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Unstable vacuum and fermion total reflection by the Klein step

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The so-called Klein tunneling is re-examined within the framework of quantum field theory, but from a different point of view on the asymptotic states. We treat it as a one-dimensional scattering process of a fermion incident to a step potential and introduce asymptotic operators as appropriate $t = \pm\infty$ limits of the field operator responsible for the process. For the so-called Klein energy range, two asymptotic vacua naturally emerge which are defined as states annihilated by the asymptotic annihilation operators. They are related by a similarity transformation, which entails an unstable vacuum. When a fermion with incident energy in the Klein region is injected to the step, it is shown to be reflected with probability one, accompanied by fermion–anti-fermion pairs that are vacuum decay products.

Subject Index B30

1. Introduction

In non-relativistic quantum mechanics, a step potential that rises abruptly to a finite value at the origin and keeps its value to infinity plays the same role as a rigid wall in classical mechanics, because the reflection probability of the stationary scattering problem for the step becomes one when the incident energy is less than the height of the step. This is because the wave function under the step is essentially a real function and the corresponding probability current vanishes. This situation changes dramatically when one considers relativistic cases. Because the relativistic dispersion relation between energy and momentum allows solutions with both positive and negative energy, an oscillating solution can exist under the step if the value of the incident energy falls in a particular range called the Klein region, named after a paradoxical phenomenon for a relativistic electron described by the Dirac equation [1]. Since the stationary solutions are understood to represent stationary flows of probability currents, the phenomenon implies the existence of a non-vanishing probability current under the step, which may be interpreted as a transmitted or tunneling current.

Even though the implication seems physically counter-intuitive and, at the same time, suggestive when one combines it with the idea of Dirac sea, which may be lifted to produce electron–positron pairs when the applied potential is strong enough, it has generally been believed that the resolution of this problem could be sought only within the framework of quantum field theory. This is because the notion of particles and anti-particles is defined in quantum field theory, while in a single-particle quantum mechanics one can just deal with positive- and negative-energy solutions with no clear association to particle and anti-particle. Even if the lack of the

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negative-energy solution might be interpreted as the presence of an anti-particle, such an interpretation is only justified on the basis of quantum field theory.

In quantum field theory, we calculate the scattering (S) matrix which describes the transition between two asymptotic states prepared at remote past $t = -\infty$ and future $t = \infty$ in terms of field operators, and therefore it is crucial that one can define asymptotic states that allow a particle picture. When the potential is localized in space, the last condition seems to be satisfied on physical grounds because particles are present only in regions far away from the potential at $t = \pm\infty$. This, on the contrary, means that for a potential that does not vanish at spatial infinity, like the step potential, it is not clear whether one can define an S-matrix as in the usual cases, even if the potential is supposed to be switched on and off adiabatically.

One may argue that such difficulty is mainly due to a mathematical idealization and oversimplification of a physical setting; however, at the same time, the problem has attracted researchers for almost 90 years because its resolution is not only sought for academic interest but is also hoped to bring some insight into the physical mechanism of pair creation of particle and anti-particle from the vacuum. In order to somehow bypass the difficulty, Nikishov proposed to interchange the role of time and spatial coordinates and to utilize stationary scattering solutions that have a single plane wave in the spatially asymptotic regions to construct the Green function [2,3]. A similar idea was introduced to quantize the field variable of the scattering problem off the step potential, where solutions of the Dirac equation that satisfy a particular boundary condition, i.e. those composed of a single plane wave in regions outside of or under the step, are used to introduce creation/annihilation operators to discuss vacuum decay and pair creations [4–10]. Notice that the dynamics, i.e. the time development of the scattering process under a somewhat smeared potential (the Sauter potential [11]), has been analyzed numerically within the framework of quantum field theory [12,13], where the field operator, initially expanded in terms of solutions of the free Dirac equation, is numerically simulated to see the effect of an incident fermion on the pair creation due to the Pauli exclusion principle. See also Ref. [14] for an introductory review.

In this paper we exclusively consider a relativistic fermion incident to a step potential with its energy lying in the Klein region and examine the scattering process within the framework of quantum field theory, but from a different point of view on the asymptotic states. The strategy adopted here may be considered more straightforward and to follow a naive physical expectation. After a brief review of the so-called Klein tunneling in Sect. 2 and the relevant stationary scattering solutions of the Dirac equation with the usual boundary condition in Sect. 3, we introduce a field variable and expand it in terms of the stationary scattering solutions in Sect. 4. It should be stressed that the fact that they form a complete orthonormal set is directly shown [15], so that the operators introduced as the expansion coefficients of the field variable are guaranteed to satisfy the standard anti-commutation relations. Then we examine the asymptotic limits $t \to \pm\infty$ of the field operator and find that four non-trivial limits exist, by which the asymptotic “in” and “out” operators are defined. It is shown that they are related through a similarity transformation, i.e. a Bogoliubov-like transformation, which turns out to be the same as that introduced in Ref. [16]. These asymptotic operators are used in Sect. 5 to define two asymptotic vacua whose overlap can be explicitly evaluated. Under such an unstable vacuum, an incident particle with energy in the Klein region is shown to be completely reflected by the step, accompanying particle and anti-particle pairs produced from the unstable vacuum

