Role of a phase factor in the boundary condition of a one-dimensional junction

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Abstract

One-dimensional quantum systems can be experimentally studied in recent nanotechnology like the carbon nanotube and the nanowire. We have considered the mathematical model of a one-dimensional Schrödinger particle with a junction and have analyzed the phase factor in the boundary condition of the junction. We have shown that the phase factor in the tunneling case appears in the situation of the non-adiabatic transition with the three energy levels in the exact Wentzel–Kramers–Brillouin analysis.

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1. Introduction

Quantum phases play a crucial role of quantum interference and coherence. It is well known that the global phase factor for the quantum state is undetectable. On the other hand, since the relative phase is detectable by interference patterns such as the Young double-slit experiment for the electron [1] and the molecule [2], this quantity is meaningful. By the experimental demonstration of the delayed choice experiment or the quantum eraser [3], we know that this quantity depends on the operational setup. Aharonov and Bohm predicted a phase of the electrically charged particle from an electromagnetic potential [4], which is known as the Aharonov–Bohm phase. Furthermore, Berry predicted a phase acquired over the course of a cycle with adiabatic processes resulting from the geometrical properties of the parameter space of the Hamiltonian [5], which is known as the Berry phase or the geometric phase. The Aharonov–Bohm phase [6–8] and the Berry phase [9–11] are experimentally realized. They
are given by the Hamiltonian decided from the operational setup. However, there also exists a phase factor in the boundary condition, which is not decided by the Hamiltonian but is decided by the situation of a quantum particle. In this paper we address the latter quantum phase under a one-dimensional system like the following physical setup.

Recent development on experimental techniques has provided a way to study the one-dimensional quantum physics, for instance, see [12]. In this paper, we focus on the one-dimensional electron transport system. The electron on the single-wall carbon nanotube [13] and the nanowire made of semiconductor materials such as InP [14], InAs/InP [15], GaAs/GaP [14] and Si/SiGe [16] can be described as the one-dimensional quantum system. This can be controlled by the application of the technique on a single-electron transistor, which is a device in which electrons tunnel one at a time through a small island connected to two leads via a tunnel junction, in the single-wall carbon nanotube [17] and the InP nanowire [18]. Furthermore, two carbon nanotubes electrically can be connected via a junction such as a gold particle [19]. See more examples on the connected carbon nanotubes in [20]. We consider a mathematical model of the one-dimensional quantum system with a junction throughout this paper.

As is well known, a physical observable is described by a self-adjoint operator [21]. Thus, the set $D(H)$ of all wavefunctions of a Hamiltonian $H$ should be determined so that $H$ becomes a self-adjoint operator. Usually, we begin with considering the action of an energy operator $H_0$ for the Hamiltonian $H$ on a domain $D(H_0)$ in which the energy operator $H_0$ is not self-adjoint, since it is smaller than $D(H)$. Thus, we seek the Hamiltonian $H$ as an extension of $H_0$. This extension is called a self-adjoint extension [22]. As the boundary condition for a physical setup is fixed, a self-adjoint extension is determined so that the extension corresponds to the boundary condition.

It is already known that a phase factor appears in a boundary condition for a self-adjoint extension of a momentum operator on a non-Euclidean space [22, 23]. In the case of Hamiltonians, however, a phase factor does not always appear in the boundary condition, for instance, example 2 in [22, section X.1], theorem 3.1.1 in [24] and equation (1.1) in [25]. Thus, in this paper we make a realization of the above physical setup to obtain a mathematical model to consider a Schrödinger particle in a line with a junction. In our mathematical idealization, the junction is represented by the closed interval $[-\Lambda, \Lambda]$ and the Schrödinger particle moves in $(-\infty, -\Lambda) \cup (\Lambda, \infty)$.

For example, we can take a non-relativistic electron as the Schrödinger particle$^4$, and then the junction is made from an insulator. We investigate the phase factor determined by the boundary conditions at the two edges ($x = -\Lambda$ and $x = \Lambda$) of the junction when the Schrödinger particle tunnels through the junction. In the near future we will consider controlling the phase factor determined by the boundary conditions using the Aharonov–Bohm phase obtained by a magnetic field through the junction only.

Our results characterize the boundary conditions for the point interaction given in [24] and [26] based on whether the Schrödinger particle tunnels through the junction or not. More precisely, the boundary condition in the case where the Schrödinger particle does not tunnel

$^4$ In the case of carbon nanotubes, the non-relativistic electron can be taken as the excitation of the Tomonaga–Luttinger liquid [20].
through the junction (as in theorem 1) corresponds to that for the point interaction given in [24] (see remark 1). On the other hand, the boundary condition in the case where the Schrödinger particle does tunnel through the junction (as in theorems 2 and 3) corresponds to that for the point interaction given in [26] (see remark 2). Namely, our results tell us that the generalized boundary condition given in the unfortunately unpublished paper [26] is important in the light of the Schrödinger particle tunneling the junction.

Our paper is organized as follows. In section 2 we recall some well-known facts and formulate our problem. In section 3 we investigate the boundary conditions of wavefunctions, dividing them into two cases. In the first case we handle the Schrödinger particle not tunneling through the junction. In this case we can completely classify the type of boundary conditions which corresponds to that in [24]. In the other case we consider the Schrödinger particle tunneling through the junction. We give another type of boundary condition which corresponds to that for the point interaction given in [26]. Furthermore, this phase corresponds to the one obtained by the exact Wentzel–Kramers–Brillouin (WKB) analysis in the model of the three-level non-adiabatic transition inside the junction. Section 4 is devoted to the summary and the discussions.

2. Preparations and our model

2.1. Mathematical notations

In this section, we develop some mathematical terms and notions. For every operator $A$ acting in a Hilbert space, $D(A)$ expresses the set of all vectors on which the operator $A$ can act. For instance, $D(A)$ is the set of all wavefunctions as $A$ is an energy operator. $D(A)$ is called the domain of the operator $A$. For the operators $A$ and $B$ we say $A$ is equal to $B$, i.e. $A = B$ if and only if $D(A) = D(B)$ and $A\psi = B\psi$ for every $\psi \in D(A) = D(B)$, where $\psi \in D(A)$ means that the vector $\psi$ belongs to the domain $D(A)$. When $D(A) \subset D(B)$ and $A\psi = B\psi$ for every $\psi \in D(A)$, we say that the operator $B$ is an extension of the operator $A$, and we express that by $A \subset B$. $D(A^*)$ expresses the set of all vectors $\psi$ satisfying the following for an operator $A$: there is a vector $\phi_A$ so that $\langle \psi | A \psi \rangle = \langle \phi_A | \psi \rangle$ for every $\psi \in D(A)$. Then the adjoint operator $A^*$ of the operator $A$ is given by $A^*\psi = \phi_A$ for every $\psi \in D(A^*)$. Note that the domain $D(A^*)$ has to be dense in the Hilbert space since the adjoint operator $A^*$ is determined uniquely. The operator $A$ is said to be symmetric as $A \subset A^*$, and moreover the operator $A$ is self-adjoint if and only if $A = A^*$. Thus, when an operator $B$ is called a self-adjoint extension of an operator $A$, the operator $B$ satisfies $B = B^*$ and $A \subset B$. $D(\overline{A})$ expresses the set of all vectors $\psi$ satisfying the following conditions for an operator $A$: there is a sequence $\{\psi_n\}_n$ of vectors $\psi_n \in D(A)$ so that the sequences $\{\psi_n\}_n$ and $\{A\psi_n\}_n$ converge and $\psi = \lim_{n \to \infty} \psi_n$. Then, the closure $\overline{A}$ of the operator $A$ is defined by $\overline{A}\psi := \lim_{n \to \infty} A\psi_n$. We say that the operator $A$ is closed if $A = \overline{A}$. It is well known that a self-adjoint operator is closed.

Following [22, example 2 in section X.1], we recapitulate some facts on the self-adjoint extension here. For the subset $\Omega$ of the line $\mathbb{R} := (-\infty, \infty)$, $C_0^\infty(\Omega)$ expresses the set of all infinitely differentiable functions on $\Omega$ with their individual compact supports in $\Omega$. Here the support of a function $\psi$ on $\Omega$ is the closure $[x \in \Omega \mid \psi(x) \neq 0]$ of the set $\{x \in \Omega \mid \psi(x) \neq 0\}$. $AC^2(\Omega)$ expresses the set of all absolutely continuous functions $\psi$ on $\Omega$ so that $\psi'$ is also absolutely continuous and $\psi''$ is square integrable on $\Omega$. It should be noted that the Lebesgue theorem states that an absolutely continuous function $\psi$ has its differentiable $\psi'$ almost everywhere.

