Levinson's theorem, zero-energy resonances, and time delay in one-dimensional scattering systems

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The one-dimensional Levinson's theorem is derived and used to study zero-energy resonances in a double-potential system. The low energy behavior of time delay is also investigated. In particular, it is shown that the quantum mechanical time delay admits a classical lower bound, in the low energy limit, if the potential has no bound-state solutions.

I. INTRODUCTION

The Levinson's theorem in its usual formulation[1,2] asserts that for a spherically symmetric potential $V(r)$ producing the phase shift $\delta_\ell(k)$ and n_ℓ bound states of angular momentum ℓ, one has, with the convention $\delta_\ell(\infty)=0$

$$\delta_\ell(0)=n_\ell\pi \tag{1.1}$$

for $\ell\geqslant 1$ and

$$\delta_0(0)=n_0\pi \tag{1.2}$$

or

$$\delta_0(0)=(n_0+\tfrac{1}{2})\pi \tag{1.3}$$

for $\ell=0$, according to whether there is a zero-energy solution (which vanishes at the origin and is finite at infinity) or not. The exceptional case (1.3) occurs when the Jost function of the S wave vanishes at threshold. One usually speaks of the occurrence of a "half bound state" [because of the additional term 1/2 in Eq. (1.3)] or of a zero-energy resonance (since the S-wave total scattering cross section approaches infinity at threshold).

A lot of literature is devoted to the proof of Levinson's theorem, Eqs. (1.1)–(1.3), for central potentials and its generalized versions for scattering by nonspherically symmetric and/or nonlocal potentials (see Ref. 3 and the references cited there). For instance, the exact analog, in the case of noncentral potentials, of the S-wave zero-energy resonance (1.3) has been obtained by Newton[4] by the method of the Fredholm theory (however, for noncentral potentials, "half bound states" do not appear to be related to specific values of the angular momentum).

Although they bring into play a variety of mathematical methods, all these extensions of Levinson's theorem are the consequence of a common simple principle. This principle is the orthogonality and completeness relation for the eigenfunctions of the total Hamiltonian, as was first noticed by Jauch.[5]

The role played by the completeness of states in the derivation of Levinson's theorem was recently emphasized by Poliatzky,[6] showing that the full information on phase shifts contained in the normalization integral for the scattering wave functions, when combined with the completeness relation, allows to derive Levinson's theorem in a simple and general way. In particular, it was pointed out in Ref. 6 that besides the well-known "half bound states," a second kind of zero-energy solution may occur for the S-wave scattering, with an additional term 1/4 instead of 1/2.

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Levinson's theorem may also be considered as the consequence of another basic principle. This principle is the spectral property of time delay which states that the total time delay experienced by an incident plane wave of energy E is proportional to the change of state density produced by the interaction (see Ref. 3).

However, the intimate relationship between the number of bound states and the energy integral of time delay (the spectral property) is also an immediate consequence of the completeness and orthogonality relation for the eigenfunctions of the total Hamiltonian. This will be emphasized in Sec. II where a general version of the one-dimensional Levinson's theorem is derived. By the way, we shall also point out that there is something missing in the derivation in Ref. 6 and that "quarter bound state" solutions are unphysical.

Levinson's theorem is then used in Sec. III to study the mechanism of the appearence of zero-energy resonances in a double-potential system, as the distance d between the two potentials is varied. The time delay at zero-energy resonance is evaluated and compared to the $E \neq 0$ resonance case. Finally, in Sec. IV, causality in the zero-energy limit is investigated. It is found that the quantum mechanical time delay obeys the classical causal bound not only in the high energy limit, when the particle hardly sees the scatterer, but also in the low energy limit, if the potential has no bound-state solutions.

II. THE ONE-DIMENSIONAL LEVINSON'S THEOREM

Consider the one-dimensional Schrödinger equation

$$\frac{\partial^2 \psi}{\partial x^2}(k,x)+(k^2-2mV(x))\psi(k,x)=0, \tag{2.1}$$

where $x \in \mathbb{R}$ is the space coordinate, $k \geq 0$ the magnitude of the incident momentum, and $V(x)$ the potential. For sake of simplicity we shall assume in what follows that $V(x)$ is bounded everywhere and that $V(x)=0$ for $x \leq x_1$ and $x \geq x_2$. Then, all the formal operations in our discussion below are easily proven to be legitimate (see, for instance, Refs. 7 and 8).

The physical solutions of Eq. (2.1) are the two linearly independent solutions $\psi_\pm(k,x)$, uniquely determined by the boundary conditions

$$\psi_+(k,x)=\begin{cases} T(k)e^{ikx}, & \text{if} \quad x \geq x_2 \\ e^{ikx}+L(k)e^{-ikx}, & \text{if} \quad x \leq x_1 \end{cases} \tag{2.2}$$

and

$$\psi_-(k,x)=\begin{cases} e^{-ikx}+R(k)e^{ikx}, & \text{if} \quad x \geq x_2 \\ T(k)e^{-ikx}, & \text{if} \quad x \leq x_1, \end{cases} \tag{2.3}$$

where $T(k)$ is the transmission coefficient and, $L(k)$ and $R(k)$ are the reflection coefficients from the left and right, respectively. The scattering matrix $S(k)$ is a 2×2 unitary matrix defined as

$$S(k)=\begin{pmatrix} T(k) & R(k) \\ L(k) & T(k) \end{pmatrix}, \tag{2.4}$$

which can be shown to be continuous and such that[7]

$$S(k)=I+O\left(\frac{1}{k}\right) \tag{2.5}$$

as $k \rightarrow \infty$. The spectrum of Eq. (2.1) is known to be complete.[7] Thus, we have the completeness relationship