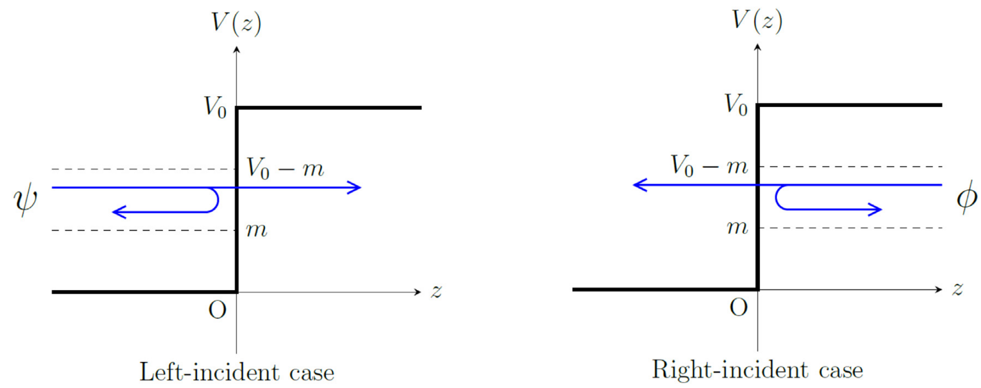

Fig. 1. Scattering states are categorized according to whether an incident flux is coming from the left (ψ) or right (ϕ) of the step potential, and the range of their energies.

in Sect. 6. The final Sect. 7 is devoted to a summary and discussions; appendices A and B are added to fix the notation and to supply additional details and information.

2. Klein tunneling in relativistic quantum mechanics

A scattering process of a Dirac fermion with mass m by a one-dimensional step potential

$$V(z) = \theta(z)V_0, \qquad V_0 > 2m, \tag{1}$$

is described by the Dirac Hamiltonian ($\hbar = c = 1$)

$$H = H_0 + V(z) = -i\alpha_z\partial_z + \beta m + V(z), \tag{2}$$

and its stationary solution is easily obtained. Here, $\theta(z)$ is the Heaviside step function, and α_z and β are two of the Dirac matrices. See Appendix A for the notation adopted here. We are mainly interested in the stationary scattering problem when the incident energy E lies in the so-called Klein region, $m < E < V_0 - m$. The stationary solution, which is nothing but an eigenfunction of H belonging to the energy eigenvalue E, is fixed once the boundary conditions and a continuity condition at $z = 0$ have been imposed on the eigenfunction (see Fig. 1). We treat the problem as an essentially one-dimensional scattering problem from the beginning, and the trivial dependence on the other coordinates x and y will be ignored completely.

Within the framework of (single-particle) relativistic quantum mechanics, when a particle with momentum $p > 0$ and spin s is incident from the left of the step, the stationary solution $\psi_s^{(E)}(z, t)$ with energy $E = \sqrt{p^2 + m^2} \equiv E_p$ is expressed, in terms of the positive frequency solution $u(\pm p, s)e^{-iE_pt\pm ipz}$ for $z < 0$ (left of the step) and the negative frequency solution $v(q, s)e^{iE_qt-iqz}$ for $z > 0$ (under the step), as ($E = E_p = V_0 - E_q$, $E_q = \sqrt{q^2 + m^2}$, $q > 0$)

$$\psi_s^{(E)}(z, t) = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m}{E}}\left[\theta(-z)\left\{u(p, s)e^{ipz} + Ru(-p, s)e^{-ipz}\right\} + \theta(z)T_{\rightarrow}\sigma_z v(q, s)e^{-iqz}\right]e^{-iEt}, \tag{3}$$

with

$$R = \frac{\sqrt{\frac{V_0-E-m}{E+m}} - \sqrt{\frac{V_0-E+m}{E-m}}}{\sqrt{\frac{V_0-E-m}{E+m}} + \sqrt{\frac{V_0-E+m}{E-m}}}, \qquad T_{\rightarrow} = \frac{2}{\sqrt{\frac{V_0-E-m}{E+m}} + \sqrt{\frac{V_0-E+m}{E-m}}}. \tag{4}$$

(Appendix A summarizes the details of the spinors.) The continuity of the current defined by $j_z = \bar{\psi}\gamma^3\psi = \psi^\dagger\alpha_z\psi$ at $z = 0$ implies the conservation of probability:

$$\frac{p}{m} - |R|^2\frac{p}{m} = |T_{\rightarrow}|^2\frac{q}{m} \quad \longrightarrow \quad P_r + P_t = |R|^2 + \frac{q}{p}|T_{\rightarrow}|^2 = 1. \tag{5}$$

Recall that this is a normal conservation law of probability, but a finite and non-vanishing transmission probability, which does not vanish even at the infinite-potential limit $V_0 \to \infty$, survives:

$$P_t = \frac{q}{p}|T_{\to}|^2 \quad \xrightarrow{V_0\to\infty} \quad \frac{2p}{E_p + p} = \frac{2\sqrt{E^2-m^2}}{E+\sqrt{E^2-m^2}} \neq 0. \tag{6}$$

This phenomenon is known as Klein tunneling [5].

