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Classical Aspects of Quantum Walls in One Dimension

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Abstract. We investigate the system of a particle moving on a half line $x \geq 0$ under the general walls at $x = 0$ that are permitted quantum mechanically. These quantum walls, characterized by a parameter L, are shown to be realized as a limit of regularized potentials. We then study the classical aspects of the quantum walls, by seeking a classical counterpart which admits the same time delay in scattering with the quantum wall, and also by examining the WKB-exactness of the transition kernel based on the regularized potentials. It is shown that no classical counterpart exists for walls with $L < 0$, and that the WKB-exactness can hold only for $L = 0$ and $L = \infty$.

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1. Introduction

Quantum systems with contact interactions (*i.e.*, point interactions or reflecting boundaries) enjoy an increasing interest recently. On the theoretical side, they have been found to exhibit a number of intriguing features, many of which have been seen before only in connection with quantum field theories. Examples include renormalization [1, 2, 3, 4, 5], Landau poles [6], anomalous symmetry breaking [5], duality [7, 8, 9], supersymmetry [9] and spectral anholonomy [9, 10, 11]. On the experimental side, the rapid developments of nanotechnology forecast that nano-scale quantum devices can be designed and manufactured into desired specifications. The description of some of these systems will involve the theory of contact interactions. As a simple example, a piece of a single nanowire would act as a one dimensional line with two reflecting endpoints between which a conduction particle moves almost freely, allowing for a quantum mechanical description with boundaries. Other applications arise, for instance, in systems with impurities which act as point scatterers. All these areas of interest lend impetus to investigate quantum systems with contact interactions further to uncover their full potential both theoretically and experimentally.

The topic of this paper is the quantum half line system, which is perhaps the simplest among those with contact interactions. This system also appears frequently as the radial part of higher dimensional systems [12]. (For the recent experimental studies, see [13] and references therein.) We consider a quantum particle that moves freely on a half line $x \geq 0$ with the endpoint $x = 0$ acting as a reflecting boundary, or an impenetrable wall. This system is known (see section 2) to admit a one-parameter family of distinct walls characterized by the boundary conditions,

$$\psi(0) + L\,\psi'(0) = 0\ , \tag{1.1}$$

where L is a parameter which takes all real numbers including $L = \infty$. Clearly, the standard wall in which we impose $\psi(0) = 0$ is obtained for $L = 0$ but it is just one of the various walls allowed, and therefore the first question one may ask is whether those nonstandard walls with $L \neq 0$ can arise in actual physical settings.

To answer this, we study how those nonstandard walls can be realized as a limit of finite (regularizing) potentials. The potentials we consider are step-like and may readily be manufactured using, *e.g.,* thin layers of different types of semiconductors. We shall show that it is indeed possible to realize such nonstandard walls out of the step-like potentials if we fine-tune the limiting procedure. We then turn to the question whether such nonstandard walls are available only quantum mechanically or not. This will be examined by looking at the time delay of the particle in scattering, which is the time difference between the moments of incidence and reflection at the wall. It will be shown that quantum nonstandard walls with $L < 0$, which are characterized by positive time delay, have no classical counterpart possessing the same time delay, which implies that these walls are purely quantum. We also consider the validity of the semiclassical WKB approximation for the transition kernel under nonstandard walls, where now one takes into account the possible two classical paths, the direct path and the bounce path, in the path integral [14]. This is of interest because it has been known that, for the standard wall as well as that of $L = \infty$, the WKB approximation becomes exact if a sign factor is properly attached to the contribution of the bounce path. We shall see that for these two values of L the required sign factor can be accounted for by the bounce effect, showing that the WKB approximation is in fact exact, whereas for other L the WKB-exactness cannot hold. Before presenting these results, we provide the basics of the quantum system on the half line below.

2. Basics of the quantum system on the half line

The system of a (nonrelativistic) free particle on a half line $x \in [0, \infty)$ is governed by the Hamiltonian $H = -\hbar^2/(2m)\, \mathrm{d}^2/\mathrm{d}x^2$, supplemented by some boundary condition imposed at the wall $x = 0$. The boundary condition is determined by the requirement that H be self-adjoint on the positive half line $x \geq 0$ and, mathematically, this is done by finding proper domains of the operator H on which it is self-adjoint. The result is that there exists a $U(1)$ family of domains of states specified by (1.1) (see, *e.g.,* [12], Appendix D), which can be readily understood by a direct inspection as well. Indeed, one sees by partial integration that for H to be self-adjoint one must have $\psi^*\psi' = \psi'^*\psi$ at $x = 0$ for any state ψ on which H acts. If $\psi'(0) \neq 0$, this implies $\psi(0)/\psi'(0) = [\psi(0)/\psi'(0)]^* = -L$ with L being some real constant, which is just the condition (1.1).[1] The case $\psi'(0) = 0$ which also fulfills the requirement can be included by allowing $L = \infty$ in (1.1). The whole family is $U(1)$ because of the range of the parameter: $L \in (-\infty, \infty) \cup \{\infty\} \cong U(1)$.

