The Spectral Structure and the WKB Approximation on a Circle with Point Interaction¹

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Abstract. Application of the theory of self-adjoint extension reveals a U(2) family of Hamiltonians to describe a quantum particle on a circle with point interaction. We provide a classification of the family by introducing a number of subfamilies and thereby analyze the spectral structure in detail. We find that the spectrum depends on a subset of U(2) parameters rather than the entire U(2), and that, in particular, there exists a subfamily in U(2) where the spectrum becomes parameterindependent. We also show that, in some specific cases, the WKB semiclassical approximation becomes exact (modulo phases) for the system.

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1. Introduction

Systems with point interaction form an important class of solvable models in quantum mechanics, allowing for a variety of applications in physics (see [1] and references therein). These systems are governed by Hamiltonian operators given by a *point perturbation* of the Laplacian on \mathbb{R}^n , that is, the self-adjoint Laplacian operators on \mathbb{R}^n with one point removed. In one dimension, it has been recognized [2, 1] that the perturbation yields a U(2) family of self-adjoint operators on $\mathbb{R}^1 \setminus \{0\}$, which implies that there is a U(2) family of distinct point interactions possible there. The physical properties of the family has been investigated in [3], and more fully in [4] including the spectra, time-dependent fundamental solutions and scattering matrices. Recent technological advances in microscopic devices have spurred a new interest in realizing these point interactions using regulated potentials [5, 6, 7, 8].

The aim of the present paper is twofold. First, we provide a study on point interaction on a circle S^1 analogous to that made on a line \mathbb{R}^1 . This is interesting for the reason that the difference in self-adjoint operators on $S^1 \setminus \{0\}$ — which are again characterized by U(2) — arises in discrete energy spectrum rather than in the scattering amplitude as on $\mathbb{R}^1 \setminus \{0\}$ whose positive energy spectrum is always continuous. We shall see that the spectra of the U(2) family exhibit remarkable characteristics; in particular, the spectral space forms a subspace of U(2), rather than the whole U(2) as apparently suggested by the theory of self-adjoint extensions. In a subfamily of U(2) (called 'separated subfamily'), the circle becomes equivalent to a box with nontrivial boundary conditions, and hence our result is also relevant to a box if such boundary conditions are available. Secondly, we show that in some specific cases our system on $S^1 \setminus \{0\}$ admits the interpretation that the WKB semicalssical approximation is exact up to a phase which is determined by the point interaction. In fact, the WKB exactness of a box system has been pointed out earlier in the path-integral for perfectly reflecting walls [9], and in this respect our cases provide a generalization of the particular case previously considered.

This paper is organized as follows. In sect. 2 we review briefly the system of a particle confined to a half line where the basic properties mentioned above, such as the dependence of the spectrum on the allowed self-adjoint extensions and the WKB exactness in the transition amplitude, can easily be seen. We then present our result on $S^1 \setminus \{0\}$ in sect. 3 by considering a particle confined to a box under the most general self-adjoint extensions of the Laplacian, a setup which is equivalent to a circle with point interaction. For our convenience we introduce a number of subfamilies defined within the U(2) family. These subfamilies are characterized by distinguished physical properties, wherein the spectra and the WKB exactness are discussed separately.

2. Particle on a Half Line

We begin by discussing a particle restricted to move on the half line $x \ge 0$. The system will be given by placing an 'infinite' potential wall at x = 0 on a line, and in quantum mechanics one conventionally imposes the vanishing boundary condition $\psi(0) = 0$ for wavefunctions. This is based on the observation (see, *e.g.*, [10]) that the boundary condition that arises under a finite constant wall V_0 at x = 0 reduces to the conventional one in the limit $V_0 \to \infty$. This, however, is too restrictive to specify the boundary condition, because other limits that also confine the particle in the half line can lead to boundary conditions which are different from the conventional one [11]. It is therefore safe to say that the only requirement for the particle to be confined on the half line is that the probability current j(x), not the wave function, vanish at the wall,

$$j(0) = 0,$$
 where $j(x) = -\frac{i\hbar}{2m} \left((\psi^*)'\psi - \psi^*\psi' \right)(x)$. (2.1)