The regions $(-\infty, -\Lambda)$ and $(\Lambda, \infty)$ are denoted as $\Omega_L$ and $\Omega_R$ for an arbitrarily fixed constant $\Lambda > 0$, respectively. We define the energy operators $H_{L,00}$ and $H_{R,00}$ by
we define the vector spaces \( H_{\alpha} \) of the energy operator with a small domain \( H_{\alpha} \) as Hamiltonians of the particle, we begin with giving the action as the proof of [27, theorem 8.25(b)] and the second part similar to the proof of [27, theorem 8.22] (see also [28, example 3 in section VIII.6]).

\[
H_{\alpha} = -\frac{d^2}{dx^2} \quad \text{with} \quad D(H_{\alpha}) = \{ \psi \in AC^2(\Omega_{\alpha}) \mid \psi'(-\Lambda) = \alpha_{\Lambda} \psi(-\Lambda) \},
\]

and for \( \alpha_{\Lambda} = \infty \), we have the self-adjoint extension

\[
H_{\infty} = -\frac{d^2}{dx^2} \quad \text{with} \quad D(H_{\infty}) = \{ \psi \in AC^2(\Omega_{\infty}) \mid \psi'(-\Lambda) = 0 \}.
\]

Similarly, for every \( \alpha_{\Lambda} \in \mathbb{R} \), we have the self-adjoint extension

\[
H_{\alpha} = -\frac{d^2}{dx^2} \quad \text{with} \quad D(H_{\alpha}) = \{ \psi \in AC^2(\Omega_{\alpha}) \mid \psi'(\Lambda) = \alpha_{\Lambda} \psi(\Lambda) \},
\]

and for \( \alpha_{\Lambda} = \infty \), we have the self-adjoint extension

\[
H_{\infty} = -\frac{d^2}{dx^2} \quad \text{with} \quad D(H_{\infty}) = \{ \psi \in AC^2(\Omega_{\infty}) \mid \psi'(\Lambda) = 0 \}.
\]

Here \( \overline{\Omega} \) denotes the closure of a set \( \Omega \subset \mathbb{R} \).

### 2.2. Mathematical setups for our model

In this paper, the closed interval \([-\Lambda, \Lambda]\) represents a junction on the line for an arbitrarily fixed constant \( \Lambda > 0 \). We define a one-dimensional, non-Euclidean space \( \Omega_{\Lambda} \) by eliminating the junction from the line \((-\infty, \infty)\), i.e. \( \Omega_{\Lambda} := (-\infty, -\Lambda) \cup (\Lambda, \infty) \). We assume that a free Schrödinger particle such as a non-relativistic electron lives in \( \Omega_{\Lambda} \). To consider the self-adjoint extensions \( H \) as Hamiltonians of the particle, we begin with giving the action \( H_{00} \) of the energy operator with a small domain \( D(H_{00}) \) in which \( H_{00} \) is not self-adjoint yet, since it is smaller than \( D(H) \). In the next section we show how a self-adjoint extension is determined so that the extension corresponds to the boundary condition of each physical setup.

We consider the Hilbert space \( L^2(\Omega_{\Lambda}) \) defined as the set of all square-integrable functions on \( \Omega_{\Lambda} \). This represents the state space to which the wavefunctions of our Schrödinger particle belong. The energy operator \( H_{00} \) is defined by

\[
H_{00} := -\frac{d^2}{dx^2} \quad \text{with} \quad D(H_{00}) := C^0_0(\Omega_{\Lambda}).
\]

Then, although the operator \( H_{00} \) is neither closed nor self-adjoint, \( H_{00} \) is symmetric. We denote the closure of \( H_{00} \) by \( H_0 \), i.e. \( H_0 := \overline{H_{00}} \). Then by the well-known theorem that \( H_0^* = H_0 \), and moreover \( H_0 \subset H_0^* \). So \( H_0 \) is symmetric, though \( H_0^* \) is not symmetric. Thus, \( H_0^* \) has some purely imaginary eigenvalues. Then, as in the definition in [22, section X.1], we define the vector spaces \( \mathcal{H}_+(H_0) \) and \( \mathcal{H}_-(H_0) \) by \( \mathcal{H}_+(H_0) := \{ \psi \in D(H_0^*) \mid H_0^* \psi = i\psi \} \) and \( \mathcal{H}_-(H_0) := \{ \psi \in D(H_0^*) \mid H_0^* \psi = -i\psi \} \), respectively. We call \( \mathcal{H}_+(H_0) \) and \( \mathcal{H}_-(H_0) \) the deficiency subspaces.

We can respectively prove the first part of the following proposition in the same way as the proof of [27, theorem 8.25(b)] and the second part similar to the proof of [27, theorem 8.22] (see also [28, example 3 in section VIII.6]).
Proposition 1. The operators $H_0$ and $H_0^*$ have the following actions with the domains respectively:

$$H_0 = -\frac{d^2}{dx^2} \quad \text{with} \quad D(H_0) = \{ \psi \in D(H_0^*) \mid \psi(\Lambda) = \psi'(-\Lambda) = \psi'(-\Lambda) = 0 \},$$

(6)

and

$$H_0^* = -\frac{d^2}{dx^2} \quad \text{with} \quad D(H_0^*) = \{ \psi \in L^2(\Omega_\Lambda) \mid \psi \in AC^2(\Omega_\Lambda) \}. \quad (7)$$

Theorem X.2 of [22], together with its corollary and proposition 1, says that for every self-adjoint extension $H_U$ of $H_0$ there is a unitary operator $U : \mathcal{H}_+(H_0) \to \mathcal{H}_-(H_0)$ so that $H_U = -d^2/dx^2$ with the domain

$$D(H_U) = \{ \psi_0 + \psi_+ + U\psi_+ \mid \psi_0 \in D(H_0), \psi_+ \in \mathcal{H}_+(H_0) \}. \quad (8)$$

Conversely, for every unitary operator $U : \mathcal{H}_+(H_0) \to \mathcal{H}_-(H_0)$, the operator $H_U = -d^2/dx^2$ with the domain given by equation (8) is a self-adjoint extension of $H_0$. That is, the self-adjoint extensions $H_U$ of $H_0$ are in one-to-one correspondence with the set of all unitary operators $U : \mathcal{H}_+(H_0) \to \mathcal{H}_-(H_0)$.

Solving simple differential equations, we can obtain the eigenfunctions $R_\pm$ and $L_\pm$ of $H_0^*$:

$$R_+(x) := \begin{cases} 0 & \text{if } -\infty < x < \Lambda, \\ N e^{-i \sqrt{2} / x} & \text{if } \Lambda < x < \infty, \end{cases} \quad (9)$$

$$R_-(x) := \begin{cases} 0 & \text{if } -\infty < x < \Lambda, \\ N e^{i \sqrt{2} / x} & \text{if } \Lambda < x < \infty, \end{cases} \quad (10)$$

and

$$L_+(x) := \begin{cases} N e^{i \sqrt{2} / x} & \text{if } -\infty < x < \Lambda, \\ 0 & \text{if } \Lambda < x < \infty, \end{cases} \quad (11)$$

$$L_-(x) := \begin{cases} N e^{-i \sqrt{2} / x} & \text{if } -\infty < x < \Lambda, \\ 0 & \text{if } \Lambda < x < \infty, \end{cases} \quad (12)$$

with the normalization factor $N = \frac{1}{\sqrt{2}} e^{\Lambda / \sqrt{2}}$ so that $H_0^* R_\pm = \pm i R_\pm$ and $H_0^* L_\pm = \pm i L_\pm$. Namely, $L_+, R_+ \in \mathcal{H}_+(H_0)$ and $L_-, R_- \in \mathcal{H}_-(H_0)$. The uniqueness of the differential equations tells us that

$$\mathcal{H}_+(H_0) = \{ c_L L_+ + c_R R_+ \mid c_L, c_R \in \mathbb{C} \}, \quad (13)$$

$$\mathcal{H}_-(H_0) = \{ c_L L_- + c_R R_- \mid c_L, c_R \in \mathbb{C} \}, \quad (14)$$