Under the boundary condition (1.1) the positive energy states are

$$\varphi_k(x) = \frac{1}{\sqrt{2\pi}} \left(e^{-ikx} + e^{i\vartheta_k} e^{ikx} \right) \tag{2.1}$$

with $\vartheta_k = 2 \operatorname{arccot} kL$. In addition, for $L > 0$, we also have one negative energy state,

$$\varphi_{\text{bound}}(x) = \sqrt{\frac{2}{L}}\, e^{-\frac{x}{L}} \qquad (L > 0)\,, \tag{2.2}$$

[1] The fact that the constant L is universal for any state ψ can be seen by considering (1.1) for all linear combinations of two states ψ_1 and ψ_2 with L_1 and L_2, from which one deduces $L_1 = L_2$ immediately.

which is a bound state localized at the wall with its characteristic size L. The existence of the bound state (2.2) can also be ensured from the minimum energy condition. Namely, for any normalized state ψ the expectation value of the energy reads

$$\langle \psi, H\psi \rangle = \frac{\hbar^2}{2m}\frac{1}{L^2}\int_0^\infty \mathrm{d}x\, |\psi(x) + L\psi'(x)|^2 - \frac{\hbar^2}{2m}\frac{1}{L^2}\ , \tag{2.3}$$

where L is the parameter in (1.1). The lower bound $-\frac{\hbar^2}{2m}\frac{1}{L^2}$ is attained if there exists a state satisfying $\psi(x) + L\psi'(x) = 0$ for all $x \geq 0$, which is just the bound state (2.2).

As seen in the bound state, the parameter L furnishes a physical scale in many of the properties of the system. An example for this is provided by the time delay that occurs when an incoming particle is reflected from the wall. The time delay in quantum scattering processes has been studied earlier (see, *e.g.,* [18, 19] and references therein) on a general basis, but here we do not need this general framework and are content with the following simple approach.

Let us consider a wave packet formed out of the positive energy states (2.1),

$$\begin{aligned}\psi(x,t) &= \int_0^\infty \mathrm{d}k\, f(k)\, e^{-\frac{i\hbar k^2}{2m}t} e^{ikx_0}\varphi_k(x)\\ &= \frac{1}{\sqrt{2\pi}}\int_0^\infty \mathrm{d}k\, f(k)\, e^{-\frac{i\hbar k^2}{2m}t} e^{ikx_0}e^{-ikx} + \frac{1}{\sqrt{2\pi}}\int_0^\infty \mathrm{d}k\, f(k)\, e^{-\frac{i\hbar k^2}{2m}t} e^{ikx_0}e^{i\vartheta_k}e^{ikx}\end{aligned} \tag{2.4}$$

where $f(k)$ is a real function peaked at $k_0 > 0$. The first term describes the incident packet whose maximum starts from x_0 at $t = 0$ and moves to the left with velocity magnitude $v_0 = \hbar k_0/m$, as can be seen from a stationary phase argument,

$$\mathrm{d}/\mathrm{d}k \left(-\hbar k^2/(2m)\, t + kx_0 - kx\right)\Big|_{k=k_0} = 0 \qquad \Longrightarrow \qquad x^{(1)}_{\max}(t) = x_0 - (\hbar k_0/m)\, t\,. \tag{2.5}$$

Similarly, the reflected packet given by the second term moves as

$$x^{(2)}_{\max}(t) = -x_0 + (\hbar k_0/m)\, t + 2L/[1 + (k_0L)^2]\,. \tag{2.6}$$

As t increases, the first packet moves towards the wall at $x = 0$, and its maximum reaches it at $t_1 = x_0/v_0$. Meanwhile, the second packet comes from the left (if we assume $x < 0$ as well) moving to the right and arrives at the wall at $t_2 = (x_0 - \frac{2L}{1+(k_0L)^2})/v_0$. The difference between the two instants gives the time delay,

$$\tau = t_2 - t_1 = -\frac{2mL}{\hbar k_0[1 + (k_0L)^2]}\,. \tag{2.7}$$

For $L = 0$ and $L = \infty$, this time delay is zero, as one would expect on the ground that for such cases there is no parameter in the system possessing the dimension of time. Note that for negative L the time delay is positive, whereas for positive L it is negative.

From the eigenfunctions (2.1) and (2.2) the Feynman kernel describing the transition of the particle from $x = a$ at $t = 0$ to $x = b$ at $t = T$ can be calculated (see [15, 16, 17]). The result is

$$K(b, T; a, 0) = \sqrt{\frac{m}{2\pi i\hbar T}} \left[e^{\frac{im}{2\hbar T}(b-a)^2} \mp e^{\frac{im}{2\hbar T}(b+a)^2} \right] , \tag{2.8}$$

for $L = 0$ ('$-$'-sign) and $L = \infty$ ('$+$'-sign). For $L < 0$ the kernel is given by