The condition (2.1) is then satisfied if

$$\psi(0) + L \,\psi'(0) = 0 \,\,, \tag{2.2}$$

with $L \in \mathbb{R}$ being an arbitrary constant of length dimension, or $\psi'(0) = 0$ which may be thought of the case $L = \infty$ in (2.2). The combined space of the solutions $\mathbb{R} \cup \{\infty\} \simeq U(1)$ to the condition (2.1) may thus be parametrized by $L := L_0 \cot \phi$ with an angle $\phi \in [0, \pi)$ and a nonvanishing constant L_0 . The same U(1) family can be obtained from the theory of self-adjoint extensions applied to the free Hamiltonian $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$ restricted to the half line [12], because self-adjointness implies probability conservation in the system as a whole.³

We then observe that, in addition to the continuum spectrum for positive energy $E_k = \hbar^2 k^2/2m$ with k > 0 formed by the states,

$$\psi_k^L(x) = \frac{1}{\sqrt{2\pi}} \left[e^{-ikx} + \left(\frac{1-ikL}{1+ikL}\right) e^{ikx} \right] , \qquad (2.3)$$

³ Here one adopts the local conservation $j(\infty) = 0$ in addition to (2.1) on the ground that the more general global conservation, $j(0) = j(\infty)$, will never be realized physically in practice unless $j(\infty) = 0$. In parallel, the possibility for a nonzero $j(\infty)$ is excluded by the results of self-adjoint extension theory, too.

the system admits a normalizable bound state

$$\psi_{bound}^L(x) = \sqrt{\frac{2}{L}} e^{-\frac{x}{L}} , \qquad (2.4)$$

for L > 0 with energy $E_B = -\hbar^2/2mL^2$. The bound state (2.4) disappears either at L = 0 or $L = \infty$ where the boundary condition becomes $\psi(0) = 0$ or $\psi'(0) = 0$.

The two exceptional cases, L = 0 and $L = \infty$, which has no scale parameter are of particular interest, because one can then evaluate the transition amplitude (Feynman kernel) in closed form. Indeed, from (2.3) the Feynman kernel K(b, T; a, 0), which describes the transition from x = a at t = 0 to x = b at t = T, is found to be

$$K(b,T;a,0) = \int_0^\infty dk \, e^{-\frac{i}{\hbar}E_k T} \psi_k^L(b) \, (\psi_k^L)^*(a) = \sqrt{\frac{m}{2\pi i\hbar T}} \left(e^{\frac{i}{\hbar}\frac{m}{2T}(b-a)^2} \mp e^{\frac{i}{\hbar}\frac{m}{2T}(b+a)^2} \right) , \qquad (2.5)$$

where the '-'-sign in (2.5) is for L = 0 whereas the '+'-sign is for $L = \infty$. In the pathintegral point of view, the result (2.5) may be interepreted as being a sum of contributions from the two possible classical trajectories, the direct path from a to b and the reflected path which starts from a and hits the wall before reaching b. We therefore see that, modulo the phase shift by π or 0 acquired at the reflection, the WKB semiclassical approximation becomes exact in the two cases of the present system. We remark that the phase shift may also be explained by the corresponding shift at the reflection in the classical action, if one considers a proper sequence of regulated potentials that leads to the infinite wall in the limit. (The path-integral treatise on the half line has been discussed earlier in [9, 13] for L = 0 and in [14, 15] for generic L.)

3. Particle in a Box or on a Circle with Point Interaction

We now consider the system of an infinite potential well, *i.e.*, a free particle confined in a box of infinite potential walls at x = 0 and x = l. It is known that there exists a U(2) family of self-adjoint Hamiltonians for the system. Using a matrix $U \in U(2)$ and the identity matrix I, the different self-adjoint extensions in the family can be described by the boundary conditions,

$$(U-I)\Psi + iL_0 (U+I)\Psi' = 0, \qquad \Psi := \begin{pmatrix} \psi(0)\\ \psi(l) \end{pmatrix}, \quad \Psi' := \begin{pmatrix} \psi'(0)\\ -\psi'(l) \end{pmatrix} , \quad (3.1)$$

where L_0 is again a constant of length dimension. As before, one can derive these boundary conditions (3.1) by requiring probability conservation of the entire system. To see this, note first that with $\Psi^{\dagger} = (\Psi^*)^t$ the probability conservation,

$$j(0) - j(l) = 0$$
, (3.2)

is equivalent to $\Psi^{\dagger}\Psi' - (\Psi^{\dagger})'\Psi = 0$, or

$$|\Psi - iL_0\Psi'|^2 - |\Psi + iL_0\Psi'|^2 = 0 , \qquad (3.3)$$

for any $L_0 \in \mathbb{R} \setminus \{0\}$. Then from this one deduces⁴ that $\Psi - iL_0\Psi' = U(\Psi + iL_0\Psi')$ with some unitary matrix $U \in U(2)$, arriving exactly at (3.1).