and thus the dimensions of $\mathcal{H}_+(H_0)$ and $\mathcal{H}_-(H_0)$ are given as $\dim \mathcal{H}_+(H_0) = 2 = \dim \mathcal{H}_-(H_0)$, respectively. This says that the set of all unitary operators $U : \mathcal{H}_+(H_0) \to \mathcal{H}_-(H_0)$ makes $SU(2)$, and thus that the unitary operator $U : \mathcal{H}_+(H_0) \to \mathcal{H}_-(H_0)$ is given either by

$$U L_+ = \gamma L_- \quad \text{and} \quad U R_+ = \gamma R_- \quad (15)$$

5 The densely defined symmetric operators can be classified by the deficiency theorem (see [36] and [37, appendix B] for physicists) using the dimensions of the deficiency subspaces. In the case of $\dim \mathcal{H}_+(H_0) = \dim \mathcal{H}_-(H_0)$, $H_0$ has a self-adjoint extension due to the deficiency theorem.
for some $\gamma_L, \gamma_R \in \mathbb{C}$ with $|\gamma_L| = 1 = |\gamma_R|$ or by

$$UL_+ = \gamma_- R_- \quad \text{and} \quad UR_+ = \gamma_- L_-$$

(16)

for some $\gamma_-, \gamma_- \in \mathbb{C}$ with $|\gamma_-| = 1 = |\gamma_-|$. Let us denote the vector $(\gamma_L, \gamma_R)$ or $(\gamma_-, \gamma_-)$ by $\gamma$. Then using the one-to-one correspondence $U \longleftrightarrow \gamma$ given by equations (15) and (16), we can represent $H_U$ by $H_\gamma$. Thus, seeking a self-adjoint extension of $H_0$ is equivalent to finding a $H_\gamma$ with $H_0 \subset H_\gamma = H_\gamma^* \subset H_\gamma^*$ for a unitary operator $U$, that is, a vector $\gamma = (\gamma_L, \gamma_R)$ or $\gamma = (\gamma_-, \gamma_-)$.

To find a boundary condition that a self-adjoint extension $H_\gamma$ of $H_0$ satisfies, we use the following tool:

$$W(\varphi, \phi) := W_{-\Lambda}(\varphi^*, \phi) - W_\Lambda(\varphi^*, \phi),$$

(17)

for all vectors $\varphi, \phi \in D(H_\Lambda^*)$, where $W_\Lambda(f, g) := f(x)g(x) - f(\pi)g(\pi)$ is the Wronskian: $W_\Lambda(f, g) := f'(x)g(x) - f(x)g'(x)$.

### 3. Phase factor in boundary conditions

In this section we investigate boundary conditions when the Schrödinger particle does and does not tunnel through the junction.

#### 3.1. Non-tunneling Schrödinger particle

Following equations (8) and (15), the wavefunctions $\psi$ of a self-adjoint extension of $H_0$ are given as $\psi = \psi_0 + (c_L L_- + c_R R_-) + (c_L U L_- + c_R U R_-)$, where $\psi_0 \in D(H_0)$, $c_L, c_R \in \mathbb{C}$. Thus, in the case where $\psi$ do not tunnel through the junction, the unitary operator $U : \mathcal{H}_\Lambda(H_0) \longrightarrow \mathcal{H}_\Lambda(H_0)$ should be given by $UL_+ = \gamma_L L_- \quad \text{and} \quad UR_+ = \gamma_R R_-$ for some $\gamma_L, \gamma_R \in \mathbb{C}$ with $|\gamma_L| = 1 = |\gamma_R|$. Namely, the wavefunctions $\psi$ have the form

$$\psi = \psi_0 + c_L(L_- + \gamma_L L_-) + c_R(R_- + \gamma_R R_-),$$

(18)

and moreover, the boundary conditions of $\psi(-\Lambda)$ and $\psi'(-\Lambda)$ are independent of those of $\psi(\Lambda)$ and $\psi'(\Lambda)$, respectively. Because any wavefunction $\psi_\Lambda$ on the island $(-\infty, -\Lambda)$ and any wavefunction $\psi_R$ on the island $(\Lambda, \infty)$ are isolated from each other. In this case, $\psi$ have to be mathematically equivalent to $\psi \equiv \psi_L \oplus \psi_R$ with $\psi_L = \psi_{L,0} + c_L(L_- + \gamma_L L_-)$ and $\psi_R = \psi_{R,0} + c_R(R_- + \gamma_R R_-)$. Here we note that there are the wavefunctions $\psi_{L,0} \in D(H_{L,0})$ and $\psi_{R,0} \in D(H_{R,0})$ so that $\psi_0 = \psi_{L,0} \oplus \psi_{R,0}$. Thus, any self-adjoint extension $H_\alpha$ without tunneling should be divided into the Schrödinger operators $H_{\alpha_L}$ and $H_{\alpha_R}$ as follows:

$$H_\alpha \equiv H_{\alpha_L} \oplus H_{\alpha_R},$$

(19)

using self-adjoint extensions shown in equations (1)–(4), where $I$ denotes the identity operator.

The following theorem and proposition establish the above physical image. Namely we can classify the self-adjoint extensions of $H_0$ the wavefunctions of which cannot tunnel through the junction in the following.

**Theorem 1.**

(i) Define the action of the Hamiltonian $H_\gamma$ by $H_\gamma : -\frac{d^2}{dx^2} + \gamma := (\gamma_L, \gamma_R)$, and give its domain $D(H_\gamma)$ by the set of all wavefunctions $\psi$ satisfying equation (18):

$$D(H_\gamma) := \{ \psi_0 + c_L(L_- + \gamma_L L_-) + c_R(R_- + \gamma_R R_-) | \psi_0 \in D(H_0), c_L, c_R \in \mathbb{C} \}. $$

(20)

If $\gamma_L$ and $\gamma_R$ are respectively given by $\gamma_L := e^{i(\theta_L + \sqrt{2}\Lambda)}$ and $\gamma_R := e^{i(\theta_R + \sqrt{2}\Lambda)}$ for $0 \leq \theta_L, \theta_R < 2\pi$, then $H_\gamma$ is a self-adjoint extension of $H_0$.

(ii) Define the action of the Hamiltonian $H_\alpha$ by $H_\alpha := -\frac{d^2}{dx^2} + \alpha := (\alpha_L, \alpha_R)$, where $\alpha_L, \alpha_R \in \mathbb{R} \cup \{\infty\}$. If the domain $D(H_\alpha)$ is given by one of (a)–(d):
(a) for $\alpha \in \mathbb{R} \times \mathbb{R}$,
\[
D(H_{\alpha}) := \{ \psi \in D(H_{0})^* \mid \psi'(-\Lambda) = \alpha_L \psi(-\Lambda) \text{ and } \psi'((\Lambda) = \alpha_R \psi((\Lambda)) \}; \tag{21}
\]
(b) for $\alpha \in \mathbb{R} \times \{\infty\}$,
\[
D(H_{\alpha}) := \{ \psi \in D(H_{0})^* \mid \psi'(-\Lambda) = \alpha_L \psi(-\Lambda) \text{ and } \psi'((\Lambda) = 0) \}; \tag{22}
\]
(c) for $\alpha \in \{\infty\} \times \mathbb{R}$,
\[
D(H_{\alpha}) := \{ \psi \in D(H_{0})^* \mid \psi'(-\Lambda) = 0 \text{ and } \psi'((\Lambda) = \alpha_R \psi((\Lambda)) \}; \tag{23}
\]
(d) for $\alpha = (\infty, \infty)$,
\[
D(H_{\alpha}) := \{ \psi \in D(H_{0})^* \mid \psi'(-\Lambda) = 0 = \psi'((\Lambda)) \}. \tag{24}
\]

then $H_{\alpha}$ is a self-adjoint extension of $H_0$

(iii) Every self-adjoint extension $H_{\gamma}$ as in part (i) and every self-adjoint extension $H_{\alpha}$ as in part (ii) become equal to each other (i.e. $H_{\alpha} = H_{\gamma}$) with the one-to-one correspondence, $(\mathbb{C} \cup \{\infty\}) \times (\mathbb{C} \cup \{\infty\}) \rightarrow [0,2\pi) \times [0,2\pi)$:
\[
\alpha_L = \frac{1 + \cos \theta_L - \sin \theta_L}{\sqrt{2}(1 + \cos \theta_L)} \quad \text{and} \quad \alpha_R = -\frac{1 + \cos \theta_R - \sin \theta_R}{\sqrt{2}(1 + \cos \theta_R)}, \tag{25}
\]

where $\alpha_2 = \infty$ if $\theta_2 = \pi, \pi = L, R$. Therefore, $H_{\alpha}$ is equivalent to $H_{\alpha_L} \oplus H_{\alpha_R}$, i.e.
\[
H_{\alpha} \cong H_{\alpha_L} \oplus H_{\alpha_R}. \tag{26}
\]

