) We introduce the notation $\rho = (h+d)/\sqrt{c}$ and consider first the “distances” of the form $\rho = \cos(m\pi/N)$, $1 \leq m \leq N-1$, $2 \leq N \leq N'$. For this, we write the potential as the sum $V_{N'+1}(x) = V_N(x) + V_{N'-N+1}(x - Nd)$, $2 \leq N \leq N'$. Then, according to Eqs. (3.5), (3.6), the phase $\alpha_{N'+1} \equiv \alpha_{T_{N'+1}}$ may be written as

$$\alpha_{N'+1} = \alpha_N + \alpha_{N'-N+1} + A. \tag{4.10}$$

By hypothesis, $V_N(x)$ supports $Nn - m$ bound states and a zero-energy resonance, and it follows from points (B) and (C) of Proposition 1 that $A=0$. Thus,

$$\alpha_{N'+1} = (Nn - m)\pi + \alpha_{N'-N+1}. \tag{4.11}$$

To determine $\alpha_{N'-N+1}$, we distinguish, for $N \neq N'$, the following two possibilities: there exist $1 \leq m' \leq N' - N$, such that (a)

$$\frac{m}{N} = \frac{m'}{N' - N + 1} \tag{4.12}$$

or (b)

$$\frac{m'}{N'-N+1} < \frac{m}{N} < \frac{m'+1}{N'-N+1}. \quad (4.13)$$

In case (a), by assumption, $\alpha_{N'-N+1} = ((N' - N + 1)n - m')\pi$, and hence

$$\alpha_{N'+1} = ((N' + 1)n - (m + m'))\pi. \quad (4.14)$$

Moreover, Eq. (4.12) is equivalent to $m/N = (m + m')/(N' + 1)$, implying $\rho = \cos((m + m')\pi/(N' + 1))$, in accordance with (iv). In case (b), we have

$$\cos\left(\frac{m'+1}{N'-N+1}\right) < \rho < \cos\left(\frac{m'}{N'-N+1}\right). \quad (4.15)$$

Thus, by assumption, $\alpha_{N'-N+1} = ((N' - N + 1)n - m' - \frac{1}{2})\pi$, yielding

$$\alpha_{N'+1} = ((N' + 1)n - (m + m') - \frac{1}{2})\pi, \quad (4.16)$$

which is in agreement with (ii), since Eq. (4.13) is equivalent to

$$\frac{m+m'}{N'+1} < \frac{m}{N} < \frac{m+m'+1}{N'+1}, \quad (4.17)$$

so that

$$\cos\left(\frac{m+m'+1}{N'+1}\right) < \rho < \cos\left(\frac{m+m'}{N'+1}\right). \quad (4.18)$$

For $N = N'$, $\alpha_{N'-N+1} = \alpha_t = (n - 1/2)\pi$, and

$$\alpha_{N'+1} = (N'n - m)\pi + (n - \frac{1}{2})\pi = ((N' + 1)n - m - \frac{1}{2})\pi, \quad (4.19)$$

which agrees with (ii), if we set $m' = 0$ in (4.17), (4.18).

Consider now the case $\rho \neq \cos(m\pi/N)$, $1 \leq m \leq N - 1$, $2 \leq N \leq N'$. Then, by assumption, none of the potentials $V_N(x)$, $N = 2, \dots, N'$, has a zero-energy resonance. Thus, writing the potential as the sum $V_{N'+1}(x) = V_{N'}(x) + v(x - N'd)$, we can apply part (A) of Proposition 1. Setting $\alpha \equiv \alpha_t$, and observing that the distance between the centers of $V_{N'}(x)$ and $v(x - N'd)$ is $(N' + 1)d/2$, we obtain

$$\alpha_{N'+1} = \alpha_{N'} + \alpha + A, \quad (4.20)$$

with

$$A = \begin{cases} \pi/2 & \text{if } H_{N'} + h + (N' + 1)d > 0 \\ 0 & \text{if } H_{N'} + h + (N' + 1)d = 0 \\ -\pi/2 & \text{if } H_{N'} + h + (N' + 1)d < 0. \end{cases} \quad (4.21)$$