$$\sqrt{\frac{m}{2\pi i\hbar T}} \left[e^{\frac{im}{2\hbar T}(b-a)^2} + e^{\frac{im}{2\hbar T}(b+a)^2} - \frac{2}{|L|} \int_0^\infty \mathrm{d}z \, e^{-z/|L|} \, e^{\frac{im}{2\hbar T}(b+a+z)^2} \right] , \tag{2.9}$$

and for $L > 0$ by

$$\sqrt{\frac{m}{2\pi i\hbar T}} \left[e^{\frac{im}{2\hbar T}(b-a)^2} + e^{\frac{im}{2\hbar T}(b+a)^2} - \frac{2}{L} \int_0^\infty \mathrm{d}z \, e^{-z/L} \, e^{\frac{im}{2\hbar T}(b+a-z)^2} \right] + \frac{2}{L} e^{\frac{i\hbar^2 T}{2mL^2}} e^{-\frac{b+a}{L}} . \tag{2.10}$$

The salient feature of the result is that, for $L = 0$ and $L = \infty$, the kernel (2.8) almost coincides with that obtained by WKB semiclassical approximation, because the two terms in (2.8) correspond to the free kernels for the direct path from $(a, 0)$ to (b, T) and for the bounce path which hits the wall once during the transition, respectively. The only problem for the complete WKB-exactness is the appearance of the $\mp$ sign factor attached to the contribution from the bounce path. We shall show later that this sign factor can be attributed to the classical action $\Delta S_{\mathrm{bounce}} = \hbar\pi$ gained by the bounce effect at the wall so that $e^{\frac{i}{\hbar}\Delta S_{\mathrm{bounce}}} = \mp 1$.

3. Realization of the wall

We now discuss how to realize the wall characterized by (1.1) in actual physical settings. For this, we shall adopt a regularization method which is analogous to those used earlier for point singularities [4, 12]. We extend the space to the entire line $-\infty < x < \infty$ and seek a potential $V(x)$ with finite support such that, in the limit of vanishing support, the boundary condition (1.1) at $x = 0$ can be realized. Obviously, since no probability flow is admitted through the wall at $x = 0$, such a regularized potential has to become infinitely high for $x < 0$ in the limit. A simple choice for the potential fulfilling the demand is

$$V(x) = \begin{cases} V_1 \, , & x < -d \qquad \text{(domain I)} \\ V_2 \, , & -d < x < 0 \qquad \text{(domain II)} \\ 0 \, , & x > 0 \qquad \text{(domain III)} \end{cases} \tag{3.1}$$

with constants $V_1 > 0$ and $V_2 < 0$. Here, the scale of the support is given by the regularization parameter d, and V_1 and V_2 are assumed to be functions of d such that V_1, $|V_2| \to \infty$ as $d \to 0$.

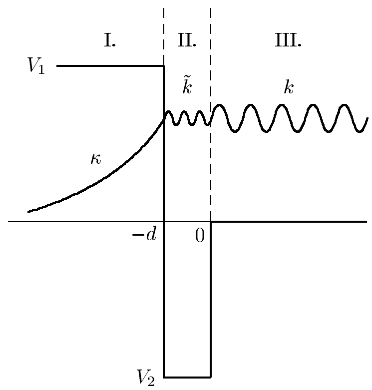

Figure 1. The regularized potential (3.1) and the eigenfunction (3.2).

To find the appropriate dependence of $V_1(d)$ and $V_2(d)$, let us consider an energy eigenstate φ in the potential (3.1) with energy $E < V_1$ (see Figure 1):

$$\varphi(x) = \begin{cases} \varphi_{\mathrm{I}}(x) = Ne^{\kappa x}, & x < -d\,, \qquad \kappa = \sqrt{\frac{2m}{\hbar^2}(V_1 - E)}\,, \\ \varphi_{\mathrm{II}}(x) = Ae^{i\tilde{k}x} + Be^{-i\tilde{k}x}, & -d < x < 0\,, \qquad \tilde{k} = \sqrt{\frac{2m}{\hbar^2}(|V_2| + E)}\,, \\ \varphi_{\mathrm{III}}(x) = Ce^{ikx} + De^{-ikx}, & x > 0\,, \qquad k = \sqrt{\frac{2mE}{\hbar^2}} \end{cases} \tag{3.2}$$

$\big($for $E < 0\,,\ \varphi_{\mathrm{III}}(x) = Me^{-\sqrt{\frac{2m|E|}{\hbar^2}}x}\big)$. Under such finite potentials (*i.e.*, without infinity or singularity), the wave function and its derivative are required to be continuous. The condition which is dynamically important is provided by the continuity of the ratio φ'/φ which is free from the ambiguity of overall normalization. From this continuity condition, we obtain

$$\kappa = \frac{i\tilde{k}(Ae^{-i\tilde{k}d} - Be^{i\tilde{k}d})}{Ae^{-i\tilde{k}d} + Be^{i\tilde{k}d}}\,, \qquad \frac{\varphi'_{\mathrm{III}}}{\varphi_{\mathrm{III}}}(0) = \frac{i\tilde{k}(A - B)}{A + B} \tag{3.3}$$