In practical settings of a box, it is natural to impose *local* probability conservation j(0) = j(l) = 0. However, it is perfectly legitimate to consider the generic boundary conditions (3.1) which derive from *global* probability conservation (3.2). The physical settings for those generic cases arise when, *e.g.*, the two ends of the box are combined to form a circle, creating a possible singularity at the junction which induces a point interaction there. The singularity or the point interaction will then be characterized by the boundary conditions (3.1). An analogous situation arises for the system on a line **R** with point interaction, where the family of self-adjoint extensions is also given by U(2) (although the local and incomplete parametrization $U(1) \times SL(2, \mathbb{R})$ instead of U(2) has been widely used in the literature; see [16] for the detail).

Let us introduce a unique parametrization for $U(2) = U(1) \times SU(2)$ by

$$U = e^{i\xi} \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix} , \qquad (3.4)$$

with $\xi \in [0, \pi)$ and $\alpha, \beta \in \mathbb{C}$ satisfying $|\alpha|^2 + |\beta|^2 = 1$, and thereby consider the energy spectra that arise under the boundary conditions (3.1). The general form of eigenfunctions for positive energy is

$$\psi_k(x) = A_k \, e^{ikx} + B_k \, e^{-ikx}, \qquad k > 0 \,, \tag{3.5}$$

where the coefficients A_k , B_k may depend on k. Then, in terms of $K_{\pm} := 1 \pm kL_0$ the boundary conditions (3.1) become

$$\begin{pmatrix} \alpha K_{-} + (\beta e^{ikl} - e^{-i\xi})K_{+} & \alpha K_{+} + (\beta e^{-ikl} - e^{-i\xi})K_{-} \\ \alpha^{*}e^{ikl}K_{+} - (\beta^{*} + e^{-i\xi}e^{ikl})K_{-} & \alpha^{*}e^{-ikl}K_{-} - (\beta^{*} + e^{-i\xi}e^{-ikl})K_{+} \end{pmatrix} \begin{pmatrix} A_{k} \\ B_{k} \end{pmatrix} = 0 .$$

$$(3.6)$$

⁴ One might think that L_0 should be regarded as a free parameter as in (2.2), but it can be shown [11] that this freedom can be absorbed by adjusting the U(2) parameters in U.

For nontrivial solutions for A_k , B_k , the following condition for the momentum k should be fulfilled,

$$2kL_0 \left(\beta_I + \sin\xi \,\cos kl\right) + \left[(\cos\xi - \alpha_R) + (\cos\xi + \alpha_R) \,(kL_0)^2 \right] \,\sin kl = 0 \,, \qquad (3.7)$$

with β_I and α_R being the imaginary part of β and the real part of α , respectively. Thus the positive spectrum consists of infinitely many discrete levels, and for large k the allowed k approaches to the equidistant values $n\pi/l$ with n integer.

On the other hand, for negative energy states,

$$\psi_{\kappa}(x) = A_{\kappa} e^{\kappa x} + B_{\kappa} e^{-\kappa x}, \qquad \kappa > 0 , \qquad (3.8)$$

one proceeds analogously by replacing k with $-i\kappa$ in (3.7) to obtain

$$2\kappa L_0 \left(\beta_I + \sin\xi \cosh\kappa l\right) + \left[\left(\cos\xi - \alpha_R\right) - \left(\cos\xi + \alpha_R\right)\left(\kappa L_0\right)^2\right] \sinh\kappa l = 0.$$
(3.9)

It is readily seen by inspection that the condition (3.9) has at most two solutions for κ . The fact that the number of negative states is at most two is a norm for a system possessing a U(2) family of self-adjoint Hamiltonians, which can be seen in the system $\mathbb{R}^1 \setminus \{0\}$ as well [3, 4]. As for the existence condition for a zero energy state, one puts the form

$$\psi_0(x) = A x + B \tag{3.10}$$

in (3.1) and finds that the condition for the existence reads

$$(\beta_I + \sin\xi) - \frac{l}{2L_0}(\alpha_R - \cos\xi) = 0 .$$
 (3.11)

An important point to observe is that the entire energy spectrum (positive, negative and zero) depends only on the parameters (ξ, α_R, β_I) rather than on the full set of U(2) parameters in (3.4). This suggests that, even though all the distinct self-adjoint extensions of Hamiltonians are furnished by the U(2) family, some of them are unitarily related and the true space of spectra, the spectral space χ_{SP} , forms a subspace of U(2). In other words, different self-adjoint extensions may *not* correspond to different physics as opposed to the common belief; see [12]. Within the U(2) family there are a number of distinguished subfamilies (some of which are not disjoint), which we shall discuss in detail in the following.