Here, $H_{N'}$ denotes the zero-energy limit of the spatial shift for $V_{N'}(x)$. On the other hand, Eqs. (3.10), (3.11) give (with obvious notation)

$$C_{N'-1} = \frac{C_{N'-2}c}{(H_{N'-2} + h + (N' - 1)d)^2}, \quad C_1 = c \quad (4.22)$$

and, with $H_1 = h$,

$$H_{N'} = H_{N'-1} + h - \frac{1}{2} (H_{N'-1} + h + N'd) - \frac{1}{2} \frac{C_{N'-1} + c}{H_{N'-1} + h + N'd}. \quad (4.23)$$

Setting $F_{N'} \equiv (H_{N'} + h + (N' + 1)d)/\sqrt{c}$, we have $F_1 = 2\rho$, and Eq. (4.22) becomes

$$C_{N'-1} = \frac{C_{N'-2}}{F_{N'-2}^2} = \frac{C_{N'-3}}{F_{N'-2}^2 F_{N'-3}^2} = \dots = \frac{c}{F_{N'-2}^2 \dots F_1^2}. \quad (4.24)$$

Moreover, Eq. (4.23) gives

$$F_{N'} = \frac{1}{2} \left(F_{N'-1} - \frac{1}{c} \frac{C_{N'-1} + c}{F_{N'-1}} + 2\rho \right) = \frac{1}{2} \left(F_{N'-1} - \frac{1}{F_{N'-1}} - \frac{1}{F_{N'-1}} \frac{1}{F_{N'-2}^2 \dots F_1^2} + 2\rho \right), \quad (4.25)$$

where, for the second equality, we have used Eq. (4.24). Then, defining

$$U_{N'} \equiv F_1 \dots F_{N'}, \quad (4.26)$$

we have $F_{N'} = U_{N'}/U_{N'-1}$ and, after multiplication by $U_{N'-1}U_{N'-2}$, Eq. (4.25) yields

$$U_{N'}U_{N'-2} = \frac{1}{2}(U_{N'-1}^2 - U_{N'-2}^2 - 1 + 2\rho U_{N'-1}U_{N'-2}). \quad (4.27)$$

Multiplying Eq. (4.4) by U_{N-2} and using Eq. (4.5), one finds that Eq. (4.27) defines the Chebyshev's polynomials of the second kind, with argument $z = \rho$. In other terms, we have shown that Eq. (4.21) may be written in the alternative form

$$A = \begin{cases} \pi/2, & \text{if } U_{N'}/U_{N'-1} > 0, \\ 0, & \text{if } U_{N'}/U_{N'-1} = 0, \\ -\pi/2, & \text{if } U_{N'}/U_{N'-1} < 0. \end{cases} \quad (4.28)$$

Assume first $\rho > \cos(\pi/(N'+1)) > \cos(\pi/N')$. Then, since the coefficient of ρ^N in the N th degree polynomial is unity, $U_{N'}/U_{N'-1} > 0$, so that $A = \pi/2$. Moreover, by assumption, $\alpha_{N'} = (N'n - \frac{1}{2})\pi$. Hence, Eq. (4.20) gives

$$\alpha_{N'+1} = \left(N'n - \frac{1}{2} \right) \pi + \left(n - \frac{1}{2} \right) \pi + \frac{\pi}{2} = \left((N'+1)n - \frac{1}{2} \right) \pi, \quad (4.29)$$

which is the desired result, in view of Eq. (2.6). Next, we assume

$$\cos\left(\frac{(m+1)\pi}{N'+1}\right) < \rho < \cos\left(\frac{m\pi}{N'+1}\right), \quad m = 1, \dots, N'-1. \quad (4.30)$$

