A Mathematical Aspect of A Tunneling Phase for Spintronic Qubit

Masao Hirokawa

Hiroshima University

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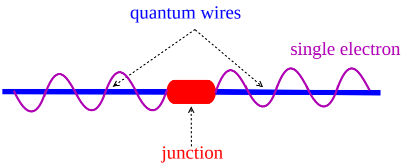
- Physical Unit:



I am interested in transportation of the electron's spin (i.e., qubit) as it passes through the junction.
In particular,

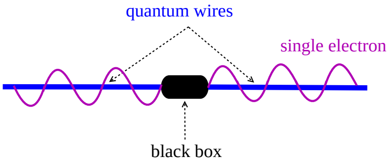
- how the tunneling makes a boundary condition of the electron's wave functions at each boundary between the junction and the quantum wire.
- how the boundary condition affects the spin.

I am studying these my interests based on von Neumann's theory, that is, under the mathematical hypothesis,

observables = self-adjoint operators

1. Introduction

- Today, we consider the part of quantum wires only.



For simplicity, we regard the quantum wires as

$$\Omega_\Lambda := (-\infty, -\Lambda) \cup (\Lambda, \infty).$$

Namely, $[-\Lambda, \Lambda]$ plays a role of the junction.

We note that

the adjoint operator H_0^* has eigenvalues $\pm i$

since it is not self-adjoint, either.

$$H_0^{**} = H_0 \subset H_0^* \text{ and } H_0^{**} = H_0 \neq H_0^*.$$

- We can easily find eigenfunctions $\psi_L^{\pm}(x)$ satisfying

$$H_0^* \psi_L^{\pm} = \pm i \psi_L^{\pm}$$

and living only in the left island $\Omega_{\Lambda,L}$:

$$\psi_L^{\pm}(x) = 0, \quad \forall x \in \Omega_{\Lambda,R}.$$

We can also find eigenfunctions $\psi_R^{\pm}(x)$ satisfying

$$H_0^* \psi_R^{\pm} = \pm i \psi_R^{\pm}$$

and living only in the right island $\Omega_{\Lambda,R}$:

$$\psi_R^{\pm}(x) = 0, \quad \forall x \in \Omega_{\Lambda,L}.$$

Precisely, $\psi_L^{\pm}(x)$ is defined by

$$\begin{cases} \psi_L^{+}(x) := N_D \begin{pmatrix} 1 \\ -\mu \end{pmatrix} \otimes \chi_L(x) e^{\sqrt{1+m^2}\, x}, \\ \psi_L^{-}(x) := N_D \begin{pmatrix} 1 \\ \mu^* \end{pmatrix} \otimes \chi_L(x) e^{\sqrt{1+m^2}\, x}. \end{cases}$$

Here χ_L is the characteristic function on the closure $\overline{\Omega}_{\Lambda,L}$ of the left island, and

$$N_D := (1+m^2)^{\frac{1}{4}} e^{-\sqrt{1+m^2}\Lambda}.$$

In the same way, $\psi_R^{\pm}(x)$ is defined by

$$\begin{cases} \psi_R^{+}(x) := N_D \begin{pmatrix} 1 \\ \mu \end{pmatrix} \otimes \chi_R(x) e^{-\sqrt{1+m^2}\,x}, \\ \psi_R^{-}(x) := N_D \begin{pmatrix} 1 \\ -\mu^* \end{pmatrix} \otimes \chi_R(x) e^{-\sqrt{1+m^2}\,x}. \end{cases}$$

Here χ_R is the characteristic function on the closure $\overline{\Omega}_{\Lambda,R}$ of the right island.

- We respectively define the eigenspaces $\mathcal{K}_{\pm}(H_0)$ as

$$
\begin{aligned}
\mathcal{K}_{+}(H_0) &:= \text{eigenspace of the eigenvalue } i \\
&= \text{the space linearly spanned by } \psi_L^{+} \text{ and } \psi_R^{+}, \\
\mathcal{K}_{-}(H_0) &:= \text{eigenspace of the eigenvalue } -i \\
&= \text{the space linearly spanned by } \psi_L^{-} \text{ and } \psi_R^{-}.
\end{aligned}
$$

Then, we obtain $U(2)$, the unitary group of the degree 2, as

$$U(2) \ni U : \mathcal{K}_{+}(H_0) \longrightarrow \mathcal{K}_{-}(H_0)$$

- Following von Neumann's theory, we can show that

all the self-adjoint extensions H of the minimal Dirac operator H_0 are parameterized by $U(2)$ as

$$\begin{cases} D(H) = \{\psi = \psi_0 + \psi^+ + U\psi^+ \,|\, \psi_0 \in D(H_0),\ \psi^+ \in \mathcal{K}_+(H_0)\}, \\ H\psi = H_0\psi_0 + i\psi^+ - iU\psi^+. \end{cases}$$

Thus, we denote by H_U every self-adjoint extension parameterized by individual $U \in U(2)$ as in the above from now on.