at $x = -d$ and $x = 0$. Note that both $\tilde{k}$ and κ are d-dependent $\tilde{k} = \tilde{k}(d)$, $\kappa = \kappa(d)$ through $V_1(d)$ and $V_2(d)$ and so are the two ratios in (3.3). If we introduce

$$R(d) = \frac{\varphi'_{\mathrm{III}}}{\varphi_{\mathrm{III}}}(0)\,, \qquad \alpha = \arctan\frac{\kappa}{\tilde{k}}\,, \qquad \beta = \tilde{k}d\,, \tag{3.4}$$

then from (3.3) we find

$$R(d) = \tilde{k}\,\frac{(Ae^{-i\beta} - Be^{i\beta})\cos\beta - i(Ae^{-i\beta} + Be^{i\beta})\sin\beta}{(Ae^{-i\beta} + Be^{i\beta})\cos\beta - i(Ae^{-i\beta} - Be^{i\beta})\sin\beta} = \tilde{k}\tan(\alpha - \beta)\,. \tag{3.5}$$

The boundary condition (1.1) is realized if

$$R(d) \to -\frac{1}{L} \qquad \text{as} \quad d \to 0\,, \tag{3.6}$$

independently of the energy E. In what follows we present a set of regularized potentials fulfilling this requirement.

To this end, we first define

$$\alpha_0 = \lim_{d\to 0} \alpha \ , \qquad \beta_0 = \lim_{d\to 0} \beta \ , \tag{3.7}$$

and note that, since $V_1(d) \to \infty$ as $d \to 0$, we always have $\kappa \to \infty$, whereas since $0 < \alpha < \pi/2$ by definition, we have $0 \le \alpha_0 \le \pi/2$. Note also that, if $V_2(d)$ used in our regularization is such that $\beta \to \infty$, then $\tan(\alpha - \beta)$ will oscillate between $-\infty$ and ∞ so $R(d)$ will not have a limit. We therefore confine ourselves to cases in which β has a finite (zero or nonzero) limit β_0. Now, let us suppose $\beta_0 \ne \alpha_0 \ (\mathrm{mod}\ \pi)$, that is, $\tan(\alpha - \beta) \to \tan(\alpha_0 - \beta_0) \ne 0$. Then, if $|V_2| \to \infty$ we have $\tilde{k} \to \infty$ and hence $R(d) \to \pm\infty$. If $|V_2|$ remains finite, on the other hand, we find $\alpha_0 = \pi/2$ and $\beta_0 = 0$ and hence $R(d) \to \infty$. We thus see that these regularizations yield necessarily the standard wall $L = 0$.

The foregoing argument shows that nonstandard walls with $L \ne 0$ can be realized only by such realizations in which V_1 and V_2 are fine-tuned as

$$\beta_0 = \alpha_0 \ (\mathrm{mod}\ \pi) \, . \tag{3.8}$$

We shall suppose (3.8) from now on, and consider the limit of $R(d)$ for the cases $\alpha_0 = 0$, $0 < \alpha_0 < \pi/2$ and $\alpha_0 = \pi/2$, separately.

<u>(i) case $\alpha_0 = 0$:</u>

We then have, as $d \to 0$, $\alpha \approx \tan\alpha = \kappa/\tilde{k} \to 0$ and $\beta - \beta_0 \to 0$ and hence $\tan(\alpha - \beta) = \tan(\alpha - \beta + \beta_0) \approx \kappa/\tilde{k} - \beta + \beta_0$. Thus the ratio is approximated as

$$R(d) \approx \kappa - \tilde{k}(\beta - \beta_0) \, . \tag{3.9}$$

Now, if $\beta_0 = 0$ then the r.h.s. reads $\kappa - \tilde{k}^2 d$. Hence, to get a finite $R(d)$, $\tilde{k}^2 d$ has to compensate the divergence of κ. This can be done if κ and $\tilde{k}$ behave as

$$\kappa \sim c\, d^{\nu} - \frac{1}{L} \, , \qquad \tilde{k} \sim c^{\frac{1}{2}}\, d^{\frac{\nu - 1}{2}} \qquad (-1 < \nu < 0) \, , \tag{3.10}$$

which is realized if, for instance, we put

$$V_1(d) = \frac{\hbar^2}{2m} \left(c^2 d^{2\nu} - \frac{2c}{L} d^{\nu} \right) \, , \qquad V_2(d) = -\frac{\hbar^2}{2m}\, c\, d^{\nu - 1} \, , \tag{3.11}$$

with a constant $c > 0$. It is then readily confirmed that this regularized potential (3.11) does lead to $R(d)$ fulfilling (3.6) for all $E > 0$. If $\beta_0 > 0$, on the other hand, then

$\beta_0 d^{-1}(\beta-\beta_0)$ on the r.h.s. of (3.9) has to cancel the divergence of κ. This means $\tilde{k} \sim \beta_0 d^{-1}+(1/\beta_0)\kappa$. The needed finite term $-\frac{1}{L}$ can be provided again by κ if $\kappa \sim c_1 d^\nu - \frac{1}{L}$. This is achieved, for example, by

$$V_1(d) = \frac{\hbar^2}{2m}\left(c^2 d^{2\nu} - \frac{2c}{L}\, d^\nu\right), \qquad V_2(d) = -\frac{\hbar^2}{2m}\left(\beta_0^2\, d^{-2} + 2c\, d^{\nu-1}\right). \tag{3.12}$$

It is again easy to confirm that (3.12) yields $R(d)$ fulfilling (3.6) for $\nu > -1/2$.

