Boundary Conditions in One-dimensional Tunneling Junction

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Abstract. The tunneling effect is first characterized in quantum mechanics. However, the mathematical analysis for the tunneling effect is so complicated. In the conventional sense, the WKB analysis is useful to analyze such effect. Here, we consider the mathematical analysis for the tunneling effect in the one-dimensional Schrödinger system from the viewpoint of functional analysis. From the rigorous analysis, we obtain the interference pattern of the tunneling particle.

1. Introduction
The tunneling effect is first appeared in quantum mechanics but cannot be characterized in classical mechanics. This effect is one of the purely quantum-mechanical effects. However, almost all cases cannot be analytically solved. On considering the tunneling effect, the WKB analysis is often used. This analysis is not rigorous in mathematics since almost all solutions are not converged but this can be well described in physical phenomena. According to the WKB analysis, the interference pattern has been appeared for the tunneling particle. To give the analytical meaning in mathematics, the exact WKB analysis was proposed to be applied the Borel summation method to the WKB solution, which is the solution in the case that the Planck constant is a sufficient small parameter [1]. Even in the exact WKB analysis, the phase factor for the WKB solution is in general appeared on the tunneling. In Ref. [2], we have considered the role of the phase factor from the viewpoint of mathematical physics.

The aim of this paper is to make clear the physical meaning of the results of Ref. [2]. Therefore, some mathematical definitions are not strictly defined in this paper.

2. Preliminaries
2.1. Our setup
In this subsection, our setup is assumed. The Schrödinger particle on the line is to be tunneled in the junction $[-\Lambda, \Lambda]$. Our question is what behavior of the tunneling particle is from the mathematical constraint. In the case of the non-tunneling particle, this only gets the global phase, see more details in Ref. [2]. The potential energy is infinity on the junction and free on
the other region. Therefore, the Hamiltonian is mathematically defined as

\[ \hat{H} := -\frac{d^2}{dx^2} \text{ on } \Omega := (-\infty, -\Lambda) \cup (\Lambda, \infty). \]  

(1)

The degrees of the freedoms at the edges of the junction are the wavefunction and its derivative defined on the edges, that is, \( U(2) \times U(2) \). However, the tunneling effect can be represented as the unitary transform \( U(1) \). Therefore, the total degree of freedom is \( U(2) \times U(2) \setminus U(1) \). This schematic figure is illustrated in Fig. 1.

From the viewpoint of physics, the tunneling effect cannot be occurred in this situation since the potential energy on the junction is infinity. However, our situation is also satisfied in the case of the point junction, \( \Lambda \to 0+ \). This case corresponds to Ref. [3] to be analyzed in the quantum graph theory. It should be noted that our result is consistent with one of Ref. [3] in the case of \( \Lambda \to 0+ \). The meaning of the mathematical generalization from the point junction is not only mathematical beauty but also to give the analytic solution for the simple model to be extended to the more realistic models, \( e.g. \), see quantum wires and fractional quantum Hall devices in Ref. [4]. From the conventional approach without the WKB analysis, we cannot obtain the interference pattern after the tunneling.

\[ \text{Quantum particle} \]

\[ -\Lambda \quad \Lambda \]

\[ \infty \]

\[ \text{Tunneling Effect} \]

\[ \text{Figure 1.} \text{ The schematic figure is our considered setup. We only consider tunneling the junction } [-\Lambda, \Lambda] \text{ of the quantum particle, especially the Schrödinger particle. The potential energy of the junction is infinity. In the case of } \Lambda \to 0+, \text{ the junction can be represented as the Dirac delta function.} \]

2.2. Mathematical notations

Due to the physical constraint that the energy spectrum is real, the Hamiltonian has to be the self-adjoint operator. It is remarked that in the case that the Hilbert space is the finite dimensional complex vector field, the Hermitian matrix is self-adjoint. This is because the Hermitian matrix must have the real eigenvalue. However, in general, in the case that the Hilbert space is the square integrable space\(^1\), the Hermite operator is completely different from the self-adjoint operator. Since the self-adjoint operator must have real spectrum, this can be taken as the observable in the von Neumann mathematical axioms of quantum mechanics [5]. The counterexamples that the Hamiltonian is not self-adjoint have been well studied, \( e.g. \), see

\(^1\) Our setup is considered in this class.
Ref. [6]. Furthermore, from the viewpoint of statistical physics, the case that the Hamiltonian has the complex eigenvalue were studied to be related with the resonance pole [7]. The symmetric operator is classified with three classes; the operator is self-adjoint, self-adjoint extendable, and the non-self-adjoint extendable, see the pedagogical explanation in Ref. [8, Appendix B]. In the case that the operator is self-adjoint extendable, the operator can be taken as the self-adjoint operator since it can be mapped by the unitary operator.