- We call H_U obtained according to von Neumann's theory the Dirac operator parameterized $U \in U(2)$.

Proposition

The unitary group $\mathbf{U(2)}$ has the following representation:

$$\mathbf{U(2)} = \mathbf{U(1)}\, \mathbf{S}\mathbb{H}$$

$$= \left\{ \gamma_3 \begin{pmatrix} \gamma_1 & -\gamma_2{}^{*} \\ \gamma_2 & \gamma_1{}^{*} \end{pmatrix} \middle| \gamma_1, \gamma_2, \gamma_3 \in \mathbb{C},\ \ |\gamma_1|^2 + |\gamma_2|^2 = |\gamma_3| = 1 \right\}.$$

Here $\mathbf{S}\mathbb{H}$ is defined by

$$\mathbf{S}\mathbb{H} := \{ A \in \mathbb{H} \,|\, \det A = 1 \}$$

for the Hamilton quaternion field $\mathbb{H}$ consisting of $\mathbf{2} \times \mathbf{2}$ matrices.

- We can then give a physical meaning to $U \in U(2)$ of von Neumann's parameterization for the self-adjoint extensions obtained by von Neumann's theory in our case:
  By the preceding proposition,

$$U(2) \ni U = \gamma_3 \begin{pmatrix} \gamma_1 & -\gamma_2{}^* \\ \gamma_2 & \gamma_1{}^* \end{pmatrix} : \begin{matrix} L^2(\Omega_{\Lambda,L}) \\ \oplus \\ L^2(\Omega_{\Lambda,R}) \end{matrix} \longrightarrow \begin{matrix} L^2(\Omega_{\Lambda,L}) \\ \oplus \\ L^2(\Omega_{\Lambda,R}) \end{matrix} .$$

$$\begin{cases} U\psi_L^+ = \gamma_3\gamma_1\psi_L^- - \gamma_3\gamma_2{}^*\psi_R^-, \\ U\psi_R^+ = \gamma_3\gamma_2\psi_L^- + \gamma_3\gamma_1{}^*\psi_R^-. \end{cases}$$

Namely,

$$\begin{cases} U\psi_L^+ = \gamma_3\gamma_1\psi_L^- - \gamma_3\gamma_2^*\psi_R^- \\ U\psi_R^+ = \gamma_3\gamma_2\psi_L^- + \gamma_3\gamma_1{}^*\psi_R^- \end{cases} \qquad \begin{cases} U\psi_L^+ = \gamma_3\gamma_1\psi_L^- - \gamma_3\gamma_2{}^*\psi_R^- \\ U\psi_R^+ = \gamma_3\gamma_2\psi_L^- + \gamma_3\gamma_1^*\psi_R^- \end{cases}$$

Thus, the parameters γ_1 and γ_2 respectively govern the reflection of the electron's wave function at the boundaries and the wave function's tunneling through the junction.

- The following theorem gives a correspondence from $\gamma_1, \gamma_2, \gamma_3$ in von Neumann's theory to the boundary-condition data $\rho \in \overline{\mathbb{R}}^2$ or $\alpha \in \mathbb{C}^4$:

$$(\gamma_1, \gamma_2, \gamma_3) \longrightarrow \rho \in \overline{\mathbb{R}}^2 \quad \text{or} \quad \alpha \in \mathbb{C}^4.$$

Theorem

i) Every diagonal $U \in U(2)$ has the representation:

$\exists \gamma_L, \gamma_R \in \mathbb{C}$

s.t.

$$U = \begin{pmatrix} \gamma_L & 0 \\ 0 & \gamma_R \end{pmatrix}, \quad |\gamma_L| = |\gamma_R| = 1.$$

That is, $\gamma_L = \gamma_3\gamma_1$ *and* $\gamma_R = \gamma_3\gamma_1^*$.
Then, for arbitrarily fixed γ_L and γ_R, a necessary and sufficient condition for $D(H_U) = D(H_\rho)$ is given by determining the vector $\rho \in \overline{\mathbb{R}}^2$ with the formulae:

(D-L1) For $\gamma_L \neq -1$,

$$\rho_- = \frac{1}{\sqrt{1+m^2}}\left(\tan\frac{\theta_L}{2} - m\right),$$

where $\theta_L := \arg\gamma_L \in [0, 2\pi)$.