Owing to the presence of negative-energy solutions to the Dirac equation, we can set up both left- and right-incident scattering problems, because even if the energy is below the potential height, there exist oscillating solutions of the equation. In fact, we obtain the right-incident solution $\phi_s^{(E)}(z,t)$ with a negative incident momentum $-q < 0$ and spin s ($E = V_0 - E_q = E_p$, $-p < 0$):

$$\phi_s^{(E)}(z,t) = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m}{V_0 - E}}\; [\theta(-z)T_{\leftarrow}\sigma_z u(-p,s)e^{-ipz} \\ +\theta(z)\{v(-q,s)e^{iqz} + Rv(q,s)e^{-iqz}\}]e^{-iEt}, \tag{7}$$

where

$$R = -\frac{\sqrt{\frac{E+m}{V_0-E-m}} - \sqrt{\frac{E-m}{V_0-E+m}}}{\sqrt{\frac{E+m}{V_0-E-m}} + \sqrt{\frac{E-m}{V_0-E+m}}}, \qquad T_{\leftarrow} = -\frac{2}{\sqrt{\frac{E+m}{V_0-E-m}} + \sqrt{\frac{E-m}{V_0-E+m}}}. \tag{8}$$

The continuity of the current results in the conservation of probability,

$$-\frac{p}{m}|T_{\leftarrow}|^2 = -\frac{q}{m} + \frac{q}{m}|R|^2, \tag{9}$$

which is essentially the same as Eq. (5). The reflection coefficient R turns out to be the same as in the left-incident case, which is nothing but a realization of reciprocity in quantum mechanics.

It is worth mentioning that a choice of $v(-q,s)e^{iqz}$ instead of $v(q,s)e^{-iqz}$ in Eq. (3) results in a negative factor in front of the transmission coefficient squared in Eq. (5) and the reflection probability becomes greater than one, which had been known as the Klein paradox [7]. It is to be observed that in such a case, the sign of the current (and also the group velocity) in the potential region ($z > 0$) becomes negative, which is not considered to satisfy the boundary condition for the left-incident scattering problem where only a positive current (transmitted current) is admissible for $z > 0$.

3. Scattering states

The stationary solutions for the left- and right-incident scattering problems are given by the eigenstates of the Hamiltonian H in Eq. (2) and are characterized by their boundary condition, i.e. left-incident (ψ) or right-incident (ϕ), and their eigenvalue E. These eigenfunctions form a complete orthonormal set. Only those cases where the potential step is higher than $2m$, $V_0 > 2m$, are considered here.

First, the orthogonality of the scattering states follows from the general argument for Hermitian Hamiltonians, i.e. eigenfunctions belonging to different eigenvalues are orthogonal to each other. Two ψs with different energies are orthogonal and normalized as

$$\int_{-\infty}^{\infty} dz \psi_s^{(E)\dagger}(z)\psi_{s'}^{(E')}(z) = \theta(EE')\delta(p-p')\delta_{s,s'}, \tag{10}$$

where $|E| = E_p$, $|E'| = E_{p'}$. Similarly, we should have

$$\int_{-\infty}^{\infty} dz \phi_s^{(E)\dagger}(z)\phi_{s'}^{(E')}(z) = \theta\left[(E - V_0)(E' - V_0)\right]\delta(q - q')\delta_{s,s'}, \tag{11}$$

where $|E - V_0| = E_q$, $|E' - V_0| = E_{q'}$, and

$$\int_{-\infty}^{\infty} dz \psi_s^{(E)\dagger}(z)\phi_{s'}^{(E')}(z) = 0. \tag{12}$$

Since the last orthogonality relation does not follow from the general argument, for both $\psi_s^{(E)}$ and $\phi_{s'}^{(E')}$ can happen to belong to the same energy $E = E'$, its validity has to be examined separately (see Appendix B). The orthonormality conditions imply that the following form of completeness relation holds:

$$\sum_{s,r=\pm}\left[\int_0^{\infty} dp \psi_s^{(rE_p)}(z)\psi_s^{(rE_p)\dagger}(z') + \int_0^{\infty} dq \phi_s^{(V_0+rE_q)}(z)\phi_s^{(V_0+rE_q)\dagger}(z')\right] = \delta(z - z')\mathbb{1}_{4\times 4}, \tag{13}$$

where $\mathbb{1}_{4\times 4}$ is the unit matrix acting in the spinor space. Notice that the fact they actually constitute a complete orthonormal set is shown in a straightforward way; the relation in Eq. (13) was shown explicitly in Ref. [15], though the proof itself first appeared more than 40 years ago [17].

4. Quantized field

In order to discuss the scattering process under the Hamiltonian H in Eq. (2) within the framework of quantum field theory, we introduce a field operator $\Psi(z, t)$ that satisfies the differential (Schrödinger) equation $i\dot{\Psi} = H\Psi$ and set up the equal-time anti-commutation relations between Ψs and $\Psi^\dagger$s; the only non-vanishing ones are

$$\{\Psi_\alpha(z, t),\ \Psi_\beta^\dagger(z', t)\} = \delta_{\alpha,\beta}\delta(z - z'). \tag{14}$$

The dynamics of Ψ is governed by the quantized Hamiltonian $\mathcal{H} = \int dz \Psi^\dagger H \Psi$ under the above equal-time anti-commutation relations. The field operator Ψ is then expanded in terms of a complete orthonormal set, and creation and annihilation operators are introduced as the expansion coefficients. Since we are interested in the scattering process described by the Hamiltonian in Eq. (2), it would be natural to choose its eigenfunctions that satisfy the boundary conditions for scattering processes, i.e. the left-incident (ψ) and right-incident (ϕ) scattering states will be chosen as the basis functions.