$$\sum_{j=1}^{N} \psi_{E_j}^*(x)\psi_{E_j}(x')+\frac{1}{2\pi}\sum_{\rho=\pm}\int_0^\infty dk\ \psi_\rho^*(k,x)\psi_\rho(k,x')=\delta(x-x'), \tag{2.6}$$

where $\psi_{E_j}(x)$, $E_j<0$ are the bound-states eigenfunctions, normalized according to

$$\int_{-\infty}^{\infty} dx|\psi_{E_j}(x)|^2=1. \tag{2.7}$$

On the other hand, for the free particle $[V(x)=0]$ there are no bound-state solutions and the completeness relation simply reads

$$\frac{1}{2\pi}\sum_{\rho=\pm}\int_0^\infty dk\ \psi_\rho^{0*}(k,x)\psi_\rho^0(k,x')=\delta(x-x'), \tag{2.8}$$

where $\psi_\pm^0(k,x)=e^{\pm ikx}$. Substracting Eq. (2.8) from Eq. (2.6), then setting $x=x'$ and integrating from $-R$ to R, one finds

$$\int_0^\infty dk\ \frac{k}{m}\ \mathrm{Tr}\ \tau(k,R)=-2\pi\sum_{j=1}^{N}\int_{-R}^{R} dx|\psi_{E_j}(x)|^2, \tag{2.9}$$

where

$$\mathrm{Tr}\ \tau(k,R)=\frac{m}{k}\sum_{\rho=\pm}\int_{-R}^{R} dx(|\psi_\rho(k,x)|^2-|\psi_\rho^0(k,x)|^2) \tag{2.10}$$

is the trace of the (on shell) time delay operator $\tau(k,R)$ for a (here one-dimensional) ball of radius R (see Ref. 3). According to Eq. (2.7), one then obtains

$$\lim_{R\to\infty}\int_0^\infty dk\ \frac{k}{m}\ \mathrm{Tr}\ \tau(k,R)=-2\pi N. \tag{2.11}$$

It is worth noting that the same reasoning leading to Eq. (2.11) can be easily generalized to the case of more than one spatial dimension as long as a completeness relation between scattering states and bound states holds. Indeed, Eq. (2.11) constitutes the most general statement on the link between time delay and bound states. To derive from Eq. (2.11) the one-dimensional Levinson's theorem (i.e., the relationship between scattering phase shifts and bound states) it is useful to consider the solutions of Eq. (2.1) of the form

$$\begin{bmatrix} u_+(k,x) \\ u_-(k,x) \end{bmatrix}=U(k)\begin{bmatrix} \psi_+(k,x) \\ \psi_-(k,x) \end{bmatrix}, \tag{2.12}$$

where

$$U(k)=\frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{R(k)/L(k)} & -1 \\ 1 & \sqrt{L(k)/R(k)} \end{pmatrix}\equiv\frac{1}{\sqrt{2}}\begin{pmatrix} e^{2i\gamma(k)} & -1 \\ 1 & e^{-2i\gamma(k)} \end{pmatrix} \tag{2.13}$$

is the k-dependent unitary transformation which diagonalizes the scattering matrix, i.e.,

$$U(k)S(k)U^{\dagger}(k)=\begin{pmatrix} e^{2i\delta_+(k)} & 0 \\ 0 & e^{2i\delta_-(k)} \end{pmatrix}, \tag{2.14}$$

with

$$e^{2i\delta_+(k)}=T(k)-\sqrt{L(k)R(k)}, \quad e^{2i\delta_-(k)}=T(k)+\sqrt{L(k)R(k)}, \tag{2.15}$$

or, equivalently,

$$T(k)=\tfrac{1}{2}(e^{2i\delta_-(k)}+e^{2i\delta_+(k)})=e^{i(\delta_-(k)+\delta_+(k))}\cos(\delta_-(k)-\delta_+(k)), \tag{2.16}$$

and

$$\sqrt{L(k)R(k)}=\tfrac{1}{2}(e^{2i\delta_-(k)}-e^{2i\delta_+(k)})=e^{i(\delta_-(k)+\delta_+(k)+(\pi/2))}\sin(\delta_-(k)-\delta_+(k)). \tag{2.17}$$

According to Eq. (2.13), we also have

$$L(k)=e^{i(\delta_-(k)+\delta_+(k)+2\gamma(k)+(\pi/2))}\sin(\delta_-(k)-\delta_+(k)) \tag{2.18}$$

and

$$R(k)=e^{i(\delta_-(k)+\delta_+(k)-2\gamma(k)+(\pi/2))}\sin(\delta_-(k)-\delta_+(k)). \tag{2.19}$$

From Eqs. (2.12) and (2.13), one finds that the solutions $u_{\pm}(k,x)$ satisfy the boundary conditions

$$u_+(k,x)=i\sqrt{2}e^{i(\delta_+(k)+\gamma(k))}\begin{cases} \sin(kx+\gamma(k)+\delta_+(k)), & \text{if} \quad x\geqslant x_2 \\ \sin(kx+\gamma(k)-\delta_+(k)), & \text{if} \quad x\leqslant x_1 \end{cases} \tag{2.20}$$

and

$$u_-(k,x)=\sqrt{2}e^{i(\delta_-(k)-\gamma(k))}\begin{cases} \cos(kx+\gamma(k)+\delta_-(k)), & \text{if} \quad x\geqslant x_2 \\ \cos(kx+\gamma(k)-\delta_-(k)), & \text{if} \quad x\leqslant x_1. \end{cases} \tag{2.21}$$