Before proving theorem 1, the following lemma is easily proved in the same way as in [22, example 2 in section X.1]:

**Lemma 1.** Let $\theta_L, \theta_R \in [0, \pi) \cup (\pi, 2\pi)$ and $\alpha_L, \alpha_R \in \mathbb{R}$ be arbitrarily given. Then, any subspace $D(H_{\gamma})$ as in theorem 1(i) and any subspace $D(H_{\alpha})$ as in theorem 1(ii) are equal if and only if the following correspondence holds:
\[
\begin{cases}
\gamma_L = e^{i(\theta_L + \gamma L)} & \text{and} & \gamma_R = e^{i(\theta_R + \gamma R)}.
\end{cases} \tag{27}
\]

**Proof.** Assume $D(H_{\gamma}) = D(H_{\alpha})$. Take an arbitrary vector $\psi \in D(H_{\gamma})$. It is equivalent to taking the vector $\psi = \psi_0 + c_L L_+ + c_R R_+ + c_L \gamma_L L_- + c_R \gamma_R R_-$ for arbitrary $c_L, c_R \in \mathbb{C}$ and arbitrary $\psi_0 \in D(H_0)$. By the same boundary condition as in theorem 1(ii), we have
\[
\begin{cases}
-\frac{1}{\sqrt{2}} c_L L_+(-\Lambda) + \frac{1}{\sqrt{2}} c_L \gamma_L L_-(-\Lambda) = \alpha_L c_L L_+(-\Lambda) + \alpha_L c_L \gamma_L L_-(-\Lambda), \\
-\frac{1}{\sqrt{2}} c_R R_+(-\Lambda) + \frac{1}{\sqrt{2}} c_R \gamma_R R_+(-\Lambda) = \alpha_R c_R R_+(-\Lambda) + \alpha_R c_R \gamma_R R_+(-\Lambda).
\end{cases} \tag{29}
\]

It should be noted that
\[
\begin{cases}
L_+(-\Lambda) = R_+(-\Lambda), \\
L_-(\Lambda) = R_-(\Lambda) = R_+(\Lambda)^*,
\end{cases} \tag{30}
\]

and
\[
R_+(\Lambda) = R_+(\Lambda)^* e^{i\gamma R}. \tag{31}
\]
Using equations (29)–(31), since \( c_L \) and \( c_R \) are arbitrary, we obtain

\[
\begin{align*}
\frac{1 - i}{\sqrt{2}} + \frac{1 + i}{\sqrt{2}} e^{\theta_k} &= \alpha_L (1 + e^{i\theta_k}), \\
\frac{-1 + i}{\sqrt{2}} + \frac{-1 - i}{\sqrt{2}} e^{\theta_k} &= \alpha_R (1 + e^{i\theta_k}),
\end{align*}
\]

which leads to equation (27).

Conversely, it is easy to check that equation (27) implies the equality \( D(H_\gamma) = D(H_0) \).

**Proof of theorem 1.** Part (i) just follows from equations (8) and (15).

We employ the same method as in [27, theorem 8.26] to prove part (ii). Note that \( D(H_0) \subseteq D(H_\alpha) \subseteq D(H_\gamma) \) and that \( \langle \phi | - \phi' \rangle = (-\phi'|\phi) + W(\psi, \phi) \) for all \( \psi, \phi \in D(H_\alpha) \) first. Simple calculations lead to the fact that \( W(\psi, \phi) = 0 \) for all \( \psi, \phi \in D(H_\alpha) \) given by one of (a)–(d). Thus, \( H_\alpha \) is symmetric, i.e. \( H_\alpha \subseteq H_\gamma \). Let \( \psi \in D(H_\alpha) \). Then \( \langle H_\alpha^* \psi | \phi \rangle = \langle \psi | H_\alpha \phi \rangle \) for every \( \phi \in D(H_\alpha) \). Thus, \( -\langle \phi'|\phi \rangle = \langle \phi | - \phi' \rangle \) by proposition 1 since \( H_\alpha \subseteq H_\gamma \subseteq H_\gamma \). It means that \( W(\psi, \phi) = 0 \). Take any function \( \phi \in D(H_\alpha) \) with \( \phi(-\Lambda) \neq 0 \) and \( \phi(\Lambda) = 0 \). Then using \( \phi = \psi \) with the boundary condition in the domain (a) we have \( \psi'(-\Lambda) = \alpha_L \psi(\Lambda) \).

Similarly, using a function \( \phi \in D(H_\gamma) \) with \( \phi(\Lambda) \neq 0 \) and \( \phi(-\Lambda) = 0 \) we reach the fact that \( \psi'(-\Lambda) = \alpha_R \psi(\Lambda) \).

Thus, \( \psi \in D(H_\alpha) \), that is, \( H_\alpha \subseteq H_\gamma \). Therefore, \( H_\alpha \) is self-adjoint. Since we can similarly handle the other cases, we complete the proof of part (ii).

Part (iii) for case (ii)(a) directly follows from lemma 1. For \( \alpha \in \mathbb{R} \times \{ \infty \} \) in case (ii)(b), we expand equation (27) to the case \( \alpha = \infty \) and \( \theta_R = \pi \) as \( 0 = 0_0 = 0_0 \). For \( \alpha \in \{ \infty \} \times \mathbb{R} \) in case (ii)(c) and \( \alpha = (\infty, \infty) \) in case (ii)(d), we expand equation (27) in the same way as in case (ii)(b). These arguments complete part (iii).

**Proposition 2.** For every vector \( \alpha = (\alpha_L, \alpha_R) \in (\mathbb{R} \cup \{ \infty \}) \times (\mathbb{R} \cup \{ \infty \}) \), there is no vector \( \gamma = (\gamma_L, \gamma_R) \) in equation (16) so that \( D(H_\alpha) \subseteq D(H_\gamma) \). Conversely, for every vector \( \gamma = (\gamma_L, \gamma_R) \) in equation (16), there is no vector \( \alpha = (\alpha_L, \alpha_R) \in (\mathbb{R} \cup \{ \infty \}) \times (\mathbb{R} \cup \{ \infty \}) \) so that \( D(H_\alpha) = D(H_\gamma) \).

**Proof.** Let a vector \( \alpha = (\alpha_L, \alpha_R) \) be in \( (\mathbb{R} \cup \{ \infty \}) \times (\mathbb{R} \cup \{ \infty \}) \). Suppose for the sake of contradiction there is a vector \( \gamma = (\gamma_L, \gamma_R) \) in equation (16) so that \( D(H_\alpha) \subseteq D(H_\gamma) \). Then simple calculations lead to a contradiction: \( e^{-i\pi/4} = \alpha_L = \alpha_R = e^{i\pi/4} \). Therefore, we prove the first part. In the same way, we can prove the last part.

**Remark 1.** We assume that the wavefunction \( \psi(x) \) is in \( D(H_\gamma) \) for every \( \Lambda > 0 \) so that

\[
\begin{align*}
\lim_{\Lambda \to -0} \psi(-\Lambda) &= \psi(0-) = \psi(0) = \psi(0+) = \lim_{\Lambda \to 0} \psi(+\Lambda), \\
\lim_{\Lambda \to 0} \psi(-\Lambda) &= \psi'(0-), \\
\lim_{\Lambda \to -0} \psi'(0+) &= \psi'(0+).
\end{align*}
\]

Let \( \alpha, \alpha_1 \) and \( \alpha_R \) be given as \( -\infty < \alpha, -\alpha_1 \leq +\infty \) and \( -\infty < \alpha_1 < +\infty \), respectively. When \( \alpha_1 \) and \( \alpha_R \) are arbitrarily given, we define \( \alpha \) by \( \alpha := \alpha_R - \alpha_1 \). Conversely, when \( \alpha \) is arbitrarily given, we divide \( \alpha \) into \( \alpha_R \) and \( \alpha_1 \) as \( \alpha = \alpha_R - \alpha_1 \). Let us assume that the boundary condition in theorem 1 holds for all \( \Lambda > 0 \). Then our boundary condition in theorem 1 tends to the boundary condition in [24, equation (3.1.9)] for the point interaction as \( \Lambda \to 0 \):

\[
\psi'(0+) - \psi'(0-) = \alpha \psi(0).
\]
equation (18) are described as in part (i) of theorem 1, since \( \theta_L \) and \( \theta_R \) are independent. On the other hand, in the case where some wavefunctions tunnel through the junction, we find another type of the boundary conditions, and then we realize that some phase factors are in this type. We show this in the next subsection.