We introduce operators $b_{l(r)}$, $d_{l(r)}^\dagger$ as expansion coefficients of Ψ expanded in terms of the scattering states $\psi(\phi)$:

$$\Psi(z, t) = \int_0^{\infty} dp \sum_s [b_l(p, s)\psi_s^{(E_p)}(z, t) + d_l^\dagger(p, s)\psi_s^{(-E_p)}(z, t)]$$
$$+ \int_0^{\infty} dq \sum_s [b_r(q, s)\phi_s^{(V_0+E_q)}(z, t) + d_r^\dagger(q, s)\phi_s^{(V_0-E_q)}(z, t)]. \tag{15}$$

The orthonormality of scattering eigenstates $\psi_s^{(E)}$ and $\phi_s^{(E)}$ guarantees the usual canonical anti-commutation relations between creation/annihilation operators. Indeed, the operators are expressed as

$$b_l(p, s) = \int_{-\infty}^{\infty} dz \psi_s^{(E_p)\dagger}(z, t)\Psi(z, t), \quad b_r(q, s) = \int_{-\infty}^{\infty} dz \phi_s^{(V_0+E_q)\dagger}(z, t)\Psi(z, t), \tag{16}$$

$$d_l^\dagger(p, s) = \int_{-\infty}^{\infty} dz \psi_s^{(-E_p)\dagger}(z, t)\Psi(z, t), \quad d_r^\dagger(q, s) = \int_{-\infty}^{\infty} dz \phi_s^{(V_0-E_q)\dagger}(z, t)\Psi(z, t), \tag{17}$$

and since the right-hand sides are all time-independent if Ψ satisfies the same equation of motion as $\psi_s^{(E)}$ and $\phi_s^{(E)}$, the equal-time anti-commutation relations in Eq. (14) and the orthonormality of $\psi_s^{(E)}$ and $\phi_s^{(E)}$, Eqs. (10)–(12), are enough to show that the operators satisfy the standard anti-commutation relations.

Since the potential extending to $z = \infty$ is present at all times, it is not clear whether the standard construction of asymptotic states at $t = \pm\infty$ is consistently applied, especially when one considers the scattering process occurring in the Klein energy range. In practice, it is not easy to conceive such asymptotic Hamiltonians that give a naive asymptotic picture where free (anti-)particles exist without potential at the far left $z = -\infty$ and, at the same time, those with a constant potential at the far right $z = \infty$, at remote past or future. This is the core problem of quantum field theory in the presence of position-dependent external fields that extend to spatial infinity, in contrast to the usual perturbative quantum field theory as well as the theory in the presence of time-dependent (local) external fields, where asymptotic Hamiltonians naturally allow global particle–anti-particle interpretations. In this sense, it can be said that previous works such as Refs. [2,3,9] provide a way to avoid the current problem, where asymptotic states are defined by interchanging the role of space and time. In order to bypass this difficulty, we take a different strategy by which the asymptotic information is extracted from the field operator itself, which will turn out to yield results consistent with the previous ones in the literature. That is, we think that the field operator Ψ contains all the scattering information; because the potential $V(z)$ is given as an external field (not quantized), we can solve the Heisenberg equation $i\dot{\Psi} = [\Psi, \mathcal{H}] = H\Psi$ to obtain the exact solution in Eq. (15) at all times. It would thus be possible to obtain asymptotic operators without resorting to asymptotic Hamiltonians. We endeavor to extract asymptotic operators from the appropriate limits of the field operator. If properly extracted, they should represent such a physical situation that at the remote past $t = -\infty$, only incoming (from the remote left and right) waves exist, and at the remote future $t = \infty$, only outgoing (towards left and right) waves exist. We consider exclusively the case where Klein tunneling occurs, i.e. the left-incident energy $E > m$ is below the potential height, $E = E_p < V_0 - m$, and these asymptotic waves are plane-wave solutions of the free Dirac equation, but with the constant potential added for the right-incident and outgoing right waves. Consider, for example, the limit

$$\lim_{t\to-\infty}\int_{-\infty}^{\infty} dz u_{p,s}^{\dagger}(z,t)\Psi(z,t), \tag{18}$$

where

$$u_{p,s}(z,t) = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m}{E_p}}u(p,s)e^{ipz-iE_pt} \qquad (p>0) \tag{19}$$

is nothing but the (normalized) positive-energy solution of the free Dirac equation moving right. The integration over z in Eq. (18) results in one of the following forms for those terms with energy lying in the range $m < E < V_0 - m$:

$$\int_{-\infty}^{0} dz e^{-ipz+iE_pt}e^{ip'z-iE_{p'}t} = \frac{-i}{p'-p-i\epsilon}e^{-i(E_{p'}-E_p)t} \to 2\pi\delta(p'-p), \tag{20}$$

$$\int_{-\infty}^{0} dz e^{-ipz+iE_pt}e^{-ip'z-iE_{p'}t} = \frac{i}{p'+p}e^{-i(E_{p'}-E_p)t} \to 0, \tag{21}$$

$$\int_{0}^{\infty} dz e^{-ipz+iE_pt}e^{\pm iq'z-i(V_0-E_{q'})t} = \frac{-i}{\pm q'-p}e^{-i(V_0-E_{q'}-E_p)t} \to 0, \tag{22}$$

in the $t \to -\infty$ limit, owing to the Riemann–Lebesgue lemma. The lemma also implies that the other terms in Eq. (18) all disappear in the limit because their energy does not match E_p and oscillates indefinitely. The limit in Eq. (18) can be interpreted as the asymptotic annihilation operator for the incoming particle $b_{\rm in}(p, s)$ since it appears as the coefficient of the positive-energy solution moving right in the field operator Ψ at $t = -\infty$, and we find that