Furthermore, $U(k)$ being unitary, they also satisfy the completeness relationship

$$\sum_{j=1}^{N} \psi^*_{E_j}(x)\psi_{E_j}(x')+\frac{1}{2\pi}\sum_{\rho=\pm}\int_0^{\infty} dk\ u^*_{\rho}(k,x)u_{\rho}(k,x')=\delta(x-x'). \tag{2.22}$$

A. The symmetric case

For a parity invariant potential $V(x)=V(-x)$, $x_2=-x_1$, we have $R(k)=L(k)$ implying $\gamma(k)=0$. Then, $u_+(k,x)$ and $u_-(k,x)$ correspond to the usual diagonal representation of the scattering matrix in terms of odd and even functions of the momentum k. In this special case, the completeness relationship between scattering solutions and bound-state solutions holds separately for the odd and even states, i.e.,

$$\sum_{j=1}^{n_\pm} \psi^*_{\pm,E_j}(x)\psi_{\pm,E_j}(x')+\frac{1}{2\pi}\int_0^{\infty} dk\ u^*_{\pm}(k,x)u_{\pm}(k,x')=\delta(x-x')\mp\delta(x+x'), \tag{2.23}$$

where $\psi_{\pm,E_j}(x)$ are, respectively, the odd and even bound-state eigenfunctions and $n_+ + n_- = N$. Substracting the completeness relation for the free particles solutions $u^0_{\pm}(k,r)$ [corresponding to $\delta_{\pm}(k)=0$] from Eq. (2.23), then setting $x=x'$ and integrating from $-R$ to R, one finds

$$\int_0^\infty dk \frac{k}{m} \tau_\pm(k,R) = -2\pi \sum_{j=1}^{n_\pm} \int_{-R}^{R} dx |\psi_{\pm,E_j}(x)|^2, \tag{2.24}$$

where

$$\tau_\pm(k,R) = \frac{m}{k} \int_{-R}^{R} dx(|u_\pm(k,x)|^2 - |u_\pm^0(k,x)|^2) \tag{2.25}$$

are, respectively, the time delays for the interval $[-R, R]$ and for an incoming odd and even wave of energy $E=k^2/2m$ (see Ref. 3). By differentiating the Schrödinger equation (2.1) with respect to k, one finds the identity[3]

$$|u_\pm(k,r)|^2 = \frac{1}{k} \frac{\partial}{\partial x} \left(\frac{\partial u_\pm^*}{\partial x} \frac{\partial u_\pm}{\partial k} - u_\pm^* \frac{\partial^2 u_\pm}{\partial x \partial k} \right)(k,x) \tag{2.26}$$

from which the time delays (2.25) are readily calculated, for large R, using the asymptotic form (2.20), (2.21) [here with $\gamma(k)=0$] with the result (we use the prime to denote the derivative with respect to k)

$$\begin{aligned}\tau_\pm(k,R) &= 2 \frac{m}{k} \delta'_\pm(k) \mp \frac{m}{k^2} [\sin(2kR + 2\delta_\pm(k)) - \sin(2kR)] \\ &= \frac{m}{k} \left(2\delta'_\pm(k) \pm \pi \sin^2 \delta_\pm(k) \frac{\sin 2kR}{\pi k} \mp \frac{\sin 2\delta_\pm(k)}{k} \cos 2kR \right).\end{aligned} \tag{2.27}$$

Inserting Eq. (2.27) into Eq. (2.24) we obtain, for R sufficiently large

$$\begin{aligned}&\delta_\pm(\infty) - \delta_\pm(0) \pm \frac{\pi}{2} \int_0^\infty dk \sin^2 \delta_\pm(k) \frac{\sin 2kR}{\pi k} \mp \frac{1}{2} \int_0^\infty dk \frac{\sin 2\delta_\pm(k)}{k} \cos 2kR \\ &= -\pi \sum_{j=1}^{n_\pm} \int_{-R}^{R} dx |\psi_{\pm,E_j}(x)|^2.\end{aligned} \tag{2.28}$$

Moreover, if we define $\delta_\pm(k)$ to be continuous for $0 \leq k < \infty$ and such that [use Eq. (2.5)]

$$\delta_\pm(k) = O\left(\frac{1}{k}\right) \tag{2.29}$$

we find from Eqs. (2.7) and (2.29) that Eq. (2.28) yields, as $R \to \infty$ [when $k=0$ we drop it from the notation, i.e., $\delta_\pm \equiv \delta_\pm(0)$]

$$\delta_\pm = n_\pm \pi \pm \frac{\pi}{2} \sin^2 \delta_\pm . \tag{2.30}$$

Furthermore, the right hand side of Eq. (2.28) being finite [because of Eq. (2.7) and the finiteness of the number of bound states], the integrals in the left hand side of Eq. (2.28) are also finite [since $\delta_\pm(\infty)=0$ and the continuous functions $\delta_\pm(k)$ have a finite limit as $k \to 0$]. Their integrability at infinity follows from Eq. (2.29) but the integrability at the origin of the second integral implies

$$\sin 2\delta_\pm = 0. \tag{2.31}$$

Clearly, the only solutions for Eqs. (2.30) and (2.31) are, for the odd states

$$\delta_+ = n_+\pi, \quad \delta_+ = (n_+ + \tfrac{1}{2})\pi \tag{2.32}$$

corresponding, respectively, to the case without and with a zero-energy solution (or zero-energy resonance or "half bound state"). On the other hand, for the even states, one finds

$$\delta_- = (n_- - \tfrac{1}{2})\pi, \quad \delta_- = n_-\pi, \tag{2.33}$$

where again the second solution corresponds to the case of a zero-energy resonance.