(D-L2) For $\gamma_L = -1$, $\rho_- = \infty$.

(D-R1) For $\gamma_R \neq -1$,

$$\rho_+ = -\frac{1}{\sqrt{1+m^2}}\left(\tan\frac{\theta_R}{2} - m\right)$$

where $\theta_R := \arg\gamma_R \in [0, 2\pi)$.

(D-R2) For $\gamma_R = -1$, $\rho_+ = \infty$.

ii) Every non-diagonal $U \in U(2)$ has the representation:
$\exists \gamma_1, \gamma_2, \gamma_3 \in \mathbb{C}$

s.t.
$$U = \gamma_3 \begin{pmatrix} \gamma_1 & -\gamma_2^* \\ \gamma_2 & \gamma_1^* \end{pmatrix}$$
with $|\gamma_1|^2 + |\gamma_2|^2 = |\gamma_3| = 1, \quad \gamma_2 \neq 0.$

Then, for arbitrarily fixed γ_1, γ_2, and γ_3, a necessary and sufficient condition for $D(H_U) = D(H_\alpha)$ is given by determining the vector $\alpha \in \mathbb{C}^4$ with the formulae:

$$\alpha_1 = i\gamma_2^{-1}\sqrt{1+m^2}\left(\Im(\gamma_1^*\mu) + \Im(\gamma_3^*\mu)\right),$$
$$\alpha_2 = \gamma_2^{-1}\sqrt{1+m^2}\,(\Re\gamma_1 + \Re\gamma_3),$$
$$\alpha_3 = \gamma_2^{-1}\sqrt{1+m^2}\left(-\Re\gamma_1 + \Re(\gamma_3^*\mu^2)\right),$$
$$\alpha_4 = i\gamma_2^{-1}\sqrt{1+m^2}\left(\Im(\gamma_1\mu) + \Im(\gamma_3^*\mu)\right),$$

where $\mu \equiv (1+im)/\sqrt{1+m^2} \in \mathbb{C}$.

We note the tunneling parameter γ_2 plays an important role because if $\gamma_2 = 0$ then $\alpha \in \mathbb{C}^4$ with $(*\alpha)$ cannot be constructed.

- We can derive a phase from the boundary-condition data $\alpha \in \mathbb{C}^4$ in the following.

Proposition

Let $\mathcal{A}$ be the set of all boundary matrices $\mathbf{B}_\alpha$ for vectors $\alpha = (\alpha_1, \alpha_2, \alpha_3, \alpha_4) \in \mathbb{C}^4$ in the class $(*\alpha)$. Then, $\alpha_1 \neq 0$ or $\alpha_3 \neq 0$. So, set $\theta \in [0, 2\pi)$ and $a_j \in \mathbb{R}$, $j = 1, 2, 3, 4$ as

$$\begin{cases} \theta := \arg(\alpha_1/|\alpha_1|); \\ a_1 := |\alpha_1|, \quad a_2 := -i(\alpha_1\alpha_2^*)^*/|\alpha_1|, \\ a_3 := -i(\alpha_1\alpha_3^*)^*/|\alpha_1|, \quad a_4 := (\alpha_1\alpha_4^*)^*/|\alpha_1|, \end{cases}$$

if $\alpha_1 \neq 0$, and

$$\begin{cases} \theta := \arg(-i\alpha_3/|\alpha_3|); \\ a_1 := i\alpha_1\alpha_3^*/|\alpha_3|, \quad a_2 := \alpha_2\alpha_3^*/|\alpha_3|, \\ a_3 := |\alpha_3|, \quad a_4 := i(\alpha_3\alpha_4^*)^*/|\alpha_3|, \end{cases}$$

if $\alpha_1 = 0$.

Then, $\mathcal{A}$, the class of the boundary matrix B_α, has the following representation:

$$\mathcal{A} = \left\{ B_\alpha \equiv \begin{pmatrix} \alpha_1 & \alpha_2 \\ \alpha_3 & \alpha_4 \end{pmatrix} = e^{i\theta} \begin{pmatrix} a_1 & ia_2 \\ ia_3 & a_4 \end{pmatrix} \middle| \ \theta \in [0, 2\pi), \right.$$

$$\left. a_j \in \mathbb{R}, \ j = 1, 2, 3, 4, \ \text{with} \ a_1 a_4 + a_2 a_3 = 1 \right\}.$$

- In the reflection case, it is clear that (D-L1)–(D-R2) make

$$\rho = (\rho_+, \rho_-) \in \overline{\mathbb{R}}^2 \overset{1-1}{\longleftrightarrow} (\gamma_L, \gamma_R) = (e^{i\theta_L}, e^{i\theta_R}) :$$

(D-L1') If $\rho_- \in \mathbb{R}$,

$$\gamma_L = \exp\left[2i \arctan\left(m + \sqrt{1+m^2}\,\rho_-\right)\right].$$

(D-L2') If $\rho_- = \infty$, $\gamma_L = -1$.
(D-R1') If $\rho_+ \in \mathbb{R}$,

$$\gamma_R = \exp\left[2i \arctan\left(m - \sqrt{1+m^2}\,\rho_+\right)\right].$$

(D-R2') If $\rho_+ = \infty$, $\gamma_R = -1$.