$$b_{\rm in}(p, s) = b_l(p, s). \tag{23}$$

Observe that the limit in Eq. (18) just extracts the coefficient of $u_{p,s}(z, t)$ in Ψ. The field operator Ψ also contains other solutions of the Dirac equation, $u_{-p,s}(z, t)$ and

$$v_{\pm q,s}(z, t) = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{m}{E_q}}\, v(\pm q, s) e^{\mp iqz - i(V_0 - E_q)t} \qquad (q > 0), \tag{24}$$

through the scattering wave functions ψ and ϕ in the Klein energy range. It would be natural to define the asymptotic creation operator for an incoming anti-particle $d^\dagger_{\rm in}(q, s)$ moving left by the limit

$$d^\dagger_{\rm in}(q, s) = \lim_{t\to-\infty} \int_{-\infty}^{\infty} dz v^\dagger_{-q,s}(z, t)\Psi(z, t), \tag{25}$$

which results in the relation

$$d^\dagger_{\rm in}(q, s) = d^\dagger_r(q, s). \tag{26}$$

Here, the direction of the particle or anti-particle is determined by that of the current for the corresponding plane-waves in Eqs. (19) or (24), which is consistent with the method using group velocity [5–7]. We understand that the limits in Eqs. (18) and (25) but with opposite momenta $p \to -p$ and $-q \to q$ give nothing,

$$\lim_{t\to-\infty} \int_{-\infty}^{\infty} dz u^\dagger_{-p,s}(z, t)\Psi(z, t) = \lim_{t\to-\infty} \int_{-\infty}^{\infty} dz v^\dagger_{q,s}(z, t)\Psi(z, t) = 0, \tag{27}$$

as expected from the directions of the incoming particle and anti-particle in the Klein region. We thus understand that the field operator Ψ in the Klein region is asymptotically expressed as

$$\lim_{t\to-\infty} \Psi(z, t) = \int_{E_p<V_0-m} dp \sum_s b_{\rm in}(p, s)u_{p,s}(z, t) + \int_{E_q<V_0-m} dq \sum_s d^\dagger_{\rm in}(q, s)v_{-q,s}(z, t), \tag{28}$$

consisting of a set of incoming plane-wave solutions for the "free" Hamiltonian $H(|z| = \infty)$. The result is essentially in accord with the idea of the standard procedure [18,19] where the asymptotic field operators are expanded in terms of the asymptotic mode functions to define asymptotic creation/annihilation operators for the case of time-dependent external fields. The quantities in Eq. (27) become non-vanishing instead in the other asymptotic limit, i.e. at $t \to \infty$, and they will be denoted as $b_{\rm out}$ and $d^\dagger_{\rm out}$, i.e. the particle–anti-particle interpretation for outgoing states, because they appear as the coefficients of the relevant positive- and negative-energy (relative to the energy gap) mode functions representing outgoing waves in the field operator Ψ at $t = \infty$. We evaluate the limit to obtain, for example,

$$b_{\rm out}(p, s) = \lim_{t\to\infty} \int_{-\infty}^{\infty} dz u^\dagger_{-p,s}(z, t)\Psi(z, t) = R(p)b_l(p, s) - \sqrt{\frac{E_q}{E_p}}\, T(p)d^\dagger_r(q, \tilde{s}), \tag{29}$$

where $E_p = V_0 - E_q$, R and $T = T_\to$ are reflection and transmission coefficients appearing in the left-incident scattering eigenfunction ψ, and the spin $\tilde{s}$ stands for the spinor $\tilde{\boldsymbol{\xi}}(\tilde{s}) = \sigma_z \boldsymbol{\xi}(s)$.

In deriving Eq. (29), the relations

$$\delta(p-p')=\frac{p}{E_p}\frac{E_q}{q}\delta(q-q'),\qquad T_{\leftarrow}(q)=-\frac{q}{p}T_{\rightarrow}(p) \tag{30}$$

were used. It is interesting to see that this operator b_{out} can be expressed as a similarity transformation of b_l multiplied by R,

$$b_{\text{out}}(p,s)=R(p)e^{B^\dagger}b_l(p,s)e^{-B^\dagger},\qquad B^\dagger=\sum_s\int_{E_p<V_0-m}dp\sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)}b_l^\dagger(p,s)d_r^\dagger(q,\tilde{s}), \tag{31}$$

and satisfies, together with its Hermitian conjugate, the standard anti-commutation relation

$$\begin{aligned}\{b_{\text{out}}(p,s),\ b^\dagger_{\text{out}}(p',s')\}&=R^2(p)\delta(p-p')\delta_{s,s'}+\frac{E_q}{E_p}T^2(p)\delta(q-q')\delta_{\tilde{s},\tilde{s}'}\\&=\left[R^2(p)+\frac{q}{p}T^2(p)\right]\delta(p-p')\delta_{s,s'}=\delta(p-p')\delta_{s,s'},\end{aligned} \tag{32}$$

where the last equality follows from the fact that the quantity in square brackets is unity, which is nothing but the current conservation condition. Another limit at $t\to\infty$ worth evaluating corresponds to the anti-particle creation operator $d^\dagger_{\text{out}}$ and yields