<u>(ii) case $0 < \alpha_0 < \pi/2$:</u>

In this case, we have $\tilde{k} \sim \beta_0 d^{-1}$ and $\kappa \sim (\beta_0 \tan\beta_0)\, d^{-1}$. Using the Taylor expansion,

$$\alpha = \arctan(\kappa/\tilde{k}) \approx \alpha_0 + \cos^2\!\alpha_0\, \big(\kappa/\tilde{k} - \tan\alpha_0\big), \tag{3.13}$$

we find

$$R(d) \approx \tilde{k}\, \tan\big[\alpha_0 - \beta_0 + \cos^2\!\alpha_0\, (\kappa/\tilde{k} - \tan\alpha_0)\big] \approx \cos^2\!\alpha_0\, (\kappa - \tilde{k}\tan\alpha_0\,). \tag{3.14}$$

Hence the choice,

$$\kappa \sim (\beta_0 \tan\beta_0)\, d^{-1} - (1/\cos^2\!\beta_0)\, \frac{1}{L} \tag{3.15}$$

may lead to (3.6). A possible regularized potential realizing (3.15) is

$$V_1(d) = \frac{\hbar^2}{2m}\left[(\beta_0^2 \tan^2\!\beta_0)\, d^{-2} - \frac{2}{L}\, (\beta_0 \tan\beta_0/\cos^2\!\beta_0)\, d^{-1}\right], \qquad V_2(d) = -\frac{\hbar^2}{2m}\, \beta_0^2\, d^{-2}, \tag{3.16}$$

which can be shown to give $R(d)$ satisfying (3.6).

<u>(iii) case $\alpha_0 = \pi/2$:</u>

We still have $\tilde{k} \sim \beta_0 d^{-1}$ but now $\kappa/\tilde{k} \to \infty$ so $\alpha \approx \pi/2 - \tilde{k}/\kappa$, and therefore

$$R(d) \approx \tilde{k} \tan\left[\frac{\pi}{2} - \frac{\tilde{k}}{\kappa} - (\beta-\beta_0) - \beta_0\right] \approx \tilde{k}\left[-\frac{\tilde{k}}{\kappa} - (\beta-\beta_0)\right]. \tag{3.17}$$

The realization (3.6) will be attained if, for example, we have $\kappa/\tilde{k}^2 \to \infty$ and provide $-\frac{1}{L}$ through $\tilde{k}$ by assuming $\tilde{k} \sim \beta_0 d^{-1} + \frac{1}{L}\frac{1}{\beta_0}$. This is the case with the regularization,

$$V_1(d) = \frac{\hbar^2}{2m}\, c_1^2\, d^{2\nu} \quad (\nu < -2), \qquad V_2(d) = -\frac{\hbar^2}{2m}\left(\beta_0^2 d^{-2} + \frac{2}{L}\, d^{-1}\right). \tag{3.18}$$

To summarize, the regularization by means of the step-like potential (3.1) leads generically to the standard wall $L = 0$. It can also lead to nonstandard walls $L \neq 0$ but only as exceptional cases under the fine-tuning (3.8). It is worth emphasizing that the crucial factor in determining the limit of $R(d)$, *i.e.*, the boundary condition at $x = 0$, is not the leading asymptotic behavior of V_1 and V_2 in $d \to 0$ but always a subleading term. A similar phenomenon has been observed for the regularization of the Dirac delta point interactions in three space dimensions [12].

The regularizations we used are based on a step-like potential. Needless to say, other types of potentials can also be used for realizing the walls. One can, for instance, look for a potential which leads to the realization for any L without involving the mass parameter m. Such a regularization may be more desirable than that we constructed — where the potentials turned out to be m-dependent — for the reason that potentials should be independent of the particle. Nonetheless, our simple regularization may well exhibit a universal feature of the realization of the (standard and nonstandard) walls, as we can see, for example, the bound state being accommodated in the negative middle part of the step-like potential we used.

4. Classical counterparts

Having seen that the quantum walls characterized by L can be realized by means of regularized potentials, we now turn to the question whether those walls have classical counterparts or not. We investigate this in the phenomena of time delay discussed in section 2, by asking if there is a classical system with some appropriate potential $V(x)$ which can account for the same amounts of time delay as those observed under the walls. Note that systems with the regularized potentials discussed above are not appropriate for this purpose, because in those systems the time a classical particle spends in a potential (3.1) tends necessarily to zero as $d \to 0$ (since as $V_2 \to -\infty$ the distance run by the particle becomes zero while its velocity becomes infinity).