Two consecutive zeros of $U_{N'}$ bracket exactly one zero of $U_{N'-1}$. More precisely,

$$\cos\left(\frac{(m+1)\pi}{N'+1}\right) < \cos\left(\frac{m\pi}{N'}\right) < \cos\left(\frac{m\pi}{N'+1}\right), \quad m = 1, \dots, N'-1. \quad (4.31)$$

If

$$\cos\left(\frac{m\pi}{N'}\right) < \rho < \cos\left(\frac{m\pi}{N'+1}\right) < \cos\left(\frac{(m-1)\pi}{N'}\right), \quad (4.32)$$

then, $\text{sgn } U_{N'} = (-1)^m$, $\text{sgn } U_{N'-1} = (-1)^{m-1}$ and $\text{sgn}(U_{N'}/U_{N'-1}) = -1$, implying

$$\alpha_{N'+1} = \left(N'n - (m-1) - \frac{1}{2} \right) \pi + \left(n - \frac{1}{2} \right) \pi - \frac{\pi}{2} = \left((N'+1)n - m - \frac{1}{2} \right) \pi, \quad (4.33)$$

and we conclude by Eq. (2.6). On the other hand, if

$$\cos\left(\frac{(m+1)\pi}{N'}\right) < \cos\left(\frac{(m+1)\pi}{N'+1}\right) < \rho < \cos\left(\frac{m\pi}{N'}\right), \quad (4.34)$$

then, $\text{sgn } U_{N'} = \text{sgn } U_{N'-1} = (-1)^m$ and $\text{sgn}(U_{N'}/U_{N'-1}) = 1$, implying

$$\alpha_{N'+1} = \left(N'n - m - \frac{1}{2} \right) \pi + \left(n - \frac{1}{2} \right) \pi + \frac{\pi}{2} = \left((N'+1)n - m - \frac{1}{2} \right) \pi. \quad (4.35)$$

In the same way, for the case $\rho < \cos(N'\pi/(N'+1)) < \cos((N'-1)\pi/N')$, we have $\text{sgn } U_{N'} = (-1)^{N'}$, $\text{sgn } U_{N'-1} = (-1)^{N'-1}$ and $\text{sgn}(U_{N'}/U_{N'-1}) = -1$, implying

$$\alpha_{N'+1} = \left(N'n - (N'-1) - \frac{1}{2} \right) \pi + \left(n - \frac{1}{2} \right) \pi - \frac{\pi}{2} = \left((N'+1)n - N' - \frac{1}{2} \right) \pi. \quad (4.36)$$

Finally, consider the case $\rho = \cos(m\pi/(N'+1))$, $m = 1, \dots, N'$. Then, $A = 0$ and

$$\cos\left(\frac{m\pi}{N'}\right) < \cos\left(\frac{m\pi}{N'+1}\right) < \cos\left(\frac{(m-1)\pi}{N'}\right). \quad (4.37)$$

Thus,

$$\alpha_{N'+1} = (N'n - (m-1) - \frac{1}{2})\pi + (n - \frac{1}{2})\pi = ((N'+1)n - m)\pi \quad (4.38)$$

and we conclude by Eq. (2.7).

(B) If $v(x)$ supports a “half bound state,” then $\alpha = n\pi$ and, by points (B) and (C) of Proposition 1, $A = 0$. Thus,

$$\alpha_{N'+1} = \alpha_{N'} + n\pi = \alpha_{N'-1} + 2n\pi = \dots = \alpha + N'n\pi = (N'+1)n\pi, \quad (4.39)$$

for all $d \geq a$, which is the desired result, according to Eq. (2.7).