Separated subfamily \mathcal{F}_1 : The first subfamily \mathcal{F}_1 of our concern is one given by the boundary conditions (3.1) with diagonal U. The boundary conditions then split into two sets, one at the left wall x = 0 and the other at the right wall x = l. In our parametrization (3.4), this occurs for $\beta = 0$, leading to the subgroup $U(1) \times U(1) \subset U(2)$ given by the torus,

$$\mathcal{F}_{1} = S^{1} \times S^{1} = \left\{ \left(\xi, \alpha_{R}, \alpha_{I}, \beta_{R}, \beta_{I}\right) \, \middle| \, \xi \in [0, \pi), \, \alpha_{R}^{2} + \alpha_{I}^{2} = 1, \, \beta_{R} = 0, \, \beta_{I} = 0 \right\} \, . \quad (3.12)$$

If we write $\alpha = e^{i\varphi}$ with $\varphi \in [0, 2\pi)$ and use the scale parameters $L_{\pm} := L_0 \cot \phi_{\pm}$ with $\phi_{\pm} = (\xi \pm \varphi)/2$, we find that the boundary conditions (3.1) reduce to

$$\psi(0) + L_+ \psi'(0) = 0$$
, $\psi(l) + L_- \psi'(l) = 0$. (3.13)

Clearly, this subfamily arises when we require local probability conservation j(0) = j(l) = 0, and therefore it describes a box in its true sense of the word — the left and the right walls of the box are disconnected physically. The corresponding subfamily appearing in the aforementioned context of a line with a point interaction is referred to as 'separated' [16], from which we adopt the name of the subfamily here.

Among this separated subfamily \mathcal{F}_1 are four special cases $(L_+, L_-) = (0, 0), (\infty, \infty),$ $(0, \infty), (\infty, 0)$ in which the theory becomes free from scale parameters (apart from l) and, consequently, solvable explicitly. Indeed, for the first two cases the eigenfunctions $\psi_n^{(L_+,L_-)}(x)$ for non-negative energies (no negative energy state is allowed)

$$E_n = \frac{\hbar^2}{2ml^2} (n\pi)^2 , \qquad (3.14)$$

are given, respectively, by

$$\psi_n^{(0,0)}(x) = \sqrt{\frac{2}{l}} \sin \frac{n\pi}{l} x, \quad \text{for} \quad n = 1, 2, 3, \dots,$$
 (3.15)

and

$$\psi_n^{(\infty,\infty)}(x) = \begin{cases} \sqrt{\frac{2}{l}} \cos \frac{n\pi}{l} x, & \text{for} \quad n = 1, 2, 3, \dots \\ \sqrt{\frac{1}{l}}, & \text{for} \quad n = 0. \end{cases}$$
(3.16)

As for the Feynman kernel we find

$$K(b,T;a,0) = \frac{1}{2l} \sum_{n=-\infty}^{\infty} e^{-\frac{i}{\hbar}E_n T} \left(e^{i\frac{n\pi}{l}(b-a)} \mp e^{i\frac{n\pi}{l}(b+a)} \right) , \qquad (3.17)$$

where the '-'-sign is for $(L_+, L_-) = (0, 0)$ whereas the '+'-sign is for (∞, ∞) . With the help of the Poisson summation formula, $\sum_{n=-\infty}^{\infty} f(n) = \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} dp f(p) e^{2\pi n i}$ which holds for well-behaved functions f(x) (*i.e.*, for $f(x) \in L_1(-\infty, \infty)$ being continuous and of bounded variation), one can rewrite (3.17) into

$$K(b,T;a,0) = \sqrt{\frac{m}{2\pi i\hbar T}} \sum_{n=-\infty}^{\infty} \left(e^{\frac{i}{\hbar} \frac{m}{2T} \{(b-a)+2nl\}^2} \mp e^{\frac{i}{\hbar} \frac{m}{2T} \{(b+a)+2nl\}^2} \right) .$$
(3.18)

As on the half line, the result (3.18) allows for the interpretation that the kernel is the sum of contributions from classical paths of two distinct classes, one hitting *n*-times the right and left walls equally while the other hitting *n*-times the left and $(n \pm 1)$ -times the right, where the signature of *n* is determined according to whether the particle hits the right wall first or not. The phase factor, -1 for (0,0) and +1 for (∞,∞) , attached to the paths in the latter class suggests that the phase shift occurs every time the particle hits the wall, and this is the only nontrivial factor for the exactness of the WKB approximation.