### 3.2. Tunneling Schrödinger particle

In this subsection, we show that the Schrödinger particle tunneling the junction comes up with another type of the boundary conditions (see definition 2). Following equation (8) again, the unitary operator \( U : \mathcal{H}_+(H_0) \rightarrow \mathcal{H}_-(H_0) \) should be given by

\[
U_L = \gamma_- R_- \quad \text{and} \quad U_R = \gamma_- L_-
\]

for some \( \gamma_- \in \mathbb{C} \) with \( |\gamma_-| = 1 = |\gamma_+| \). Namely, all wavefunctions \( \psi \) of any self-adjoint extension of \( H_0 \) satisfying equation (35) have the following form:

\[
\psi = \psi_0 + c_1(L_+ + \gamma_- R_-) + c_R(R_+ + \gamma_- L_-),
\]

and moreover the boundary conditions of \( \psi(\Lambda) \) and \( \psi'(\Lambda) \) are dependent on those of \( \psi(-\Lambda) \) and \( \psi'(-\Lambda) \), respectively. For the wavefunctions with the form of equation (36), we can find a phase factor in some boundary conditions.

We define some mathematical notions.

**Definition 1.** A vector \( \vec{a} = (\alpha_1, \alpha_2, \alpha_3, \alpha_4) \in \mathbb{C} \) belongs to the class \( A \) (i.e. \( \vec{a} \in A \)) if the vector \( \vec{a} \) satisfies

(A1) \( \alpha_1\alpha_2^* = \alpha_2^*\alpha_1 = 1 \);

(A2) \( \alpha_1\alpha_3^*, \alpha_2\alpha_4^* \in \mathbb{R} \).

**Definition 2.** Fix \( \vec{a} = (\alpha_1, \alpha_2, \alpha_3, \alpha_4) \in \mathbb{C} \). Then a wavefunction \( \psi \in D(H_0^+) \) satisfies the boundary conditions \( BC(\vec{a}) \) if the wavefunction \( \psi \) satisfies

\[
\begin{align*}
\psi(\Lambda) &= \alpha_1\psi(-\Lambda) + \alpha_2\psi'(-\Lambda), \\
\psi'(\Lambda) &= \alpha_3\psi(-\Lambda) + \alpha_4\psi'(-\Lambda).
\end{align*}
\]

(37)

We define a function \( F : \mathbb{C}^2 \rightarrow \mathbb{C} \) by

\[
F(z_1, z_2) := |z_1|^2 + \sqrt{2}z_1z_2 + |z_2|^2 - 1
\]

(38)

for every \( (z_1, z_2) \in \mathbb{C}^2 \).

**Definition 3.** A vector \( \vec{a} = (\alpha_1, \alpha_2, \alpha_3, \alpha_4) \in \mathbb{C} \) is a solution of the system \( S \) if the vector \( \vec{a} \) satisfies

(S1) \( F(\alpha_1, \alpha_2) = 0 = F(\alpha_3, \alpha_4) \);

(S2) \( \alpha_1 + \alpha_2 e^{-i\pi/4} = (\alpha_3 + \alpha_4 e^{-i\pi/4}) e^{i\pi/4} \);

(S3) \( \alpha_1 + \alpha_2 e^{i\pi/4} = (\alpha_3 + \alpha_4 e^{i\pi/4}) e^{-i\pi/4} \).

**Example 1.** Fix \( \theta \) with \( 0 \leq \theta < 2\pi \) arbitrarily. Set \( \vec{a} \) as \( \alpha_1 = 0, \alpha_2 = -e^{i\theta}, \alpha_3 = e^{i\theta} \) and \( \alpha_4 = 0 \). Then, the vector \( \vec{a} \) belongs to the class \( A \) and it is a solution of the system \( S \).

Example 1, together with the following theorem, secures that the boundary condition \( BC(\vec{a}) \) can include some phase factors.
Theorem 2.

(i) Fix a vector \( \vec{a} \in A \) arbitrarily. Define the action of the Hamiltonian \( H_\vec{a} \) by

\[
D(H_\vec{a}) := \{ \psi \in D(H_0^\gamma) \mid \psi \text{ satisfies the boundary condition } BC(\vec{a}) \}.
\]

Then \( H_\vec{a} \) is a self-adjoint extension of \( H_0 \).

(ii) Assume that the vector \( \vec{a} \) belongs to the class \( A \) and is a solution of the system \( S \). Define the action of the Hamiltonian \( H_\vec{y} \) by \( H_\vec{y} := -\frac{\partial^2}{\partial x^2} \) with \( \vec{y} := (y_-, y_+) \), and give its domain \( D(H_\vec{y}) \) by the set of all wavefunctions \( \psi \) satisfying equation (18):

\[
D(H_\vec{y}) := \{ \psi_0 + c_1 f + c_2 g \mid \psi_0 \in D(H_0), c_1, c_2 \in \mathbb{C} \}.
\]

If \( y_L \) and \( y_R \) are given by

\[
y_- := (\alpha_1 + \alpha_2 e^{-\pi i/4}) e^{\pi i/2} = (\alpha_3 + \alpha_4 e^{-\pi i/4}) e^{\pi i/2},
\]

and

\[
y_- := (\alpha_1 + \alpha_2 e^{\pi i/4}) e^{-\pi i/2} = (\alpha_3 + \alpha_4 e^{\pi i/4}) e^{-\pi i/2},
\]

then \( H_\vec{y} \) is a self-adjoint extension of \( H_0 \). Moreover, \( H_0 = H_\vec{y} \).

Before proving theorem 2 we note the following five lemmas.

Lemma 2. If \( \alpha_1, \alpha_2, \alpha_3, \alpha_4 \in \mathbb{C} \) satisfy

\[
\alpha_1 \alpha_4^* - \alpha_2^2 \alpha_3 = 1,
\]

\[
\alpha_1 \alpha_4^*, \alpha_2 \alpha_4^* \in \mathbb{R},
\]

then \( \alpha_j \alpha_j^* \in \mathbb{R} \) for each \( j, j' = 1, 2, 3, 4 \).

Proof. In the case of \( j = j' \), the statement of our lemma is trivial. Thus, we suppose that \( j \neq j' \). Equation (43) leads to

\[
\alpha_4^* = \alpha_3^* (\alpha_1 \alpha_4^* - \alpha_2^2 \alpha_3) = \alpha_1 \alpha_4^* \alpha_4^* - \alpha_2^2 \alpha_3^2.
\]

Due to condition (44), multiplying \( \alpha_2 \) by both sides of this equation gives \( \alpha_2^2 \alpha_3^* \in \mathbb{R} \). Also this fact and equation (43) say that \( \alpha_1 \alpha_4^* = 1 + \alpha_2^2 \alpha_3 \in \mathbb{R} \) at the same time. Similarly, since equation (43) leads to \( \alpha_2 = \alpha_2 (\alpha_1 \alpha_4^* - \alpha_2^2 \alpha_3) = \alpha_1 \alpha_2^* \alpha_4^* - |\alpha_2|^2 \alpha_3 \), we have \( \alpha_2^* \alpha_2 \in \mathbb{R} \). Using equation (45), we reach \( \alpha_1 \alpha_4^* = \alpha_1 \alpha_4^* |\alpha_4^*|^2 - \alpha_2^2 \alpha_3^2 \in \mathbb{R} \) by condition (44). We can conclude all the results we desire from the facts that we showed above.

Lemma 3. If \( \alpha_1 \alpha_2^*, \alpha_3 \alpha_4^* \in \mathbb{R} \), then

\[
\alpha_1 + \alpha_2^* e^{\pi i/4} \neq 0 \quad \text{and} \quad \alpha_3 + \alpha_4^* e^{\pi i/4} \neq 0.
\]

Proof. Suppose for the sake of contradiction (i) \( \alpha_1 = -\alpha_2^* e^{\pi i/4} \) or (ii) \( \alpha_3 = -\alpha_4^* e^{\pi i/4} \) holds. In the case where (i) holds, \( \mathbb{R} \ni \alpha_1 \alpha_2^* = -|\alpha_2|^2 e^{\pi i/4} \), which is a contradiction. In the same way as we did now, we have a contradiction in the case where (ii) holds.