To find a potential of classical systems that reproduces the identical time delay, we shall first consider the walls with $L > 0$. In this case the time delay (2.7) is negative, and if the classical picture is available, the incident particle with velocity magnitude $v = \frac{\hbar k}{m}$ must return earlier by

$$|\tau| = \frac{2L}{v} \, \frac{1}{1 + \left(\frac{mL}{\hbar}\, v\right)^2} \tag{4.1}$$

than we would expect when it collided with the wall at $x = 0$. Observe that, for small v the (minus) delay $|\tau|$ approaches $\frac{2L}{v}$. This indicates that a slow particle sees the wall at (around) $x = L$, not $x = 0$. Consequently, the reflecting potential $V(x)$ must begin to grow at $x = L$. For definiteness, let us search for the potential in the qualitative form as shown in Figure 2. (This fixes an arbitrariness in the choice of the potential. As we will

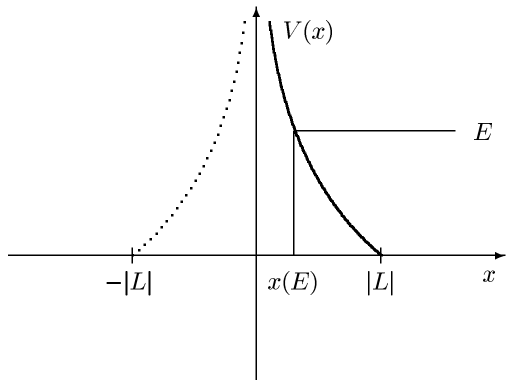

Figure 2. The realizing potential (4.7) is shown by the solid line for $L > 0$. For $L < 0$ the obtained potential becomes the dotted line and is unphysical.

see, demanding a positive, monotonically decreasing potential determines the potential uniquely.) Now, let us introduce

$$\tilde{\tau} = \frac{2L}{v} + \tau = \sqrt{2mL^2E}\Big/\left(\frac{\hbar^2}{2mL^2} + E\right), \tag{4.2}$$

(where $E = \frac{1}{2}mv^2$ is the incoming energy) which is the time spent by the particle in the region left to the point $x = L$. Our problem is then an inverse problem: determine a potential $V(x)$ from a given $\tilde{\tau}(E)$ as a function of E. This can be answered if we follow the well-known argument [20] used for the problem of determining a well-shaped potential from the period time with which a particle moves.

We start by writing the relationship between the potential and $\tilde{\tau}$ as

$$\tilde{\tau}(E) = \sqrt{2m}\int_{x(E)}^{L} \frac{\mathrm{d}x}{\sqrt{E - V(x)}} = \sqrt{2m}\int_0^E \left(-\frac{\mathrm{d}x(V)}{\mathrm{d}V}\right)\frac{\mathrm{d}V}{\sqrt{E-V}}\,. \tag{4.3}$$

Dividing by $\sqrt{W-E}$ with W being an auxiliary parameter, and integrating with respect to E from 0 to W, we find

$$\int_0^W \frac{\tilde{\tau}(E)\,\mathrm{d}E}{\sqrt{W-E}} = \sqrt{2m}\int_0^W \mathrm{d}V\left(-\frac{\mathrm{d}x}{\mathrm{d}V}\right)\int_V^W \frac{\mathrm{d}E}{\sqrt{(W-E)(E-V)}}\,. \tag{4.4}$$

The inner integral (the one with respect to E) gives π, and hence we have

$$\int_0^W \frac{\tilde{\tau}(E)\,\mathrm{d}E}{\sqrt{W-E}} = \pi\sqrt{2m}\,[L - x(W)]\,. \tag{4.5}$$

On the other hand, from (4.2) we can evaluate the integral on the l.h.s. explicitly as

$$\int_0^W \frac{\tilde{\tau}(E)\,\mathrm{d}E}{\sqrt{W-E}} = \pi\sqrt{2m}\,L\left(1 - 1\Big/\sqrt{1 + \tfrac{2mL^2}{\hbar^2}\,W}\right)\,. \tag{4.6}$$

Combining this with (4.5), we obtain $x(W) = L\big[1 + \frac{2mL^2}{\hbar^2}\,W\big]^{-\frac{1}{2}}$, and inverting it we get[2]

$$V(x) = \frac{\hbar^2}{2mL^2}\left(\frac{L^2}{x^2} - 1\right). \tag{4.7}$$

For $L < 0$, the time delay is positive and the quantum wave packet returns later than expected. In this case the time delay that the corresponding classical particle must reproduce reads

$$\tau = \frac{2|L|}{v}\,\frac{1}{1 + \left(\frac{m|L|}{\hbar}\,v\right)^2}. \tag{4.8}$$

For small v, this becomes $\frac{2|L|}{v}$, which shows that a slow particle enters the $x < 0$ region and sees the wall near $x = -|L|$. For this, the realizing potential $V(x)$ has to start to increase at $x = -|L|$, and for smaller x, the potential is expected to increase. However, if one repeats the same argument used for the $L > 0$ case, one ends up with (4.7) again, with now the left branch of this function (see Figure 2). The problem with this branch is obvious: it increases for x to the right of $-|L|$ rather than to the opposite and is unphysical. It is not hard to check that no potential in $-|L| < x < 0$ or in $0 < x$ can help the situation, because for large v the leading order term of the time delay is at least $\frac{2|L|}{v}$, while (4.8) would require only a $\frac{1}{v^3}$ asymptotic behavior. Hence, interestingly enough, the walls with negative L do not admit a classical counterpart, *i.e.*, they are genuinely quantum.