Notice that the scattering problem for $u_+(k,x)$ is the same as the three-dimensional S-wave scattering problem and yields the same solutions (1.2), (1.3) with n_+ replaced by the total number n_0 of bound states of zero angular momentum. On the other hand, the even solutions (2.33) differ from the odd ones by an additional term $-1/2$.

In Ref. 6 it was pointed out that

$$\delta_\pm = (n_\pm \pm \tfrac{1}{4})\pi \tag{2.34}$$

are also solutions of Eq. (2.30). However, they cannot represent a second kind of physically realizable zero-energy solutions, since they break condition (2.31).

A physical zero-energy solution of the one-dimensional Schrödinger equation (2.1) is a nonzero constant solution outside the range of the potential. Thus, it is not normalizable and it is part of the continuum. However, contrary to the continuous spectrum which is doubly degenerate (the particle can come either from the left or from the right), a zero-energy solution is nondegenerate (as it is in the case for the discrete spectrum). Indeed, the Wronskian of two solutions of a one-dimensional Schrödinger equation is a constant which, for linearly independent solutions, differs from zero. But the Wronskian of two zero-energy solutions, which are constant far from the potential, is clearly zero implying that they must be linearly dependent. Thus, we must have $\psi_+(0,x) = \alpha\psi_-(0,x)$, $\alpha \in \mathrm{C}$, which implies, according to Eqs. (2.2), (2.3) [here with $L(k) = R(k)$ and we have set $L \equiv L(0)$, $T \equiv T(0)$]

$$1 + L = T \quad \text{or} \quad 1 + L = -T \tag{2.35}$$

corresponding, respectively, to the even and odd solutions. Moreover, from the unitarity of the scattering matrix (2.4), it follows that

$$|T|^2 + |L|^2 = 1, \quad \mathrm{Re}\, TL^* = 0. \tag{2.36}$$

Equations (2.35) and (2.36) may then be easily solved and one finds that the only solutions are

$$T = 0, \quad L = -1 \tag{2.37}$$

or

$$T = -1, \quad L = 0 \tag{2.38}$$

or

$$T = 1, \quad L = 0. \tag{2.39}$$

According to Eqs. (2.16), (2.17) we find that Eq. (2.37) corresponds to the choice

$$\delta_+ = n_+\pi, \quad \delta_- = (n_- - \tfrac{1}{2})\pi, \tag{2.40}$$

without zero-energy resonance. On the other hand, Eqs. (2.38) and (2.39) correspond, respectively, to

$$\delta_+ = (n_+ + \tfrac{1}{2})\pi, \quad \delta_- = (n_- - \tfrac{1}{2})\pi, \tag{2.41}$$

with an odd zero-energy resonance and to

$$\delta_+ = n_+ \pi, \quad \delta_- = n_- \pi, \tag{2.42}$$

with an even zero-energy resonance. In other terms, the reflection probability $|R(k)|^2$ is "normally" unity at threshold, when the potential supports no zero-energy solution. On the contrary, when a zero-energy solution exists, one observes a resonance transmission (i.e., a vanishing reflection coefficient) at threshold.

B. The nonsymmetric case

Consider now the case of a nonsymmetric potential $V(x)$. Then, expressing the trace (2.10) in terms of the solutions (2.12) and using again the identity (2.26), we find, for a large R

$$\begin{aligned}
\mathrm{Tr}\ \tau(k,R) &= \frac{m}{k} \sum_{\rho=\pm} \int_{-R}^{R} dx(|u_\rho(k,x)|^2 - |u_\rho^0(k,x)|^2) \\
&= 2\,\frac{m}{k}\,(\delta'_+(k) + \delta'_-(k)) - \frac{m}{k^2} \cos 2\gamma(k)[\sin(2kR + 2\delta_+(k)) - \sin(2kR + 2\delta_-(k))] \\
&= \frac{m}{k} \left\{ 2\delta'_+(k) + 2\delta'_-(k) + \cos 2\gamma(k) \left[(\pi \sin^2 \delta_+(k) - \pi \sin^2 \delta_-(k))\, \frac{\sin 2kR}{\pi k} \right.\right. \\
&\quad \left.\left. + \frac{2}{k} \sin(\delta_-(k) - \delta_+(k)) \cos(\delta_-(k) + \delta_+(k)) \cos 2kR \right] \right\}.
\end{aligned} \tag{2.43}$$

Inserting Eq. (2.43) into Eq. (2.9), then taking the limit $R \to \infty$ and using Eq. (2.29), we find [with $\gamma \equiv \gamma(0)$]

$$\delta_+ + \delta_- = \pi N + \frac{\pi}{2} \cos 2\gamma (\sin^2 \delta_+ - \sin^2 \delta_-) = \pi N - \frac{\pi}{2} \cos 2\gamma \sin(\delta_- - \delta_+) \sin(\delta_- + \delta_+) \tag{2.44}$$

together with the condition [the analog of Eq. (2.31)]

$$\cos 2\gamma \sin(\delta_- - \delta_+) \cos(\delta_- + \delta_+) = 0. \tag{2.45}$$

To solve Eqs. (2.44),(2.45), we start by considering the case $\cos 2\gamma \neq 0$. Then, Eq. (2.45) gives $\sin(\delta_- - \delta_+)\cos(\delta_- + \delta_+) = 0$. If $\cos(\delta_- + \delta_+) = 0$, then Eq. (2.44) yields $|\cos 2\gamma \sin(\delta_- - \delta_+)| = 1$. For the case $\cos 2\gamma = 1$, the solutions are clearly of the form (with n and m positive integers)

$$\delta_+ = n\pi, \quad \delta_- = (m - \tfrac{1}{2})\pi, \quad n + m = N \tag{2.46}$$

and

$$\delta_+ = (n + \tfrac{1}{2})\pi, \quad \delta_- = m\pi, \quad n + m = N. \tag{2.47}$$