Straightforward calculations lead to the following two lemmas.

Lemma 4. If \( z_1, z_2 \in \mathbb{C} \) satisfy \( z_1 z_2^* = \frac{1 - (|z_1|^2 + |z_2|^2)}{\sqrt{2}} \), then

\[
|z_1 + z_2^* e^{\pi i/4}| = 1.
\]
Proof. We have
\[
(z_1 + z_2 e^{i\pi/4})(z_1^* + z_2^* e^{i\pi/4}) = |z_1|^2 + |z_2|^2 + z_1 z_2^* \left( \frac{1 + i}{\sqrt{2}} + \frac{1 - i}{\sqrt{2}} \right) 
= |z_1|^2 + |z_2|^2 + z_1 z_2^* \sqrt{2} = 1,
\]
noting \(z_1 z_2^* \in \mathbb{R}\) and using the assumption. \(\square\)

Lemma 5. Let \(\alpha_1, \alpha_2, \alpha_3, \alpha_4 \in \mathbb{C}\) be given so that equation (43) and condition (44) hold. If \(\psi, \phi \in D(H_0^\alpha)\) satisfy the boundary condition \(BC(\bar{a})\), then \(W(\psi, \phi) = 0\).

Proof. It follows directly from equation (43) and condition (44) that
\[
W(\psi, \phi) = \varphi(-\Lambda)^* \varphi'(-\Lambda)(-1 + \alpha_1^* \alpha_4 - \alpha_2^* \alpha_3) + \varphi(-\Lambda)^* \varphi(-\Lambda)(\alpha_1^* \alpha_3 - \alpha_4^* \alpha_2) 
+ \varphi'(-\Lambda)^* \varphi(-\Lambda)\alpha_2^* \alpha_3 + 1 - \alpha_1^* \alpha_4) + \varphi'(-\Lambda)^* \varphi(-\Lambda)(\alpha_2^* \alpha_4 - \alpha_3^* \alpha_1) 
= 0,
\]
since \(\psi, \phi \in D(H_0^\alpha)\) satisfy the boundary condition \(BC(\bar{a})\). \(\square\)

We state the last of five lemmas:

Lemma 6. Let \(\alpha_1, \alpha_2, \alpha_3, \alpha_4 \in \mathbb{C}\) be given so that equation (46) holds. Then, the boundary condition \(BC(\bar{a})\) is equivalent to the following conditions:
\[
\begin{align*}
\gamma_+ &= (\alpha_1 + \alpha_2 e^{-i\pi/4}) e^{i\Lambda} = (\alpha_1 + \alpha_4 e^{-i\pi/4}) e^{i\Lambda}, \\
\gamma_- &= (\alpha_1 + \alpha_2 e^{i\pi/4})^{-1} e^{i\Lambda} = (\alpha_3 + \alpha_4 e^{i\pi/4})^{-1} e^{i\Lambda}.
\end{align*}
\]

Proof. Let \(\psi \in D(H_0^\alpha)\) be an arbitrary wavefunction satisfying the boundary condition \(BC(\bar{a})\). Then we note that taking this \(\psi\) is equivalent to giving \(\psi\) with arbitrary \(c_L, c_R \in \mathbb{C}\) so that \(\psi = \psi_0 + c_L (L_+ + \gamma_+ R_+) + c_R (R_+ + \gamma_- L_-)\) by equations (35) and (36). Thus, while the wavefunction \(\psi\) is written as \(x = \Lambda\) as \(\psi(\Lambda) = c_L \gamma_+ R_+ (\Lambda)^* + c_R R_+ (\Lambda)\) by equation (30), we have
\[
\psi(\Lambda) = \alpha_1^* \psi(-\Lambda) + \alpha_2^* \psi'(-\Lambda) 
= c_L (\alpha_1^* + \alpha_2^* e^{-i\pi/4}) R_+ (\Lambda) + c_R (\alpha_1^* + \alpha_2^* e^{i\pi/4}) \gamma_+ R_+ (\Lambda)^*.
\]
Since \(c_L\) and \(c_R\) are arbitrary, we obtain the first equality of \(\gamma_+\) and \(\gamma_-\) in equation (50) individually. Employing the same argument we can express \(\gamma_+\) and \(\gamma_-\) by \(\alpha_1, \alpha_2\) as in the second equality of equation (50) individually.

We can show directly that equation (50) leads to the boundary condition \(BC(\bar{a})\) with some straightforward calculations. \(\square\)

Proof of theorem 2. We employ the same method as in [27, theorem 8.26] to prove part (i). Note that, in the same way as noted in the proof of theorem 1, \(D(H_0) \subseteq D(H_0^\alpha) \subseteq D(H_0^\alpha)^\alpha\), and moreover \((\psi| - \phi'' = - \varphi''(\phi) + W(\psi, \phi)\) for all \(\psi, \phi \in D(H_0^\alpha)\). Let the wavefunctions \(\varphi\) and \(\phi\) be in \(D(H_0)\). Then, there are \(\varphi_0, \phi_0 \in D(H_0)\) and \(a_L, a_R, b_L, b_R \in \mathbb{C}\) so that the wavefunctions \(\varphi\) and \(\phi\) are written as \(\varphi = \varphi_0 + a_L f + a_R g\) and \(\phi = \phi_0 + b_L f + b_R g\), respectively. Straightforward calculations lead to
\[
W(\psi, \phi) = a_L^* b_L [- f(-\Lambda)^* f'(-\Lambda) + f(\Lambda)^* f'(-\Lambda) + f'(-\Lambda)^* f(-\Lambda) - f'(\Lambda)^* f(\Lambda)] 
+ a_R^* b_R [- f(-\Lambda)^* g'(-\Lambda) + f(\Lambda)^* g'(-\Lambda) + f'(-\Lambda)^* g(-\Lambda) - f'(\Lambda)^* g(\Lambda)] 
+ a_L^* b_L [- g(-\Lambda)^* f'(-\Lambda) + g(\Lambda)^* f'(-\Lambda) + g'(-\Lambda)^* f(-\Lambda) - g'(\Lambda)^* f(\Lambda)] 
+ a_R^* b_R [- g(-\Lambda)^* g'(-\Lambda) + g(\Lambda)^* g'(-\Lambda) + g'(-\Lambda)^* g(-\Lambda) - g'(\Lambda)^* g(\Lambda)] 
\]
\[
= \sum_{\alpha=1,2} \sum_{\beta=0,1}(a_{L\alpha} b_{L\beta} - a_{R\alpha} b_{R\beta}) \begin{cases} 
\frac{1}{\sqrt{2}} (1 - i) \left( \frac{1}{\sqrt{2}} + \frac{1 - i}{\sqrt{2}} \right) \right) 
\end{cases}
\]
Using equation (30), we have
\begin{align}
\begin{aligned}
f(-\Lambda) &= R_\alpha(\Lambda), \\
f'(\Lambda) &= e^{-i\pi/4}R_\alpha(\Lambda), \\
g(-\Lambda) &= \gamma_- R_\alpha(\Lambda), \\
g'(\Lambda) &= e^{-i\pi/4}R_\alpha(\Lambda).
\end{aligned}
\end{align}
(53)

Inserting these values into \(W(\phi, \phi)\) obtained above, we have
\begin{align}
W(\phi, \phi) &= \frac{a^*_b b_a R_\alpha(\Lambda)^* R_\alpha(\Lambda)}{\sqrt{2}} \left[ (-1 + i) + |\gamma_-|^2(-1 - i) + (1 + i) + |\gamma_-|^2(1 - i) \right] \\
&\quad + \frac{a^*_b b_a}{\sqrt{2}} (R_\alpha(\Lambda)^2 \gamma_-(-1 - i) + R_\alpha(\Lambda)^2 \gamma_+^*(1 + i)) \\
&\quad + \frac{a^*_b b_a}{\sqrt{2}} (R_\alpha(\Lambda)^2 \gamma_+^*(1 + i) + R_\alpha(\Lambda)^2 \gamma_-(-1 - i)) \\
&\quad + \frac{a^*_b b_a}{\sqrt{2}} (R_\alpha(\Lambda)^2 \gamma_+^*(1 + i) + R_\alpha(\Lambda)^2 \gamma_-(-1 - i)) \\
&\quad + \frac{a^*_b b_a R_\alpha(\Lambda) R_\alpha(\Lambda)^*}{\sqrt{2}} \left[ |\gamma_-|^2(-1 - i) + (1 + i) + |\gamma_-|^2(1 - i) + (1 + i) \right] \\
&= 0.
\end{align}
(55)