$$d^\dagger_{\text{out}}(q,s)=\lim_{t\to\infty}\int_{-\infty}^{\infty}dz v^\dagger_{q,s}(z,t)\Psi(z,t)=R(p)d_r^\dagger(q,s)+\frac{q}{p}\sqrt{\frac{E_p}{E_q}}T(p)b_l(p,\tilde{s}), \tag{33}$$

where use has been made of $R(p)\equiv R_{\leftarrow}(p)=R_{\rightarrow}(q)$ (the reciprocity). This operator is written as

$$d^\dagger_{\text{out}}(q,s)=R(p)e^{-C}d_r^\dagger(q,s)e^{C}, \tag{34}$$

where the operator C turns out to be the same as B,

$$\begin{aligned}C&=\sum_s\int_{E_q<V_0-m}dq\frac{q}{p}\sqrt{\frac{E_p}{E_q}}\frac{T(p)}{R(p)}d_r(q,s)b_l(p,\tilde{s})\\&=\sum_s\int_{E_p<V_0-m}dp\sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)}d_r(q,\tilde{s})b_l(p,s)=B,\end{aligned} \tag{35}$$

and satisfies

$$\begin{aligned}\{d_{\text{out}}(q,s),\ d^\dagger_{\text{out}}(q',s')\}&=R^2(p)\delta(q-q')\delta_{s,s'}+\left(\frac{q}{p}\right)^2\frac{E_p}{E_q}T^2(p)\delta(p-p')\delta_{\tilde{s},\tilde{s}'}\\&=\delta(q-q')\delta_{s,s'}.\end{aligned} \tag{36}$$

Since only the limits in Eqs. (29) and (33) yield non-vanishing results at $t=\infty$, we understand that the field operator Ψ is asymptotically given, in the Klein region, by

$$\lim_{t\to\infty}\Psi(z,t)=\int_{E_p<V_0-m}dp\sum_s b_{\text{out}}(p,s)u_{-p,s}(z,t)+\int_{E_q<V_0-m}dq\sum_s d^\dagger_{\text{out}}(q,s)v_{q,s}(z,t), \tag{37}$$

which is now expanded in the basis of outgoing solutions for the “free” Hamiltonian $H(|z|=\infty)$. The field operator in other energy regions can be obtained by the same method as described above.

5. Asymptotic vacua

We are now in a position to define asymptotic vacuum states. We define an asymptotic vacuum state at $t=-\infty$, called the “in” vacuum, as the state that is annihilated by the asymptotic operators $b_{\rm in}$ and $d_{\rm in}$:

$$b_{\rm in}(p,s)\,|0\rangle_{\rm in} = d_{\rm in}(q,s)\,|0\rangle_{\rm in} = 0. \tag{38}$$

The "in" vacuum $|0\rangle_{\rm in}$ is nothing but the normalized state $|0\rangle$ that is annihilated by the operators b_l and d_r:

$$|0\rangle_{\rm in} = |0\rangle\,, \qquad b_l(p,s)\,|0\rangle = d_r(q,s)\,|0\rangle = 0, \qquad \langle 0|0\rangle = 1. \tag{39}$$

We also introduce another asymptotic vacuum state at $t = \infty$, called the "out" vacuum, defined as the state that is annihilated by the operators $b_{\rm out}$ and $d_{\rm out}$:

$$b_{\rm out}(p,s)\,|0\rangle_{\rm out} = R(p)\left(b_l(p,s) - \sqrt{\tfrac{E_q}{E_p}}\tfrac{T(p)}{R(p)}d_r^\dagger(q,\tilde{s})\right)|0\rangle_{\rm out} = 0, \tag{40}$$

$$d_{\rm out}(q,\tilde{s})\,|0\rangle_{\rm out} = R(p)\left(d_r(q,s) + \tfrac{q}{p}\sqrt{\tfrac{E_p}{E_q}}\tfrac{T(p)}{R(p)}b_l^\dagger(p,\tilde{s})\right)|0\rangle_{\rm out} = 0. \tag{41}$$

It is not difficult to see that the "out" vacuum is explicitly constructed as

$$|0\rangle_{\rm out} = \prod_{p,s} R(p)\left(1 + \frac{2\pi}{L}\sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)}b_l^\dagger(p,s)d_r^\dagger(q,\tilde{s})\right)|0\rangle\,, \tag{42}$$

where L is the (infinite) size of the physical system and is formally equal to $2\pi\delta(p-p)$. To see that it is annihilated by $b_{\rm out}(p,s)$ and $d_{\rm out}(q,\tilde{s})$, we only need to confirm that for all $p > 0$ ($E_p = V_0 - E_q$) and for all s, the relations

$$\left(b_l(p,s) - \sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)}d_r^\dagger(q,\tilde{s})\right)\left(1 + \frac{2\pi}{L}\sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)}b_l^\dagger(p,s)d_r^\dagger(q,\tilde{s})\right)|0\rangle = 0, \tag{43}$$

$$\left(d_r(q,s) + \frac{q}{p}\sqrt{\frac{E_p}{E_q}}\frac{T(p)}{R(p)}b_l^\dagger(p,\tilde{s})\right)\left(1 + \frac{2\pi}{L}\sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)}b_l^\dagger(p,s)d_r^\dagger(q,\tilde{s})\right)|0\rangle = 0 \tag{44}$$

hold. The "out" vacuum $|0\rangle_{\rm out}$ is normalized to unity, as can be shown explicitly:

$$\begin{aligned} {}_{\rm out}\langle 0|0\rangle_{\rm out} &= \langle 0|\prod_{p,s} R^2(p)\left(1 + \frac{2\pi}{L}\sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)}d_r(q,\tilde{s})b_l(p,s)\right) \\ &\qquad \times\left(1 + \frac{2\pi}{L}\sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)}b_l^\dagger(p,s)d_r^\dagger(q,\tilde{s})\right)|0\rangle \\ &= \prod_{p,s} R^2(p)\left(1 + \frac{q}{p}\frac{T^2(p)}{R^2(p)}\right) = 1, \end{aligned} \tag{45}$$

where the last equality follows from the current conservation condition $R^2(p) + \frac{q}{p}T^2(p) = 1$. It may be interesting to see that the "out" vacuum state can be expressed as $|0\rangle_{\rm out} = \mathcal{N}e^{B^\dagger}\,|0\rangle$, where the operator $B^\dagger$ is the same as in Eq. (31) and the normalization constant is formally given by $\mathcal{N} = \prod_{p,s} R(p)$. Notice that the meaning of an infinite product over the continuous variable p is unclear and its precise meaning will be addressed below.

We are interested in the transition amplitudes to find specific asymptotic states at $t = \infty$ when the initial state is prepared at $t = -\infty$. It is thus convenient to express "in" states in terms of "out" states. We can, for example, invert the relations in Eqs. (29) and (33) to express "in" operators in terms of "out" operators:

$$\begin{pmatrix} b_{\rm in}(p,s) \\ d_{\rm in}^\dagger(q,\tilde{s}) \end{pmatrix} = \begin{pmatrix} R(p) & \sqrt{\frac{E_q}{E_p}}T(p) \\ -\frac{q}{p}\sqrt{\frac{E_p}{E_q}}T(p) & R(p) \end{pmatrix}\begin{pmatrix} b_{\rm out}(p,s) \\ d_{\rm out}^\dagger(q,\tilde{s}) \end{pmatrix}; \tag{46}$$

we also have, instead of Eq. (42),

$$|0\rangle_{\rm in} = \prod_{p,s} R^{-1}(p) \left(1 - \frac{2\pi}{L}\sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)} b^\dagger_{\rm in}(p,s) d^\dagger_{\rm in}(q,\tilde{s})\right) |0\rangle_{\rm out} . \tag{47}$$

It is not difficult to see that the last expression is actually symmetric between "in" and "out" since it can be rewritten, in terms of "out" operators, as

$$|0\rangle_{\rm in} = \prod_{p,s} R(p) \left(1 - \frac{2\pi}{L}\sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)} b^\dagger_{\rm out}(p,s) d^\dagger_{\rm out}(q,\tilde{s})\right) |0\rangle_{\rm out} . \tag{48}$$

Notice that the expression in Eq. (48), which is formal and somewhat ambiguous, can be written as

$$|0\rangle_{\rm in} = \mathcal{N} e^{-B^\dagger_{\rm out}} |0\rangle_{\rm out} , \tag{49}$$

where

$$B^\dagger_{\rm out} = \sum_s \int_{E_p < V_0 - m} dp \sqrt{\frac{E_q}{E_p}} \frac{T(p)}{R(p)} b^\dagger_{\rm out}(p,s) d^\dagger_{\rm out}(q,\tilde{s}). \tag{50}$$

It is easily seen that the state $e^{-B^\dagger_{\rm out}} |0\rangle_{\rm out}$ is actually annihilated by $b_{\rm in}$ and $d_{\rm in}$:

$$\begin{aligned} b_{\rm in}(p,s)\,|0\rangle_{\rm in} &\propto \left(R(p) b_{\rm out}(p,s) + \sqrt{\frac{E_q}{E_p}} T(p) d^\dagger_{\rm out}(q,\tilde{s})\right) e^{-B^\dagger_{\rm out}} |0\rangle_{\rm out} \\ &= e^{-B^\dagger_{\rm out}} R(p) b_{\rm out}(p,s)\,|0\rangle_{\rm out} = 0, \end{aligned} \tag{51}$$

$$\begin{aligned} d_{\rm in}(q,\tilde{s})\,|0\rangle_{\rm in} &\propto \left(R(p) d_{\rm out}(q,\tilde{s}) - \frac{q}{p}\sqrt{\frac{E_p}{E_q}} T(p) b^\dagger_{\rm out}(p,s)\right) e^{-B^\dagger_{\rm out}} |0\rangle_{\rm out} \\ &= e^{-B^\dagger_{\rm out}} R(p) d_{\rm out}(q,\tilde{s})\,|0\rangle_{\rm out} = 0. \end{aligned} \tag{52}$$

The constant $\mathcal{N}$ is calculated from the normalization condition $\mathcal{N}^{-2} = {}_{\rm out}\langle 0| e^{-B_{\rm out}} e^{-B^\dagger_{\rm out}} |0\rangle_{\rm out}$.