On the other hand, for $\cos 2\gamma = -1$, one finds

$$\delta_+ = (n - \tfrac{1}{2})\pi, \quad \delta_- = m\pi, \quad n+m=N \tag{2.48}$$

and

$$\delta_+ = n\pi, \quad \delta_- = (m+\tfrac{1}{2})\pi, \quad n+m=N. \tag{2.49}$$

However, for the solutions (2.47) and (2.49), $u_+(0,x)$ and $u_-(0,x)$ are readily seen to be linearly independent. Thus, they must be discarded (we recall that a physical zero-energy solution is nondegenerate). Moreover, by Eqs. (2.18) and (2.19) one finds that Eqs. (2.46) and (2.48) correspond to $L=R=-1$, i.e., to a reflection probability which is unity at threshold.

If $\cos(\delta_- + \delta_+) \neq 0$, then $\sin(\delta_- - \delta_+)=0$ and Eq. (2.44) gives $\delta_+ + \delta_- = N\pi$. Thus, the solutions are of the form

$$\delta_+ = (n \pm \tfrac{1}{2})\pi, \quad \delta_- = (m \mp \tfrac{1}{2})\pi, \quad n+m=N \tag{2.50}$$

or

$$\delta_+ = n\pi, \quad \delta_- = m\pi, \quad n+m=N \tag{2.51}$$

yielding, respectively, [use Eq. (2.16)] $T=-1$ and $T=1$, i.e., a vanishing reflection coefficient at threshold.

Finally, for $\cos 2\gamma=0$, we also have $\delta_+ + \delta_- = N\pi$ but the difference $\delta_- - \delta_+$ may now in principle take any value and one can only say that a finite portion of the incident particles is transmitted at threshold. Notice however that $T \neq 0$. Indeed, if $T=0$, then $\psi_\pm(0,x)=0$ for all x, so that we must have $L=R=-1$. But for $\cos 2\gamma=0$, it follows from Eqs. (2.18) and (2.19) that $L=-R$, in contradiction to the assertion hereabove.

To summarize, let us reformulate the results hereabove in terms of the phases $\alpha_T(k) = \arg T(k)$, $\alpha_L(k) = \arg L(k)$, and $\alpha_R(k) = \arg R(k)$ of the transmission and reflection coefficients. For this, we observe from Eqs. (2.16) and (2.17) that, modulo π

$$\alpha_T(k) = \delta_-(k) + \delta_+(k), \quad \tfrac{1}{2}(\alpha_L(k) + \alpha_R(k)) = \delta_-(k) + \delta_+(k) + \frac{\pi}{2}. \tag{2.52}$$

Thus, setting

$$\alpha_T(\infty) = 0, \quad \tfrac{1}{2}(\alpha_L(\infty) + \alpha_R(\infty)) = \frac{\pi}{2} \tag{2.53}$$

we obtain the solutions (dropping the $k=0$ argument)

$$\alpha_T = (N - \tfrac{1}{2})\pi, \quad \tfrac{1}{2}(\alpha_L + \alpha_R) = N\pi, \quad L=R=-1 \tag{2.54}$$

and

$$\alpha_T = N\pi, \quad \tfrac{1}{2}(\alpha_L + \alpha_R) = (N + \tfrac{1}{2})\pi, \quad T \neq 0 \tag{2.55}$$

corresponding, respectively, to the case without and with zero-energy resonance. For the special case of a symmetric potential we have $L(k)=R(k)$ and, according to Eqs. (2.37)–(2.42), Eqs. (2.54),(2.55) are, respectively, to be replaced by

$$\alpha_T = (N - \tfrac{1}{2})\pi, \quad \alpha_L = N\pi, \quad L=-1 \tag{2.56}$$

and

$$\alpha_T = N\pi, \quad \alpha_L = (N+\tfrac{1}{2})\pi, \quad L=0. \tag{2.57}$$

A different proof of the one-dimensional Levinson's theorem, with the help of the analytic properties of the Jost functions, is given in Ref. 9. Note that the theorem is incorrectly stated in Ref. 9 but subsequently corrected in Ref. 10, footnote 20; see also Ref. 11. A very simple heuristic derivation of the one-dimensional Levinson's theorem is also given in Ref. 12 for the special case of a reflectionless potential. However, since for a reflectionless potential $L(k)=0$ for all k, the authors find result (2.55) with a zero-energy resonance (or "half bound state"), i.e., they find the "exceptional" case instead of the "generic" one.

III. ZERO-ENERGY RESONANCES IN A DOUBLE-POTENTIAL SYSTEM

The purpouse of the present section is to use the results (2.53)–(2.57) to study the mechanism of the appearance of zero-energy resonances in the one-dimensional scattering by the potential

$$V(x) = v\left(x+\frac{d}{2}\right) + v\left(x-\frac{d}{2}\right), \tag{3.1}$$

where $v(x)$ is a finite range potential with support in the interval $[-a/2,\ a/2]$ and $d \geqslant a$. For this, we first observe that, in one dimension, the scattering matrix (2.4) for a potential $V(x)$ can be expressed in a rather simple way in terms of the scattering matrices of the fragments of that potential. To be more precise, we write the potential $V(x)$ as the sum

$$V(x) = V_1(x) + V_2(x), \tag{3.2}$$

where we have defined ($y \in \mathrm{R}$)

$$V_1(x) \equiv V(x)\chi_{(-\infty,y)}(x), \quad V_2(x) \equiv V(x)\chi_{(y,\infty)}(x), \tag{3.3}$$