It is not difficult to check that, for a nonsymmetric $v(x)$, the result of Proposition 2 remains true. For this, notice that (4.3) holds for any shape of the composing potential $v(x)$, so the same is true for the resonance conditions (4.9). For a nonsymmetric $v(x)$ the proof remains essentially the same, apart from the case $\rho \neq \cos(m\pi/N)$ where one has to use the condition $\alpha'_{r_1} + \alpha'_{r_2} + 2d$ instead of $h_1 + h_2 + 2d$, and the corresponding formulas for the reflection coefficients.^{3,4}

Condition (i) is always realized for a d sufficiently large and is consistent with the limiting case of N infinitely separated potentials. As d approaches one of the resonance distances (4.9), for instance d_1 , a bound-state level approaches the onset of the continuum and give rise to a vanishing reflection coefficient at threshold. Then, the zero-energy “bound state” becomes unbound when $d < d_1$, and transforms into a resonance. In other terms, a superlattice composed of N identical potentials admits, in general, at most $N-1$ zero-energy resonance distances and can lose at most $N-1$ bound states by decreasing the spacing d separating the potentials. On the contrary, if the composing potential supports itself a “half bound state” [point (B) of the proposition], then the number of bound states of the entire superlattice remains constant as the “period” d varies.

To illustrate the content of Proposition 2, we have plotted in Fig. 1 the bound-state levels and resonances for a system of $N=7$ attractive delta-function potentials $\lambda\delta(x)$, $\lambda < 0$, as a function of

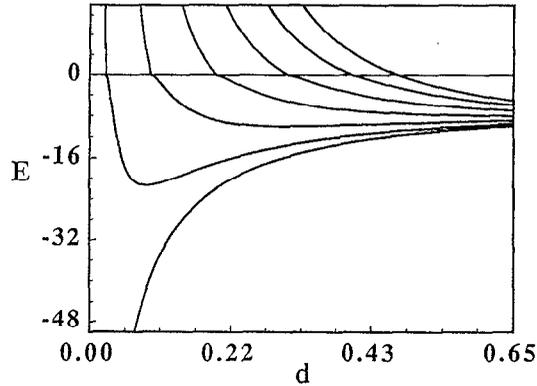


FIG. 1. Bound-state levels and resonances of a superlattice of $N=7$ attractive delta-function potentials $\lambda\delta(x)$, as a function of the “period” $d \geq 0$. The plot is for $\lambda=-4$ and $m=1$.

$d \geq 0$ ($a=0$ for a delta-function potential). In this case $h = -\sqrt{c} = -1/m|\lambda|$, where m is the mass of the incoming particle and we have set $\hbar=1$. In the limiting case $d \rightarrow \infty$, $V_N(x)$ has one bound-state level of energy $E = -m\lambda^2/2$, seven times degenerate, which corresponds to the only bound-state level of the single potential. In accordance with point (A) of the proposition, the superlattice loses, one by one, six of its seven bound states (which transform into resonances) as d approaches each of the resonant distances $d_j = (1/m|\lambda|)(1 - \cos(j\pi/7))$, $j=1, \dots, 6$. Finally, for $d=0$, the seven delta-function potentials are superimposed at the origin and one is left with only one bound state of energy $-m(7\lambda)^2/2$. For the plot we have chosen $\lambda=-4$ and $m=1$.

Figure 2 illustrates point (B) of Proposition 2. For this, we have considered the single potential $v(x) = \lambda(\delta(x) + \delta(x - 1/m|\lambda|))$, which has exactly one bound state and a zero-energy resonance. Contrary to the case of Fig. 1, we now observe that the number of bound states remains constant as d varies from infinity to $a = 1/m|\lambda|$.