Thus, \(H_\alpha\) is symmetric, i.e. \(H_\alpha \subset H_\alpha^\perp\). Let \(\psi \in D(H_\alpha^\perp)\). Then \(\langle H_\alpha^\perp \psi | \phi \rangle = \langle \psi | H_\alpha \phi \rangle\) for every \(\phi \in D(H_\alpha)\). Thus, \((-\psi^\dagger | \phi \rangle = \langle \psi - \phi^\dagger \rangle\) by proposition 1 since \(H_\alpha \subset H_\alpha^\perp\). It means that \(W(\phi, \phi) = 0\). Take any function \(\phi \in D(H_\alpha)\) with \(\phi(-\Lambda) \neq 0\) and \(\phi'(-\Lambda) = 0\). Then using this \(\phi\) with the boundary condition \(BC(\bar{a})\), we have
\begin{align}
\alpha_4 \phi(-\Lambda) - \alpha_1 \phi'(-\Lambda) = -\phi(-\Lambda)^*.
\end{align}
(56)

In the same way, take any function \(\phi \in D(H_\alpha)\) with \(\phi(-\Lambda) = 0\) and \(\phi'(-\Lambda) \neq 0\). Then using this function \(\phi\) with the boundary condition \(BC(\bar{a})\), we have
\begin{align}
\alpha_4 \phi(-\Lambda) - \alpha_2 \phi'(-\Lambda) = \phi(-\Lambda)^*.
\end{align}
(57)

It follows from equations (56) and (57) that
\begin{align}
\begin{aligned}
\left\{ -\alpha_2^* \alpha_3^* \phi(-\Lambda)^* + \alpha_1 \alpha_2^* \phi'(-\Lambda)^* \right\} \\
\left\{ \alpha_1^* \alpha_4 \phi(-\Lambda)^* - \alpha_1 \alpha_2 \phi'(-\Lambda)^* \right\} &= \alpha_2^* \phi(-\Lambda)^*.
\end{aligned}
\end{align}
(58)

Summing these two equations gives the equation
\begin{align}
(\alpha_4^* \alpha_4 - \alpha_2^* \alpha_2) \phi(-\Lambda)^* + (\alpha_1 \alpha_2^* - \alpha_1^* \alpha_2) \phi'(-\Lambda)^* = (\alpha_1 \phi(-\Lambda) + \alpha_2 \phi'(-\Lambda))^*.
\end{align}
(59)

Since \(\alpha_1 \alpha_2^* \in \mathbb{R}\) by lemma 2, we have
\begin{align}
\alpha_1 \alpha_2^* - \alpha_1^* \alpha_2 = 0.
\end{align}
(60)

Since \(\alpha_1 \alpha_2^* \in \mathbb{R}\) by lemma 2 again, we have \(\alpha_1 \alpha_4 = \alpha_1 \alpha_2^*\). It follows from this fact and (A1) that
\begin{align}
\alpha_4^* \alpha_4 - \alpha_2^* \alpha_2 = 1.
\end{align}
(61)

Combining equations (59)-(61), we can conclude that \(\phi(-\Lambda) = \alpha_1 \phi(-\Lambda) + \alpha_2 \phi'(-\Lambda)\). In the same way as demonstrated above, we obtain \(\phi'(-\Lambda) = \alpha_2 \phi(-\Lambda) + \alpha_4 \phi'(-\Lambda)\). Thus, \(\phi \in D(H_\alpha)\), that is, \(H_\alpha^\perp \subset H_\alpha\). Hence it follows from the two arguments that \(H_\alpha\) is self-adjoint, and thus part (i) is completed.

Part (ii) directly follows from lemma 6.
To see the correspondence of our boundary condition and equation (2.2) of [26], we show the following lemma:

**Lemma 7.** Let \( \bar{\alpha} \) be in the class \( A \). If \( \alpha_j \neq 0 \), then \( \alpha_j \alpha_j^{-1} \in \mathbb{R} \) for \( j, j' = 1, 2, 3, 4 \).

**Proof.** Since \( \alpha_j \alpha_j^{-1} = \alpha_j \alpha_j'^{-1} |\alpha_j'|^2 \in \mathbb{R} \) by lemma 2, we obtain the desired result. \( \square \)

**Remark 2.** We assume that the wavefunction \( \psi(x) \) is in \( D(H_0^{\alpha}) \) for every \( \lambda > 0 \) so that

\[
\begin{align*}
\lim_{\lambda \to 0} \psi(-\Lambda) &= \psi(0^-), \\
\lim_{\lambda \to 0} \psi(+\Lambda) &= \psi(0^+), \\
\lim_{\lambda \to 0} \psi'(-\Lambda) &= \psi'(0^-), \\
\lim_{\lambda \to 0} \psi'(+\Lambda) &= \psi'(0^+).
\end{align*}
\]

Let \( \bar{\alpha}, a, b \) and \( c \) be given as \( \bar{\alpha} \in A, a, b \in \mathbb{R} \), and \( c \in \mathbb{C} \), respectively. When \( \bar{\alpha} \) with \( \alpha_2 \neq 0 \) is given arbitrarily, based on lemma 7, we set \( a, b \) and \( c \) as

\[
a := \alpha_2 \alpha_2^{-1} \in \mathbb{R}, \quad b := \alpha_1 \alpha_2^{-1} \in \mathbb{R}, \quad c := -(\alpha_2^{-1}) \in \mathbb{C}.
\]

So we have \( \alpha_1 = -(c^*)^{-1}(|c|^2 - ab) \). Conversely, when \( a, b \in \mathbb{R} \) and \( c \in \mathbb{C} \) with \( c \neq 0 \) are given arbitrarily, we set \( \bar{\alpha} \) as

\[
\begin{align*}
\alpha_1 &= -(c^*)^{-1} b, \\
\alpha_2 &= -(c^*)^{-1}, \\
\alpha_3 &= (c^*)^{-1}(|c|^2 - ab), \\
\alpha_4 &= -(c^*)^{-1} a.
\end{align*}
\]

Let us assume that the boundary condition in theorem 2 holds for all \( \lambda > 0 \). Then our boundary condition in theorem 2 tends to the boundary condition (2.2) of [26] as \( \Lambda \to 0 \):

\[
\begin{align*}
\psi'(0+) &= a \psi(0+) + c \psi(0^-), \\
-\psi'(0-) &= c^* \psi(0+) + b \psi(0^-).
\end{align*}
\]

As a special case of theorem 2, we take \( \bar{\alpha} \) given in example 1. That is, we set \( \alpha_2 = \alpha_3 = e^{i\theta} \) for every \( \theta \in [0, 2\pi] \) and \( \alpha_1 = 0 = \alpha_4 \). For \( \alpha := (\alpha_2, \alpha_3) \) we define the action of the Hamiltonian \( H_0 \) by \( H_0 := -d^2/dx^2 \), and the domain \( D(H_0) \) by

\[
D(H_0) := \{ \psi \in D(H_0^{\alpha}) \mid \psi(\Lambda) = \alpha_2 \psi'(-\Lambda) \text{ and } \psi'(\Lambda) = \alpha_3 \psi(-\Lambda) \}.
\]

Then theorem 2(i) says that \( H_0 \) is a self-adjoint extension of \( H_0 \). This comes up with a concrete phase factor in the boundary condition as an example. Let \( \gamma_- \) and \( \gamma_+ \) be given by

\[
\gamma_- := e^{i[\theta + \sqrt{2\Lambda}(3\pi/4)]} \quad \text{and} \quad \gamma_+ := e^{i[-\theta + \sqrt{2\Lambda}(3\pi/4)]}
\]

for arbitrary \( \theta \) with \( \theta \in [0, 2\pi] \). For \( \gamma := (\gamma_-, \gamma_+) \) we define the action of the Hamiltonian \( H_{\gamma} \) by \( H_{\gamma} := -d^2/dx^2 \) and give its domain \( D(H_{\gamma}) \) by the set of all wavefunctions \( \psi \) satisfying equation (36):

\[
D(H_{\gamma}) := \{ \psi_0 + c_L (L_+ + \gamma_- R_-) + c_R (R_+ + \gamma_+ L_-) \mid \psi_0 \in D(H_0), c_L, c_R \in \mathbb{C} \}.
\]

Then theorem 2 says that \( H_{\gamma} \) is a self-adjoint extension of \( H_0 \), and that \( H_{\alpha} \) is represented by \( H_{\gamma} \). Moreover, \( H_{\alpha} \) and \( H_0 \) have the one-to-one correspondence as in the following theorem.