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

$$S_i(k) = \begin{pmatrix} T_i(k) & R_i(k) \\ L_i(k) & T_i(k) \end{pmatrix} \tag{3.4}$$

be the scattering matrix for the potential $V_i(x)$, $i=1,2$. Then, we have the factorization formula[13]

$$\begin{pmatrix} \dfrac{1}{T(k)} & -\dfrac{R(k)}{T(k)} \\ \dfrac{L(k)}{T(k)} & \dfrac{1}{T(k)^*} \end{pmatrix} = \begin{pmatrix} \dfrac{1}{T_1(k)} & -\dfrac{R_1(k)}{T_1(k)} \\ \dfrac{L_1(k)}{T_1(k)} & \dfrac{1}{T_1(k)^*} \end{pmatrix} \begin{pmatrix} \dfrac{1}{T_2(k)} & -\dfrac{R_2(k)}{T_2(k)} \\ \dfrac{L_2(k)}{T_2(k)} & \dfrac{1}{T_2(k)^*} \end{pmatrix}. \tag{3.5}$$

Clearly, the double-potential (3.1) is the sum of two compactly supported fragments and we may apply the factorization formula (3.5). For this, let

$$s(k) = \begin{pmatrix} t(k) & r(k) \\ l(k) & t(k) \end{pmatrix} \tag{3.6}$$

be the scattering matrix for the potential $v(x)$. Under the transformation $v(x) \to v(x \pm d/2)$ it is transformed as

$$s(k) \to s_\pm(k) = \begin{pmatrix} t(k) & e^{\pm ikd} r(k) \\ e^{\mp ikd} l(k) & t(k) \end{pmatrix}. \tag{3.7}$$

Thus, with $S_1(k)=s_+(k)$ and $S_2(k)=s_-(k)$, Eq. (3.5) yields for the transmission coefficient

$$T(k)=\frac{t^2(k)}{1-l(k)r(k)e^{2ikd}}. \tag{3.8}$$

For sake of simplicity, let us first consider the case of a parity invariant potential $v(x)$, i.e., $l(k)=r(k)$. Then, setting $\alpha_t(k)=\arg t(k)$ and $\alpha_l(k)=\arg l(k)$, we may also write

$$|T(k)|^2=\frac{|t(k)|^4}{1-2|l(k)|^2\cos(2\alpha_l(k)+2kd)+|l(k)|^4} \tag{3.9}$$

and

$$\alpha_T(k)=2\alpha_t(k)+A(k), \tag{3.10}$$

where we have defined

$$A(k)=\arctan\left(\frac{|l(k)|^2\sin(2\alpha_l(k)+2kd)}{1-|l(k)|^2\cos(2\alpha_l(k)+2kd)}\right). \tag{3.11}$$

It immediately follows from Eq. (3.9) that for a given $k\neq 0$, the transmission probability $|T(k)|^2=1$, if the resonance condition

$$\cos(2\alpha_l(k)+2kd)=1 \tag{3.12}$$

is fulfilled. In other terms, for a given potential $v(x)$ and $k\neq 0$, there is always an infinite number of resonance distances

$$d_n(k)=d_0(k)+\frac{n\pi}{k},\quad n=1,2,\ldots,$$
$$d_0(k)=\inf\{d|\cos(2\alpha_l(k)+2kd)=1,\quad d\geqslant a\} \tag{3.13}$$

for which the transmission probability for the double-potential (3.1) is unity. On the other hand, if $v(x)$ supports no zero-energy solution, we find from Eq. (2.56) that

$$\cos(2\alpha_l(k)+2kd)=1-2(\alpha_l'+d)^2k^2+O(k^4). \tag{3.14}$$

Thus, as $k\to 0$, the resonance condition (3.12) becomes $[h\equiv h(0)]$

$$h+d=0, \tag{3.15}$$

where we have defined the spatial shift

$$h(k)\equiv\frac{k}{m}\tau(k) \tag{3.16}$$

caused by the time delay

$$\tau(k)=|t(k)|^2\tau_t(k)+|l(k)|^2\tau_l(k)=|t(k)|^2\frac{m}{k}\alpha_t'(k)+|l(k)|^2\frac{m}{k}\alpha_l'(k)=\frac{m}{k}\alpha_t'(k)=\frac{m}{k}\alpha_l'(k). \tag{3.17}$$

For the last two equalities in (3.17), we have used $|t(k)|^2+|l(k)|^2=1$ and the fact that, according to Eq. (2.52), $\tau_t(k)=\tau_l(k)$, i.e., transmission and reflection time delays are equal for a symmetric potential (transmission and reflection time delays can be determined by a stationary phase argument; for a more general treatement see Ref. 14). Thus, contrary to the case with $k\neq 0$, as $k\to 0$, there is at most one resonance distance $d=-h$. Moreover, since we must have $d\geqslant a$, such a resonance condition can be realized only if $h\leqslant -a$, which can be the case or not depending on the particular choice for the potential $v(x)$. More precisely, we have the following:

Proposition 1: Let $V(x)=v(x+d/2)+v(x-d/2)$, $d\geqslant a$, with $v(x)$ a parity invariant potential such that $v(x)=0$ if $|x|\geqslant a/2$.

(A) Assume that $v(x)$ has $n\neq 0$ bound states and there exist $\epsilon>0$ such that $h\leqslant-(d+\epsilon)$. Then, V(x) has

(i) $N=2n$ bound states for $d>-h$;
(ii) $N=2n-1$ bound states and a "half bound state" for $d=-h$;
(iii) $N=2n-1$ bound states for $d<-h$.

(B) Assume that $v(x)$ has n bound states and a "half bound state." Then, $V(x)$ has 2n bound states and a "half bound state" for all $d\geqslant a$.