One can proceed analogously for the third case $(L_+, L_-) = (0, \infty)$ and for the fourth $(L_+, L_-) = (\infty, 0)$, the latter being obtained from the former by the parity operation $x \mapsto l - x$, where one has the eigenfunctions,

$$\psi_n^{(0,\infty)}(x) = \sqrt{\frac{2}{l}} \sin \frac{(n+\frac{1}{2})\pi}{l} x, \quad \text{for} \quad n = 0, 1, 2, \dots,$$
 (3.19)

and

$$\psi_n^{(\infty,0)}(x) = \sqrt{\frac{2}{l}} \cos \frac{(n+\frac{1}{2})\pi}{l} x, \quad \text{for} \quad n = 0, 1, 2, \dots,$$
 (3.20)

of energy

$$E_n = \frac{\hbar^2}{2ml^2} \left[\left(n + \frac{1}{2} \right) \pi \right]^2 . \tag{3.21}$$

(Again, no negative energy state is allowed.) Then the Feynman kernel turns out to be

$$K(b,T;a,0) = \sqrt{\frac{m}{2\pi i\hbar T}} \sum_{n=-\infty}^{\infty} (-1)^n \left(e^{\frac{i}{\hbar} \frac{m}{2T} \{(b-a)+2nl\}^2} \mp e^{\frac{i}{\hbar} \frac{m}{2T} \{(b+a)+2nl\}^2} \right) , \quad (3.22)$$

where the '-'-sign is for $(L_+, L_-) = (0, \infty)$ and the '+'-sign is for $(\infty, 0)$. The status of the WKB exactness remains similar, where now one observes that the phase shift occurs only when the particle hits the left wall for $(0, \infty)$ or the right wall for $(\infty, 0)$. (The spectrum decomposition of the Feynman kernel has been obtained in [17] for generic boundary conditions, and the WKB exactness for the case $(L_+, L_-) = (0, 0)$ has been mentioned earlier [9, 13] based on the ideas developed in [18, 19].) In passing we note that all of the Feynman kernels obtained in closed form here can be cast into expressions in the theta-function, $\vartheta_3(z,\tau) = \sum_{n=-\infty}^{\infty} e^{i\pi\tau n^2 + i2n\pi z}$. For example, the kernel (3.22) can be written as

$$K(b,T;a,0) = \sqrt{\frac{m}{2\pi i\hbar T}} \left\{ \vartheta_3 \left(\frac{ml(b-a)}{\pi\hbar T} - \frac{1}{2}, \frac{2ml^2}{\pi\hbar T} \right) e^{\frac{i}{\hbar} \frac{m}{2T}(b-a)^2} \\ \mp \vartheta_3 \left(\frac{ml(b+a)}{\pi\hbar T} - \frac{1}{2}, \frac{2ml^2}{\pi\hbar T} \right) e^{\frac{i}{\hbar} \frac{m}{2T}(b+a)^2} \right\}.$$
(3.23)

Scale independent subfamily \mathcal{F}_2 : The second subfamily \mathcal{F}_2 arises when the derivative terms become decoupled from non-derivative terms in (3.1). This occurs if and only if

$$det(U - I) = det(U + I) = 0.$$
(3.24)

The conditions in (3.24) state that the two eigenvalues for the matrix U are ± 1 , and hence U is symmetric $U^{\dagger} = U$, as can also be confirmed explicitly using (3.4). Then, from the unitarity of U one deduces that each term in (3.1) must vanish separately,

$$(U-I)\Psi = 0$$
, $(U+I)\Psi' = 0$. (3.25)

The set of U satisfying (3.25) forms a $U(2)/(U(1) \times U(1)) \simeq S^2$ subspace in U(2), where the second U(1) is the Cartan subgroup of the $SU(2) \subset U(2)$. Explicitly, the sphere is given by the constraint in the parameter space of U(2),

$$\mathcal{F}_{2} = S^{2} = \left\{ \left(\xi, \alpha_{R}, \alpha_{I}, \beta_{R}, \beta_{I}\right) \left| \xi = \frac{\pi}{2}, \, \alpha_{R} = 0, \, \alpha_{I}^{2} + \beta_{R}^{2} + \beta_{I}^{2} = 1 \right. \right\} \,. \tag{3.26}$$

This subfamily is distinguished in that the dimensionful parameter L_0 drops out from the boundary conditions, leaving the width l of the well as the only independent scale parameter. One may therefore expect that the theory becomes scale invariant in the limit $l \to \infty$ where no scale parameter survives.