**Theorem 3.** Let \( \theta \in [0, 2\pi] \) and \( \alpha_2, \alpha_3 \in \mathbb{C} \) be given arbitrarily. Then any subspace \( D(H_{\alpha}) \) and any subspace \( D(H_{\gamma}) \) are equal if and only if the correspondence

\[
\alpha_2 = -e^{i\theta} \quad \text{and} \quad \alpha_3 = e^{i\theta}
\]

holds.
Proof. Assume $D(H_γ) = D(H_0)$. Take an arbitrary vector $ψ ∈ D(H_γ)$. It is equivalent to take the vector $ψ = ψ_0 + c_L L_+ + c_R R_+ + c_L γ_+ R_− + c_R γ_− L_−$ for arbitrary $c_L, c_R ∈ ℂ$ and arbitrary $ψ_0 ∈ D(H_0)$. By the boundary condition, we have

$$\begin{cases}
γ_− R_−(Λ) - e^{−iπ/4}α_2 L_+(-Λ) = 0, \\
R_+(Λ) - e^{iπ/4}α_2 γ_− L_−(-Λ) = 0,
\end{cases}$$

(69)

and

$$\begin{cases}
e^{−i3π/4}γ_− R_−(Λ) - α_3 L_+(-Λ) = 0, \\
e^{i3π/4}R_+(Λ) - α_3 γ_− L_−(-Λ) = 0.
\end{cases}$$

(70)

Using equations (30), (31), (69) and (70), we obtain

$$\begin{cases}
γ_− - e^{−iπ/4}α_2 e^{i√2Λ} = 0, \\
e^{i√2Λ} γ_− - e^{iπ/4}α_2 γ_− = 0,
\end{cases}$$

(71)

and

$$\begin{cases}
e^{−i3π/4}γ_− - α_3 e^{i√2Λ} = 0, \\
e^{i3π/4} e^{i√2Λ} - α_3 γ_− = 0.
\end{cases}$$

(72)

Equation (68) follows from these four equations.

Conversely, as a corollary of theorem 2(ii), equation (68) implies the equality $D(H_γ) = D(H_0)$. □

For $γ_+$ and $γ_−$ determined by $α_2 = −e^{iθ}$ and $α_3 = e^{iθ}$ in theorem 3, we define the two functions $f$ and $g$ by

$$f := L_+ + γ_− R_− \quad \text{and} \quad g := R_+ + γ_− L_−,$$

(73)

respectively. We introduce a new inner product ( ) by $(ψ|φ) := (φ|ψ) + (ψ''|φ'')$. We say that $ψ$ and $φ$ are $H_θ$-diagonal if $(ψ|φ) = 0$. Then, we obtain the following.

Proposition 3. Fix an arbitrary $θ$ with $0 ≤ θ < 2π$. Define $γ_+$ and $γ_−$ by $γ_+ := e^{iθ+√2Λ+(3π/4)}$ and $γ_− := e^{iθ−√2Λ+(3π/4)}$, respectively. Then the following (i)–(iii) hold:

(i) $f$ and $g$ defined in equation (73) are $H_θ$-diagonal;

(ii) $f(Λ) = e^{iθ+(3π/4)} f(−Λ)$ and $g(Λ) = e^{iθ−(3π/4)} g(−Λ)$;

(iii) for every $ψ ∈ D(H_γ)$,

$$ψ = ψ_0 + c_L f + c_R g,$$

(74)

where $ψ_0 ∈ D(H_0)$ and $c_L, c_R ∈ ℂ$ are uniquely determined by equation (36), and moreover $ψ_0, f$ and $g$ are mutually $H_θ$-diagonal.

Proof. Condition (i) is an easy application of lemma on page 138 of [22]. Simple calculations lead to condition (ii). Condition (iii) directly follows from theorem 3. □

Remark 3. Proposition 3 says that the functions $f$ and $g$ play essential roles to determine the wavefunction $ψ$ around the junction since $ψ_0(x) = 0$ for $x$ in the neighborhood of the junction.

Remark 4. Proposition 3(ii) says that the function $f$ (resp. $g$) has the standard Ramsauer–Townsend (RT) effect when $θ = π/4 + 2nπ$ (resp. $−π/4 + 2nπ$) for each $n ∈ ℤ$. Thus, the functions $f$ and $g$ have a generalization of the RT effect.
### 3.3. Phase of the tunneling Schrödinger particle and the exact WKB analysis

In this subsection, we explain a physical meaning of proposition 3 using the model of the non-adiabatic transition with the three energy levels.

Proposition 3 tells us that the Schrödinger particle leads to the interference by the tunneling effect except for \( f = g = 0 \) since the wavefunctions \( f \) and \( g \) get the phase factors \( \frac{3\pi}{4} \) and \( -\frac{3\pi}{4} \) from the boundary conditions, respectively. As a naive guess, we state the following remark:

**Remark 5.** By definitions \( S1 \) and \( S2 \), we can rewrite the boundary condition in proposition 3(ii) as

\[
f(\Lambda) = -e^{i(\theta - \pi/4)} f(-\Lambda) \quad \text{and} \quad g(\Lambda) = -e^{i(\theta + \pi/4)} g(-\Lambda).
\]

(75)

We recall that, when we apply the WKB approximation to the Schrödinger particle’s barrier-penetration problem, the phase factor \( \pi/4 \) appears because of the connection formulas (see [31, section 12]). It should be noted that we have not yet shown whether there is a relation between that phase factor \( \pi/4 \) and our \( \pi/4 \).

We discuss a connection between our phase factors and the WKB analysis in the following. Let us assume the model of the Landau–Zener transition for three levels [29] in the tunneling junction as

\[
\frac{d}{dt} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} = \eta \begin{bmatrix} b_{11} & a & 0 \\ 0 & b_{22} & 0 \\ 0 & 0 & b_{33} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} + \frac{1}{\sqrt{\eta}} \begin{bmatrix} 0 & c_{12} & c_{13} \\ c_{21} & 0 & c_{23} \\ c_{31} & c_{32} & 0 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix},
\]

(76)

where \( a > 0 \) is constant and \( b_3 > b_2 > b_1 > 0 \). The WKB solution of equation (76) is given by equation (2.4) of [29]. The phase factors, which correspond to the one obtained by proposition 3, appear in a particular model with the connection matrix for the WKB solution, given by equation (2.41) of [29] from the exact WKB analysis up to the order \( \eta^{-1/2} \). The connection matrix is computed through the connection formulas (equations (2.27), (2.32), and (2.37) of [29]). Furthermore, equation (76) can be mapped onto the BNR equation [30]. According to [30], the phase factors are obtained by the turning point of the Stokes and anti-Stokes lines. This situation may be experimentally realizable in the systems introduced in section 1.

A keen reader may note a relationship between the energy crossing and the self-adjointness. However, in this system, the total energy can be preserved while the energy crossing occurs inside the junction. That is, the concept of the self-adjoint extension may effectively lead to the energy crossing inside the junction remaining the preservation of the total energy. This might be an example of physical meanings on the self-adjointness.

### 4. Conclusion and discussions

We have considered the phase factor of the one-dimensional Schrödinger particle with the junction like the connected carbon nanotubes and shown that this phase factor depends on the situation of the particle, whether the particle goes through the junction or not. Theorem 1 means that the phase factor of the non-tunneling Schrödinger particle does not appear from the boundary condition of the junction. Proposition 3 means that the phase factor of the tunneling Schrödinger particle appears from the boundary condition of the junction. Physically speaking, the wavefunction of the tunneling Schrödinger particle shows the interference pattern. This phase factor corresponds to one obtained by the exact WKB analysis in the model of the non-adiabatic transition with the three energy levels inside the tunneling junction.
There remain the following problems. First, the geometry of the tunneling junction can be taken as the Y-junction scheme [32] in the complex plane. The relationship between the Y-junction scheme and our obtained phase factor has not been shown. Second, our considered model may also be analyzed by the duality of the quantum graph [25, 33]. Finally, the extension to the Dirac particle has not yet been done. This situation can be experimentally realized by the helical edge state in the quantum spin Hall system by the application to the quantum point contact technique [34, 35].

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