Proof: Let us apply Levinson's theorem to Eqs. (3.10),(3.11). For this, we first observe that $\alpha_T(\infty)=\alpha_t(\infty)=0$ implies $A(\infty)=\arctan(0)=0$ [$|l(\infty)|=0$, by Eq. (2.5)]. Moreover, since $|l(k)|\neq 1$ for all $k\neq 0$, the denominator in Eq. (3.11) never vanishes for $k\neq 0$, so that $A(k)$ is continuous for all k.

(A) According to Eq. (2.56), if $v(x)$ has n bound states, then $\alpha_t=(n-1/2)\pi$ and Eq. (3.10) becomes, as $k\to 0$ [$A\equiv A(0)$]

$$\alpha_T=(2n-1)\pi+A. \tag{3.18}$$

To determine A, we recall that (Ref. 9) $l(-k)=l^*(k)$, i.e., $|l(-k)|=|l(k)|$ and $\alpha_l(-k)=-\alpha_l(k)$. Thus, since [by Eq. (2.56)] $\alpha_l=n\pi$ and $|l|=1$, we have, as $k\to 0$

$$\begin{aligned}|l(k)|^2&=1-ck^2+O(k^4),\quad c>0,\\ \alpha_l(k)&=n\pi+hk+O(k^3).\end{aligned} \tag{3.19}$$

Assuming $h+d>0$, we clearly obtain

$$A=\lim_{k\to 0}\arctan\left(\frac{2(h+d)k+O(k^3)}{2(h+d)^2k^2+ck^2+O(k^4)}\right)=\frac{\pi}{2} \tag{3.20}$$

and Eq. (3.20) substituted into Eq. (3.18) yields

$$\alpha_T=(2n-\tfrac{1}{2})\pi, \tag{3.21}$$

which proves (i), according to Eq. (2.56). In the same way, for $h+d<0$, we get $A=-\pi/2$, yielding

$$\alpha_T=((2n-1)-\tfrac{1}{2})\pi \tag{3.22}$$

and establishing (iii). For the case $h+d=0$, we get from Eq. (3.11)

$$A=\lim_{k\to 0}\arctan\left(\frac{O(k^3)}{ck^2+O(k^6)}\right)=0 \tag{3.23}$$

yielding

$$\alpha_T=(2n-1)\pi \tag{3.24}$$

and proving (ii), according to Eq. (2.57). In the same way, using Eq. (3.9), it is easy to check that $|T|=0$ for the case (i) and (iii) and that $|T|=1$ for the case (ii).

(B) If $v(x)$ has n bound states and a "half bound state," then $|l|=0$ and Eqs. (3.10),(3.11) immediately yield

$$\alpha_T=2n\pi, \quad \forall d\geqslant a, \tag{3.25}$$

which is the desired result according to Eq. (2.57).

Condition (i) is always realized for a d sufficiently large, which is consistent with the limiting case of two infinitely separated potentials. As d approaches the critical value $d=-h$, 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 $d<-h$.

Finally, let us investigate the behavior of the time delay

$$\tau^V(k)=\frac{m}{k}\,\alpha_T'(k)=\frac{m}{k}\,\alpha_L'(k) \tag{3.26}$$

for the double-potential $V(x)$. Writing Eq. (3.8) in the form [here with $l(k)=r(k)$]

$$T(k)=t(k)^2+t(k)^2l(k)^2e^{2ikd}+t(k)^2l(k)^4e^{4ikd}+\cdots \tag{3.27}$$

we observe that the transmitted wave represents a sum of waves passing through the two potentials once, or after any number $2n$, $n=1,2,...,$ of internal reflections. Thus, according to Eqs. (3.10),(3.17), we find that

$$\tau^V(k)=2\tau(k)+\tau^{\text{int}}(k) \tag{3.28}$$

is the sum of the time delay for the passage through the two potentials once, plus the time delay caused by the internal back and forth of the particle in between the two potentials

$$\tau^{\text{int}}(k)=\frac{m}{k}\,A'(k). \tag{3.29}$$

When the resonance condition (3.12) is met one finds, after a straightforward calculation

$$\tau^V(k)=2\tau(k)+\frac{2|l(k)|^2}{1-|l(k)|^2}\left(\tau(k)+\frac{m}{k}\,d\right) \tag{3.30}$$

and for the spatial shift $H(k)\equiv\tau^V(k)k/m$, we have

$$H(k)=2h(k)+\frac{2|l(k)|^2}{1-|l(k)|^2}\,(h(k)+d). \tag{3.31}$$

As $|l(k)|\to 1$ (with k fixed), the multiple reflection mechanism is enhanced and it follows from Eq. (3.30) [or Eq. (3.31)] that the time delay (or the spatial shift) approaches in general plus infinity (provided that the resonance distance d is chosen sufficiently large). This is in agreement with the intuitive picture of a long lived metastable state associated with a resonance.

In the low energy limit the situation is however rather different. Indeed, the zero-energy resonance condition (3.15) has the following simple meaning: as $k\to 0$, the time delay $\tau(k)$ caused by the potential $v(x)$ approaches the value $-dm/k$, which is nothing but minus the time taken by the particle to go from one potential to the other. Thus, everything happens as if the internal back and forth of the particle takes no time in this limit. As a consequence, even though $|l(k)| \to 1$ as $k \to 0$, one finds a spatial shift $H \equiv H(0)$ at threshold which remains finite at resonance. Indeed, expanding Eq. (3.29) in powers of k, one obtains for $h+d=0$

$$H=-2d+\frac{1}{3c}\frac{\partial^3 \alpha_l}{\partial k^3}(0). \tag{3.32}$$

Notice however that if $h+d \neq 0$, one finds

$$H=2h-\frac{2(h+d)^2+c}{2(h+d)} \tag{3.33}$$

and the spatial shift H approaches plus (minus) infinity when the resonance condition is approached from negative (positive) values of $h+d$. The results of this section may be considered as a generalization of Ref. 15, where the special case of the double delta-function potential was considered.