The energy spectra in this subfamily are characteristic, due to the absence of the scale parameter L_0 . First, the condition (3.9) does not admit any negative states, while (3.11) allows one zero energy state $\psi_0(x) = \sqrt{1/l}$ if and only if $\beta_I = -1$ (in which case $\alpha = 0$, $\beta = -i$). Further, the positive energy spectra can be determined explicitly from (3.7), which reduces to $\beta_I + \cos kl = 0$, yielding the two sets of solutions for the momenta $k = k_s$ labeled by $s = \pm$,

$$k_n^s = s \, k_n \,, \qquad k_n := \frac{1}{l} (\theta + 2n\pi) \,, \qquad n = \begin{cases} 0, 1, 2, \dots, & \text{for } s = +, \\ -1, -2, -3, \dots, & \text{for } s = -, \end{cases}$$
(3.27)

where we have used

$$heta := \arccos\left(-eta_I
ight)$$
 . (3.28)

Thus the positive energy spectra are found to be

$$E_n = \frac{\hbar^2}{2ml^2} (\theta + 2n\pi)^2 , \qquad n \in \mathbb{Z}.$$
(3.29)

It is also readily seen that normalized eigenfunctions are given by

$$\psi_n^s(x) = A_s \, e^{ik_n^s x} - A_{-s} \, e^{-ik_n^s x} \,, \tag{3.30}$$

with

$$A_{\pm} = \frac{(1+\alpha_I) + (\beta_I - i\beta_R)e^{\pm i\theta}}{2\sqrt{l(1+\alpha_I)(1+\beta_I\cos\theta)}} , \qquad (3.31)$$

for $\alpha_I \neq -1$ and $\beta_I \neq \pm 1$. The cases $\alpha_I = \pm 1$ in \mathcal{F}_2 are identical to the special cases $(L_+, L_-) = (0, \infty)$, $(\infty, 0)$ of the subfamily \mathcal{F}_1 , which are the only two points of the intersection $\mathcal{F}_1 \cap \mathcal{F}_2$. We note that, for $\beta_I = \pm 1$, the coefficients A_{\pm} are undetermined, which implies that all the energy levels but one, *i.e.*, the zero energy ground state for $\beta_I = -1$, are doubly degenerated. This is also seen from (3.29) where the two sets of levels $s = \pm$ coincide for $\theta = 0$ and π . Note also that the spectra are solely determined by the angle θ , that is, the subfamily \mathcal{F}_2 has S^1 as its image in the spectral space \mathcal{X}_{SP} . In contrast, the coefficients, and hence the eigenfunctions are dependent on the parameters (α_I, β_R) as well, even though the spectra are independent of them.

Having obtained the eigenfunctions in closed form, we shall now resort the same procedure used before to evaluate the Feynman kernel. To this end, let us denote by $\sum_{n=0}^{\prime} f_n$ the summation $\sum_{n=0}^{\infty}$ for s = + and $\sum_{n=-1}^{-\infty}$ for s = -. We then have

$$K(b,T;a,0) = \sum_{s=\pm} \sum_{n}' e^{-\frac{i}{\hbar}E_{n}T} \psi_{n}^{s}(b) (\psi_{n}^{s}(a))^{*}$$

$$= \sum_{n}' e^{-\frac{i}{\hbar}E_{n}T} \left\{ |A_{+}|^{2} \left(e^{ik_{n}^{+}(b-a)} + e^{-ik_{n}^{-}(b-a)} \right) + |A_{-}|^{2} \left(e^{ik_{n}^{-}(b-a)} + e^{-ik_{n}^{+}(b-a)} \right) - A_{+}A_{+}^{*} \left(e^{ik_{n}^{-}(b+a)} + e^{-ik_{n}^{+}(b+a)} \right) - A_{-}A_{+}^{*} \left(e^{ik_{n}^{-}(b+a)} + e^{-ik_{n}^{+}(b+a)} \right) \right\}.$$

$$(3.32)$$

Recombining the terms in the summation, and using the Poisson summation formula, we end up with