In our setup, the Hamiltonian should mathematically defined by

\[
\hat{H}_0 = -\frac{d^2}{dx^2}
\]

with \( \text{Dom}(\hat{H}_0) = \{ \psi \in \text{Dom}(\hat{H}_0^*) \mid \psi(-\Lambda) = \psi(\Lambda) = \psi'(-\Lambda) = \psi'(\Lambda) = 0 \} \),

where

\[
\hat{H}_0^* := -\frac{d^2}{dx^2}
\]

with \( \text{Dom}(\hat{H}_0^*) = \{ \psi \in \mathcal{L}^2(\Omega_\Lambda) \mid \psi \in AC^2(\Omega_\Lambda) \} \),

and \( \text{Dom}(\hat{A}) \) expresses is the domain of the operator \( \hat{A} \). Here, \( \overline{S} \) is the closure of the set \( S \), \( \mathcal{L}^2(S) \) is the square integrable space on the space \( S \), and \( AC^2(S) \) is that every function defined on the space \( S \) is absolutely contentious on the space \( S \). Now, the deficiency subspaces\(^2\) for the Hamiltonian \( \hat{H}_0 \) are defined by

\[
\mathcal{H}_+(\hat{H}_0) := \{ \psi \in \text{Dom}(\hat{H}_0^*) \mid \hat{H}_0^*\psi = i\psi \},
\]

\[
\mathcal{H}_-(\hat{H}_0) := \{ \psi \in \text{Dom}(\hat{H}_0^*) \mid \hat{H}_0^*\psi = -i\psi \}.
\]

Roughly speaking, any wavefunction \( \psi \in \mathcal{L}^2(\Omega_\Lambda) \) can be decomposed to three components,

\[
\psi = \psi_0 + c_+\psi_+ + c_-\psi_-, \quad \text{with} \quad \psi_+ \in \mathcal{H}_+(\hat{H}_0) \quad \text{and} \quad \psi_- \in \mathcal{H}_-(\hat{H}_0),
\]

where \( c_+, c_- \in \mathbb{C} \). The wavefunction \( \psi_0 \) has the eigenfunction with the real eigenvalue for the operator \( \hat{H}_0 \).

3. Main result

**Theorem 1 (Furuhashi, Hirokawa, Nakahara, Shikano [2])** From the physical constraint that the Hamiltonian \( \hat{H}_0 \) should be self-adjoint extendable, we obtain

\[
\psi_+(\Lambda) = e^{i(\theta+3\pi/4)}\psi_+(-\Lambda),
\]

\[
\psi_-(\Lambda) = e^{i(\theta-3\pi/4)}\psi_-(\Lambda),
\]

where \( \theta \) is the arbitrary real number.

This means that the tunneling Schrödinger particle always leads to the interference pattern after the tunneling by the effect of \( \psi_\pm(x) \). Also, this phase is independent of the width of the junction \( 2\Lambda \). While we simply set \( \psi = \psi_0 \) and \( \psi_0(\pm\Lambda) = \psi'_0(\pm\Lambda) = 0 \) as the boundary condition in the standard approach, the more general boundary condition should be considered in the quantum-mechanical system by the von Neumann axiom. It should be noted that our result is globally defined. Therefore, the incoming Schrödinger particle for the tunneling cannot be dealt

\(^2\) The deficiency subspaces are useful to classify the symmetric operator, which is called a deficiency theorem. See more details in Ref. [8, Appendix B].
from the viewpoint of mathematical physics. This interference pattern is not always occurred. As the future problem, the concrete example of our system should be constructed. However, the tunneling effect is often analyzed by the WKB analysis. The tunneling effect can be taken as one kind of the scattering problem. Therefore, in the approximate solution for the quantum mechanical system, the interference after the tunneling can be considered. However, our result is not approximated while the potential energy on the junction is infinity. Our result may help us consider the relationship between the self-adjointness and the scattering process in quantum mechanics.

4. Conclusion
We have considered the phase factor of the one-dimensional Schrödinger particle with the junction. The tunneling particle leads to the interference from the viewpoint of the mathematical rigorous analysis. In this paper, we have explained its meaning and the comparison to the conventional setting from the viewpoint of physics.

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