The analysis hereabove of the double-potential system is readily generalized to the case of a nonsymmetric potential $v(x)$. In that case, one can easily check that Proposition 1 still holds if the (global) time delay $\tau(k)$ is replaced by the averaged (total) time delay

$$\frac{1}{2}\,\mathrm{Tr}\ \tau(k)=\frac{m}{k}\,\alpha_t'(k)=\frac{1}{2}\frac{m}{k}\,(\alpha_l'(k)+\alpha_r'(k)). \tag{3.34}$$

IV. CLASSICAL CAUSALITY AT ZERO ENERGY

Classical causality says that the particle cannot leave the interaction region before entering it. For a finite range potential $v(x)$, with support in the interval $[-a/2,\ a/2]$, it means that the classical sojourn time $T_{\mathrm{cl}}(k,a/2)$ in $[-a/2,\ a/2]$ must be non-negative. Thus, causality implies that the classical time delay

$$\tau_{\mathrm{cl}}(k)=T_{\mathrm{cl}}(k,a/2)-T_{\mathrm{cl}}^{v=0}(k,a/2)\geqslant -T_{\mathrm{cl}}^{v=0}(k,a/2)=-a\,\frac{m}{k}\,. \tag{4.1}$$

For the spatial shift $h_{\mathrm{cl}}(k)=\tau_{\mathrm{cl}}(k)k/m$, we thus find

$$h_{\mathrm{cl}}(k)\geqslant -a, \quad \forall k. \tag{4.2}$$

The corresponding quantum mechanical causality principle is simply the fact that the quantum sojourn time $T(k,a/2)$ is non-negative.[3] If $v(x)$ is assumed to be parity invariant, we find for the odd and even scattering states

$$T_\pm(k,a/2)=\frac{m}{k}\int_{-a/2}^{a/2} dx|u_\pm(k,x)|^2=a\,\frac{m}{k}+2\,\frac{m}{k}\,\delta_\pm'(k)\mp\frac{m}{k^2}\sin(ka+2\delta_\pm(k))\geqslant 0 \tag{4.3}$$

and therefore

$$\delta_\pm'(k)\geqslant -\frac{a}{2}\pm\frac{1}{2k}\sin(ka+2\delta_\pm(k)). \tag{4.4}$$

For the quantum spatial shift $h(k)$, we thus find

$$h(k)=\frac{k}{m}\,\tau(k)=\delta'_+(k)+\delta'_-(k)\geqslant -a+\frac{1}{2k}\,[\sin(ka+2\delta_+(k))-\sin(ka+2\delta_-(k))]\geqslant -a-\frac{1}{k}\,. \tag{4.5}$$

Because of the presence of the additional interference terms, Eq. (4.5) differs in general appreciably from Eq. (4.2). However, in the high energy limit $k\to\infty$, Eq. (4.5) clearly agrees with the classical bound (4.2). A similar result holds in the low energy limit $k\to 0$, when the potential $v(x)$ has no bound-state solutions. More precisely, we have the following:

Proposition 2: Let $v(x)$ be a parity invariant potential, with no bound-state solutions and such that $v(x)=0$ if $|x|\geqslant a/2$. Then

$$h=\lim_{k\to 0} h(k)\geqslant -a. \tag{4.6}$$

Proof: Assume, to the contrary, that $h<-a$. Then, according to Proposition 1, it is always possible to find a distance $a\leqslant d<-h$ for which the double-potential (3.1) gives $\alpha_T=((2n-1)-1/2)\pi$, with n being the number of bound states of $v(x)$. If $n=0$, we find $\alpha_T=-3\pi/2$, in contradiction with Levinson's theorem, Eqs. (2.56)–(2.57).

The same result clearly holds for a nonsymmetric potential $v(x)$ if $\tau(k)$ is replaced by $\mathrm{Tr}\,\tau(k)/2$.

To conclude, let us illustrate the content of Proposition 2 in the simple case $v(x)=\lambda\,\delta(x)$. The transmission coefficient is

$$t(k)=\frac{ik}{ik-m\lambda} \tag{4.7}$$

and

$$\alpha_t(k)=-\arctan\left(\frac{m\lambda}{k}\right). \tag{4.8}$$

If we define $\arctan(0)=0$, we find $\alpha_t(\infty)=0$ and

$$\alpha_t(0)=\begin{cases}(0-1/2)\pi, & \text{if}\quad \lambda>0\\ (1-1/2)\pi, & \text{if}\quad \lambda<0.\end{cases} \tag{4.9}$$

Thus, according to Eq. (2.56), for $\lambda>0$ the potential has no bound states and one bound state for $\lambda<0$. The spatial shift is

$$h(k)=\frac{m\lambda}{(m\lambda)^2+k^2} \tag{4.10}$$

and yields, in the low energy limit

$$h=\lim_{k\to 0} h(k)=\frac{\lambda}{|\lambda|}\,\frac{1}{m|\lambda|}\,. \tag{4.11}$$

For $\lambda>0$ (no bound states), we find

$$h=\frac{1}{m|\lambda|}>0 \tag{4.12}$$

in agreement with Proposition 2 (for a delta-function potential $a=0$). On the other hand, for $\lambda<0$, the spatial shift at threshold is

$$h=-\frac{1}{m|\lambda|}<0 \tag{4.13}$$

and thus disagrees with the classical bound (4.2).

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