$$K(b,T;a,0) = \sum_{n=-\infty}^{\infty} e^{-\frac{i}{\hbar}E_n T} \left(|A_+|^2 e^{ik_n(b-a)} + |A_-|^2 e^{-ik_n(b-a)} - A_+ A_-^* e^{ik_n(b+a)} - A_- A_+^* e^{-ik_n(b+a)} \right)$$

$$= \sqrt{\frac{m}{2\pi i\hbar T}} l \sum_{n=-\infty}^{\infty} \left\{ C_n e^{\frac{i}{\hbar}\frac{m}{2T} \{(b-a)+nl\}^2} - D_n e^{\frac{i}{\hbar}\frac{m}{2T} \{(b+a)+nl\}^2} \right\}$$
(3.33)

with

$$C_n = |A_+|^2 e^{-i\theta n} + |A_-|^2 e^{i\theta n}, \qquad D_n = A_+ A_-^* e^{-i\theta n} + A_- A_+^* e^{i\theta n} .$$
(3.34)

The result (3.33) suggests that the WKB approximation yields the exact kernel, if the factors C_n , D_n are properly interpreted.

Smooth subfamily \mathcal{F}_3 : Among \mathcal{F}_2 is the U(1) subfamily $\mathcal{F}_3 \subset \mathcal{F}_2$ obtained by

$$\mathcal{F}_{3} = S^{1} = \left\{ \left(\xi, \alpha_{R}, \alpha_{I}, \beta_{R}, \beta_{I}\right) \, \middle| \, \xi = \frac{\pi}{2}, \, \alpha_{R} = 0, \, \alpha_{I} = 0, \, \beta_{R}^{2} + \beta_{I}^{2} = 1 \right\} \,. \tag{3.35}$$

This subfamily is distinguished in that with the remaining parameter $\theta \in [0, \pi)$ in (3.28) the boundary conditions (3.1) become

$$\psi(0) + e^{-i\theta}\psi(l) = 0$$
, $\psi'(0) + e^{-i\theta}\psi'(l) = 0$, (3.36)

which are actually the boundary conditions familiar on a smooth circle (*i.e.*, one without singularity; see [9]) with θ representing possible phase change around a 2π rotation. Here we find $A_{+} = \sqrt{1/l}$ and $A_{-} = 0$, and accordingly the Feynman kernel (3.33) takes the well-known form on the circle,

$$K(b,T;a,0) = \sqrt{\frac{m}{2\pi i\hbar T}} \sum_{n=-\infty}^{\infty} e^{-i\theta n} e^{\frac{i}{\hbar} \frac{m}{2T} \{(b-a)+nl\}^2} .$$
(3.37)

It is worth pointing out that the freedom expressed by the U(1) θ -parameter, which is a prototype of the θ -parameter of the QCD vacua, is usually ascribed to the ambiguity in quantization on the circle which is topologically nontrivial (see, e.g., [20, 21]). Here it arises as part of the U(2) family of systems allowed on a circle, where the $U(1) \subset U(2)$ subgroup emerges upon demanding translational invariance of the system, that is, the smoothness given by the boundary conditions (3.36). (The role of translational invariance among the U(2) family has been remarked in [9].)

Isospectral subfamily \mathcal{F}_4 : The energy spectra obtained explicitly for the preceding subfamilies are solutions of the spectral condition (3.7) (and (3.11)). Conversely, one may look for specific cases where other solutions can be found directly from (3.7). One then finds, for instance, that for $\xi = 0$ and $\beta_I = 0$ the condition (3.7) simplifies to $\sin kl = 0$ and admits equidistant $k = n\pi/l$ with $n = 1, 2, 3, \ldots$ for the solutions. Hence, the subfamily \mathcal{F}_4 defined by

$$\mathcal{F}_4 = S^2 = \left\{ (\xi, \alpha_R, \alpha_I, \beta_R, \beta_I) \, \middle| \, \xi = 0, \, \alpha_R^2 + \alpha_I^2 + \beta_R^2 = 1, \, \beta_I = 0 \, \right\} \,, \tag{3.38}$$

possesses the unique spectrum given by (3.14), even though the sphere (3.38) retains α_R as a free parameter for the spectra. In other words, the sphere \mathcal{F}_4 maps to a point in \mathcal{X}_{SP} . Note that $\mathcal{F}_4 \cap \mathcal{F}_1 = S^1$ while \mathcal{F}_4 is disjoint from \mathcal{F}_2 .