5. WKB-exactness

The fact that for walls with $L = 0$ and $L = \infty$ the transition kernel is almost WKB-exact alludes us to examine whether this implies a complete exactness or not, and if so, whether such a feature persists to nonstandard walls as well. More precisely, we wish to see if the sum of amplitudes along the classical two paths, the direct world line from $(x,t) = (a,0)$ to (b,T) and the bouncing path which hits the wall $x = 0$ before arriving at (b,T), give the exact result (see Figure 3). The question, therefore, is if the kernels (2.8), (2.9) and (2.10) can be rewritten as a sum of the corresponding two terms as

$$K(b,T;a,0) = \sqrt{\frac{m}{2\pi i\hbar T}}\left[e^{\frac{im}{2\hbar T}(b-a)^2} + A_L(a,b,T)\right], \tag{5.1}$$

with

$$A_L(a,b,T) = e^{\frac{i}{\hbar}S_{\rm bounce}(b,T;a,0)}, \tag{5.2}$$

[2] We remark that, while this potential reproduces the time delay classically, it does not reproduce the boundary condition (1.1) and hence cannot serve as a potential to realize the walls.

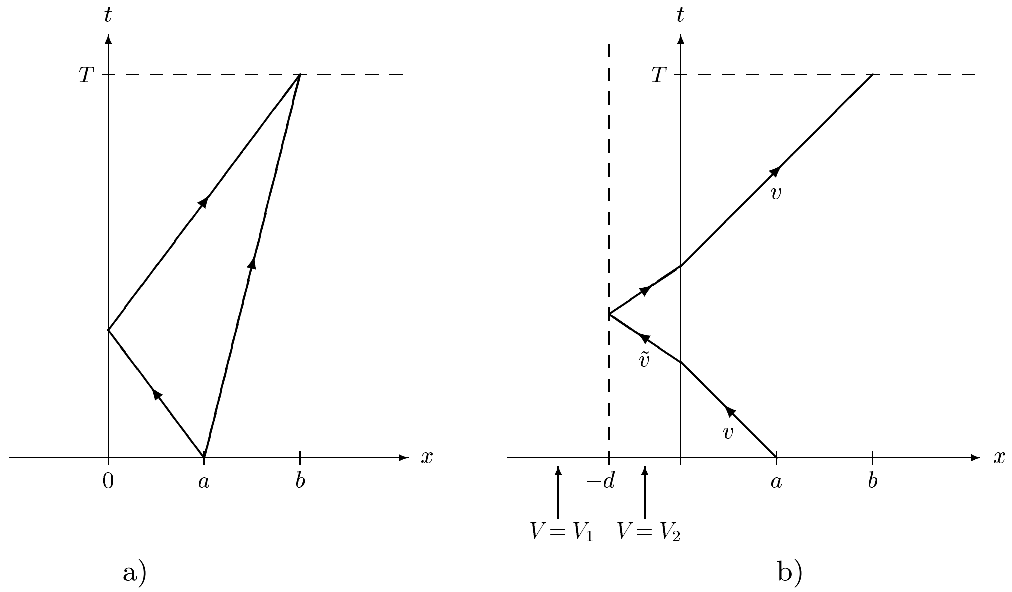

Figure 3. a) The direct and the bounce paths. b) The bounce path under the regularized potential (3.1).

where $S_{\text{bounce}}(b, T; a, 0)$ is the classical action for the bounce path.

Let us begin by examining the complete WKB-exactness for the $L = 0$ and $L = \infty$ cases. For definiteness let us use the regularized potentials (3.1) for evaluating the classical action for the bouncing path. Then we get

$$S_{\text{bounce}}(b, T; a, 0) = \int_0^T \mathrm{d}t\,(E - 2V) = ET - 2V_2 \left(\frac{2d}{\tilde{v}}\right) , \tag{5.3}$$

for $V_1 > E$, where $\tilde{v} = \sqrt{2(E + |V_2|)/m}$ is the velocity of the particle in domain II. Since the time $2d/\tilde{v}$ spent by the particle in the domain vanishes as $d \to 0$, we find

$$\frac{a}{v} + \frac{b}{v} \to T \qquad \Longrightarrow \qquad v \to \frac{a+b}{T}, \qquad E \to \frac{m(a+b)^2}{2T^2}, \tag{5.4}$$

which shows that the first ET term on the r.h.s. of (5.3) tends to $S^{(0)}_{\text{bounce}} = \frac{m(a+b)^2}{2T}$, which is the action corresponding to the bounce path without taking account of the bounce effect at $x = 0$. The second term in (5.3) represents, therefore, the extra contribution by the bounce effect,

$$\Delta S_{\text{bounce}} = \lim_{d\to 0} \left[\sqrt{8md^2\,|V_2(d)|^2} \Big/ \sqrt{E + |V_2(d)|}\ \right] . \tag{5.5}$$