A comment is in order. According to Proposition 2, one may be tempted to conclude that a multipotential system of N nonoverlapping potentials can only lose bound states by decreasing the distances separating the potentials. However, this is true only in the case where all the distances and potentials are the same, i.e., in the special case of a finite periodic potential. To see this,

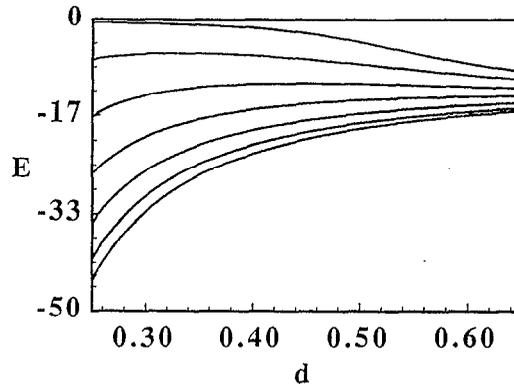


FIG. 2. Bound-state levels of a superlattice of $N=7$ double delta-function potentials $\lambda(\delta(x) + \delta(x - 1/m|\lambda|))$, as a function of the “period” $d \geq 1/m|\lambda|$. The plot is for $\lambda=-4$ and $m=1$.

consider for instance the potential $v(x) + v(x-d) + v(x-d-\gamma)$, where $d \geq a$ and $\gamma > 0$ is fixed. It is then an easy exercise to show that the system loses a bound state when d decreases below the value $-h + \frac{1}{2}(\sqrt{\gamma^2 + c} - \gamma)$, but subsequently gets it back at $d = -h$, when the double potential $v(x) + v(x-d)$ has a zero-energy resonance.

V. A LOWER BOUND FOR THE TIME DELAY AT THRESHOLD

For the potential $v(x)$, with support in the interval $[-a/2, a/2]$, we define the reduced time delay

$$\tilde{\tau}(k) = \frac{k}{ma} \tau(k) = \frac{1}{a} h(k) = \frac{1}{a} \alpha'_t(k). \quad (5.1)$$

For a classical particle, causality implies $\tilde{\tau}_{cl}(k) \geq -1$, for all k . In quantum mechanics, the same lower bound holds, in general, in the high energy limit.¹⁰ In Ref. 5, it was shown that it also holds in the low energy limit, when the potential has no bound-state solutions. Actually, according to the analysis hereabove, a stronger lower bound can be proven in this case. More precisely, we have the following.

Proposition 3: Let $v(x)$ be a finite range potential, with support in the interval $I = [-a/2, a/2]$, supporting no bound state solutions. Then,

$$\tilde{\tau} = \lim_{k \rightarrow 0} \tilde{\tau}(k) \geq -1 + \frac{\sqrt{c}}{a}. \quad (5.2)$$

Proof: According to Proposition 2, one has, for $a \leq d \leq d_1 = -h + \sqrt{c} \cos(\pi/N)$, $\alpha_N \leq (Nn-1)\pi$. If the potential has no bound states, then $n=0$ and $\alpha_N \leq -\pi$, in contradiction with Levinson's theorem (2.6), (2.7). Thus $a > -h + \sqrt{c} \cos(\pi/N)$ or, equivalently,

$$\tilde{\tau} > -1 + \cos(\pi/N) \frac{\sqrt{c}}{a}. \quad (5.3)$$

Then, taking the limit $N \rightarrow \infty$, we find (5.2).

Consider, as an illustration, the case $v(x) = \lambda \chi_I(x)$, $\lambda > 0$. Then, a straightforward calculation yields

$$\tilde{\tau} = -1 + \cosh(\sqrt{2m\lambda a}) \frac{\sqrt{c}}{a}, \quad \sqrt{c} = \frac{2}{\sqrt{2m\lambda} |\sinh(\sqrt{2m\lambda a})|}, \quad (5.4)$$

in agreement with Proposition 3, since $\cosh(\sqrt{2m\lambda a}) \geq 1$. It is worth noting that, in the limit of a delta-function potential ($\lambda \rightarrow \lambda/a, a \rightarrow 0$), $\cosh(\sqrt{2m\lambda a}) \rightarrow 1$. Hence, the inequality (5.2) is in fact an equality in this special case.

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