Despite the triviality of the spectrum, the eigenfunctions turn out to be nontrivial in that the coefficients appearing in the solution (3.5) become dependent on the level n, in sharp contrast to the coefficients in (3.30) in the scale independent subfamily \mathcal{F}_2 where they become independent (except the $s = \pm$ dependence). Because of this complication, it does not seem to be possible to proceed analogously to obtain the Feynman kernel in a form in which the WKB exactness can be examined.

Semi-isospectral subfamily \mathcal{F}_5 : An extension of the isospectral subfamily \mathcal{F}_4 is given by those cases with the property $\sin \xi = \pm \beta_I$, that is,

$$\mathcal{F}_5 = \left\{ \left(\xi, \alpha_R, \alpha_I, \beta_R, \beta_I\right) \mid \sin \xi = \pm \beta_I, \ \alpha_R^2 + \alpha_I^2 + \beta_R^2 + \beta_I^2 = 1 \right\} \ . \tag{3.39}$$

Generically, in \mathcal{F}_5 the solutions of the spectral condition (3.7) consists of two infinite sequences, one that is equidistant and parameter independent — like for the isospectral subfamily \mathcal{F}_4 which arises at $\beta_I = 0$ in \mathcal{F}_5 — and another that is parameter dependent and given by transcendental roots. For example, on the positive branch $\sin \xi = +\beta_I$, the roots of $\cos kl = -1$, $k = n\pi/l$ with $n = 1, 3, 5, \ldots$, are the parameter independent solutions. By inspection, one finds from (3.7) that the other roots are an infinite sequence of nontrivial, transcendental solutions. The two sequences of roots are alternating, one transcendental root between any two succeeding equidistant roots and vice versa. For the negative branch $\sin \xi = -\beta_I$, the isospectral roots are now given by the solutions, $k = n\pi/l$ with n = 2, 4, 6, ..., of $\cos kl = +1$ and the transcendental roots are also different from the previous ones, but the qualitative picture of the spectrum remains the same.

We observe that the two branches meet each other in \mathcal{F}_4 at $\beta_I = 0$, where both sequences become isospectral and equidistant. The other special points in \mathcal{F}_5 are the two points with $\beta_I = \pm 1$, where the two sequences coincide and hence the energy levels become doubly degenerate. These points, $\beta_I = 0, \pm 1$, are in fact exceptional in \mathcal{F}_5 in the sense that a single ξ corresponds to the respective β_I . Since there exist two ξ for a generic β_I except the above three, we see from (3.39) that, topologically, the subfamily \mathcal{F}_5 is given by two S^3 sharing their equators ($\beta_I = 0$) and the North and South Poles ($\beta_I = \pm 1$); see Fig.1. We also note that $\mathcal{F}_5 \cap \mathcal{F}_1 = \mathcal{F}_4 \cap \mathcal{F}_1 = S^1$, and that $\mathcal{F}_5 \cap \mathcal{F}_2 = \mathcal{F}_5 \cap \mathcal{F}_3$ consists of the two special points $\beta_I = \pm 1$.

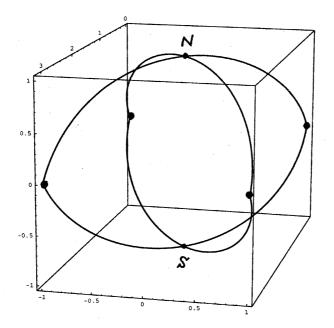


Figure 1. A schematical picture of Semi-isospectral subfamily \mathcal{F}_5 obtained by setting $\alpha_{\rm I} = \beta_{\rm R} = 0$ in (3.39). The North and South Poles are shared by the two S^3 which are shown here by two circles. The four points marked by dots • correspond to a sphere S^2 which is the shared equator of the two S^3 .

Finally, we stress that it is important to analyze the spectral space \mathcal{X}_{SP} thoroughly in order to understand fully, *e.g.*, the intriguing double spiral structure and a certain 'fermion-boson' duality on \mathcal{X}_{SP} recently reported [22, 23]. We suspect that behind them underlie certain symmetries, such as those associated with parity, time-reversal and scale transformations studied in [16] for $\mathbb{R}^1 \setminus \{0\}$. The analysis is also important with regard to quantum mechanical symmetry breaking, in view of the fact that in two and three dimensions the conformal SO(2, 1) symmetry is seen to be broken dynamically under the presence of the delta-function interaction [24]. Our investigation on these issues, including a fuller account of the result presented here, will be reported elsewhere [11].

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