Now, for the standard $L = 0$ system, if we choose

$$V_1(d) = \text{const.}\, d^{-1}, \qquad V_2(d) = -\frac{\hbar^2}{2m}\left(\frac{\pi}{2}\right)^2 d^{-2}, \tag{5.6}$$

for which $\alpha_0 = 0$ and $\beta_0 = \pi/2$, then from (5.5) we obtain $\Delta S_{\rm bounce} = \hbar\pi$ in the limit $d \to 0$, thus providing the correct sign factor $e^{i\Delta S_{\rm bounce}} = -1$ as required. For the $L = \infty$ system, we choose (3.11) and set $\nu = -1/2$, say, to get

$$V_1(d) = \frac{\hbar^2}{2m}\, c^2\, d^{-1}\,, \qquad V_2(d) = -\frac{\hbar^2}{2m}\, c\, d^{-\frac{1}{2}}\,, \tag{5.7}$$

which immediately leads to $\Delta S_{\rm bounce} = 0$.

It should be pointed out, however, that the action $\Delta S_{\rm bounce}$ associated to the bounce effect is highly ambiguous, as one can see that it depends only on the behavior of $V(d)$ in the $d \to 0$ limit and hence may be changed while maintaining the value of L. The crucial property for the WKB-exactness is, therefore, found not in the actual value of $\Delta S_{\rm bounce}$ but in the fact that the factor $A_L(a,b,T)$ is of modulus one, $|A_L(a,b,T)| = 1$. In fact, this is no longer true for L other than these two values of L, which we shall prove now.

For this, we first consider the case $L < 0$ and observe that the term $A_L(a,b,T)$ in (2.9) depends on its four variables a, b, T and L only through the two combinations,

$$p = (a+b)/|L|\,, \qquad q = m|L|^2/(2\hbar T)\,, \tag{5.8}$$

and hence can be written as

$$A_L(a,b,T) \equiv A(p,q) = e^{ip^2q} - 2\int_0^\infty {\rm d}s\, e^{-s}\, e^{i(p+s)^2 q}\,, \tag{5.9}$$

using $s = z/|L|$. If $A(p,q)$ is on the unit circle for all p and q, then both $\partial_p A(p,q)$ and $\partial_q A(p,q)$ have to be orthogonal to $A(p,q)$ in the complex plane. This implies

$$A(p,q)^*\, \partial_p A(p,q) + {\rm c.c.} = 0\,, \qquad A(p,q)^*\, \partial_q A(p,q) + {\rm c.c.} = 0\,, \tag{5.10}$$

for all p and q. From (5.9) one finds that $\partial_p A(p,q)$ and $\partial_q A(p,q)$ can be expressed as

$$\begin{aligned} \partial_p A(p,q) &= 2(1+ipq)\, e^{ip^2q} - 2\int_0^\infty {\rm d}s\, e^{-s}\, e^{i(p+s)^2 q}\,, \\ \partial_q A(p,q) &= \left(\frac{p}{q} + ip^2 - \frac{i}{2q^2}\right) e^{ip^2q} + \left(\frac{1}{q} + \frac{i}{2q^2}\right)\int_0^\infty {\rm d}s\, e^{-s}\, e^{i(p+s)^2 q}\,. \end{aligned} \tag{5.11}$$

Using (5.9) and (5.11) together with new variables u, v defined by

$$\frac{1}{u+iv} = e^{-ip^2q} A(p,q)\,, \tag{5.12}$$

we find that the two orthogonality conditions (5.10) become

$$u - 2pqv = -1\,, \qquad (1+2p)u + \left(1/2q - 2p^2q\right) v = 1\,. \tag{5.13}$$

This set of linear equations has a unique solution

$$u = \frac{4pq^2(1+p)-1}{4pq^2(1+p)+1}, \qquad v = \frac{4q(1+p)}{4pq^2(1+p)+1}\,. \tag{5.14}$$

Note that (5.12) implies that, if $A(p,q)$ is on the unit circle in the complex plane, so is $u+iv$. However, this is not fulfilled by the solution (5.14) which never satisfies $u^2+v^2=1$ for positive values of p and q. We therefore find that $A(p,q)$ fails to be on the unit circle and, consequently, the WKB-exactness cannot hold for $L<0$. The proof for $L>0$ can also be done analogously.

We thus learn that quantum walls with $L=0$ and $L=\infty$, which correspond to the Dirichlet $\psi(0)=0$ and the Neumann $\psi'(0)=0$ boundary condition, respectively, are distinguished in the $U(1)$ family of walls, at least with respect to the WKB-exactness. These two cases are distinguished also by their scale invariance which arises due to the absence of the scale parameter. The relationship between the two, the WKB-exactness and scale invariance, is however still unclear.

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