- In the tunneling case, we can also seek the formulae which give the correspondence from the boundary condition data to $\alpha \in \mathbb{C}^4$ to γ_1, γ_2, and γ_3 in von Neumann's theory,

$$\alpha = (\alpha_1, \alpha_2, \alpha_3, \alpha_4) \in \mathbb{C}^4 \longrightarrow (\gamma_1, \gamma_2, \gamma_3).$$

Theorem

For every B_α with $\alpha \in \mathbb{C}^4$ in the class $(*\alpha)$, the corresponding non-diagonal $U \in U(2)$ is determined as:

$$\begin{cases} \gamma_1 = \Gamma_0 e^{-i(\theta-\pi/2)} (-\mu^*\alpha_1 + \alpha_2 - \alpha_3 + \mu\alpha_4), \\ \gamma_2 = (2/\sqrt{1+m^2})\Gamma_0 e^{-i(\theta-\pi/2)}, \\ \gamma_3 = \Gamma_0 e^{-i(\theta-\pi/2)} \mu (\alpha_1 + \mu^*\alpha_2 + \mu\alpha_3 + \alpha_4)^*, \end{cases}$$

where $\mu := (1 + im)/\sqrt{1+m^2}$,

$$\Gamma_0 := \left(\frac{4}{1+m^2} + \left| -\mu^*\alpha_1 + \alpha_2 - \alpha_3 + \mu\alpha_4 \right|^2 \right)^{-1/2},$$

and the phase θ is determined as folows:

The phase factor $e^{i\theta}$ appears if and only if the tunneling parameter $\gamma_2 \neq 0$, and then, there exists a certain $\nu \in \mathbb{Z}$ such that

$$\theta = -\arg \gamma_2 + \left(\frac{1}{2} + \nu\right)\pi.$$

Thus, the phase θ appearing in the boudary matrix B_α can be called the tunneling phase.

Once the material of the physical unit is determined,
$\Downarrow$
self-adjointness of the Dirac operator is determined.
$\Downarrow$
Then, its corresponding boundary condition of
the Dirac particle's wave functions is fixed.
$\Downarrow$
The spin may be affected by the boundary condition,
and there are cases that the phase factor special to
the tunneling appears in the boundary condition.

In one of those cases,
wave functions have to satisfy the fixed boundary condition
and have the fixed phase factor to live in the physical unit
as residents there.

$\Downarrow$

Othewise, they are ejected from the physical unit.

So,

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Can we prepare the home for them?

6. Summary

My question:

Can we control and change their own phase in the junction?

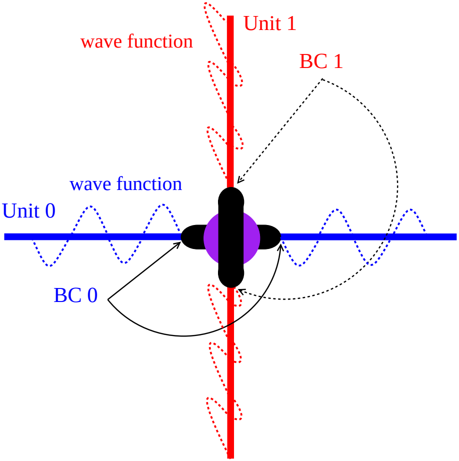
If it is possible, they have to find another home in somewhere.

Next my question:

Can we prepare the home for them?

If it is possible, the electron switches its homes and becomes a resident of new quantum unit.

6. Summary



For more details, please see

- Y. Furuhashi, M. Hirokawa, K. Nakahara, and Y. Shikano,
  "*Role of a phase factor in the boundary condition of a one-dimensional junction*"
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- M. Hirokawa and T. Kosaka,
  "*One-dimensional tunnel-junction formula for Schrödinger particle*"
  SIAM J. Appl. Math. **73** (2013) 2247,
- M. Hirokawa and T. Kosaka,
  "*A Mathematical Aspect of A Tunnel-Junction for Spintronic Qubit*"
  J. Math. Anal. Appl. **417** (2014) 856.

Thank you very much for your attention!