In order to estimate $\mathcal{N}$, consider the functional

$$F[a] \equiv \langle 0| e^{-B[a]} e^{-B^\dagger[a]} |0\rangle , \qquad B[a] = \sum_s \int_{E_p < V_0 - m} dp\, a(p,s) d(q,\tilde{s}) b(p,s), \tag{53}$$

where the index "out" has been suppressed for notational simplicity. A functional derivative of F brings down operators db and $b^\dagger d^\dagger$,

$$\frac{\delta}{\delta a(p,s)} F[a] = -\langle 0| e^{-B[a]} (d(q,\tilde{s}) b(p,s) + b^\dagger(p,s) d^\dagger(q,\tilde{s})) e^{-B^\dagger[a]} |0\rangle . \tag{54}$$

These operators can be moved to, say, just the right of $\langle 0|$

$$\begin{aligned} &-\langle 0| \left[d(q,\tilde{s}) b(p,s) + \left(b^\dagger(p,s) - a(p,s) d(q,\tilde{s})\right)\left(d^\dagger(q,\tilde{s}) + \frac{q}{p}\frac{E_p}{E_q} a(p,s) b(p,s)\right)\right] \\ &\quad \times e^{-B[a]} e^{-B^\dagger[a]} |0\rangle \\ &= a(p,s)\,\langle 0| d(q,\tilde{s}) d^\dagger(q,\tilde{s}) |0\rangle\,\langle 0| e^{-B[a]} e^{-B^\dagger[a]} |0\rangle \\ &\quad - \langle 0| d(q,\tilde{s}) b(p,s) e^{-B[a]} e^{-B^\dagger[a]} |0\rangle \left(1 - \frac{q}{p}\frac{E_p}{E_q} a^2(p,s)\right) . \end{aligned} \tag{55}$$

The last matrix element satisfies the relations

$$
\begin{aligned}
&\langle 0|d(q,\tilde{s})b(p,s)e^{-B[a]}e^{-B^\dagger[a]}|0\rangle \\
&= \langle 0|\, e^{-B[a]}e^{-B^\dagger[a]} \left(d(q,\tilde{s}) + \frac{q}{p}\frac{E_p}{E_q} a(p,s) b^\dagger(p,s) \right) \left(b(p,s) - a(p,s) d^\dagger(q,\tilde{s}) \right) |0\rangle \\
&= -a(p,s)\, \langle 0|e^{-B[a]}e^{-B^\dagger[a]}|0\rangle\, \langle 0|d(q,\tilde{s})d^\dagger(q,\tilde{s})|0\rangle \\
&\quad - \langle 0|e^{-B[a]}e^{-B^\dagger[a]} b^\dagger(p,s) d^\dagger(q,\tilde{s})|0\rangle\, \frac{q}{p}\frac{E_p}{E_q} a^2(p,s) \\
&= -a(p,s) \left(1 - \frac{q}{p}\frac{E_p}{E_q} a^2(p,s) \right) \langle 0|e^{-B[a]}e^{-B^\dagger[a]}|0\rangle\, \langle 0|d(q,\tilde{s})d^\dagger(q,\tilde{s})|0\rangle \\
&\quad + \langle 0|d(q,\tilde{s})b(p,s)e^{-B[a]}e^{-B^\dagger[a]}|0\rangle \left(\frac{q}{p}\frac{E_p}{E_q} a^2(p,s) \right)^2 ,
\end{aligned} \tag{56}
$$

resulting in

$$
\langle 0|d(q,\tilde{s})b(p,s)e^{-B[a]}e^{-B^\dagger[a]}|0\rangle = -\frac{a(p,s)}{1+\frac{q}{p}\frac{E_p}{E_q}a^2(p,s)} \langle 0|e^{-B[a]}e^{-B^\dagger[a]}|0\rangle\, \langle 0|d(q,\tilde{s})d^\dagger(q,\tilde{s})|0\rangle\, . \tag{57}
$$

We thus understand that $F[a]$ satisfies

$$
\begin{aligned}
\frac{\delta}{\delta a(p,s)} F[a] &= \frac{2a(p,s)}{1+\frac{q}{p}\frac{E_p}{E_q}a^2(p,s)} \langle 0|d(q,\tilde{s})d^\dagger(q,\tilde{s})|0\rangle\, F[a] \\
&= \frac{2\frac{q}{p}\frac{E_p}{E_q}a(p,s)}{1+\frac{q}{p}\frac{E_p}{E_q}a^2(p,s)} \langle 0|b(p,s)b^\dagger(p,s)|0\rangle\, F[a],
\end{aligned} \tag{58}
$$

the solution of which with the condition $F[0] = 1$ reads

$$
F[a] = \exp\left[\sum_s \int_{E_p<V_0-m} dp \ln\left(1 + \frac{q}{p}\frac{E_p}{E_q} a^2(p,s) \right) \langle 0|b(p,s)b^\dagger(p,s)|0\rangle \right]. \tag{59}
$$

This shows that the normalization constant $\mathcal{N}$, which is reproduced by the functional $F[a]$ once $a(p,s)$ is replaced with $\sqrt{E_q/E_p}\, T(p)/R(p)$, is given by[1]

$$
\begin{aligned}
\mathcal{N} &= \exp\left[-\frac{1}{2} \sum_s \int_{E_p<V_0-m} dp \ln\left(1 + \frac{q}{p}\frac{T^2(p)}{R^2(p)} \right) \langle 0|b(p,s)b^\dagger(p,s)|0\rangle \right] \\
&= \exp\left[\frac{1}{2} \sum_s \int_{E_p<V_0-m} dp \ln R^2(p)\, \langle 0|b(p,s)b^\dagger(p,s)|0\rangle \right] \\
&= \exp\left[\frac{L}{2\pi} \int_m^{V_0-m} \frac{dE_p}{v_p} \ln R^2(p) \right],
\end{aligned} \tag{60}
$$

where $v_p = p/E_p$ is the group velocity.

The expressions in Eqs. (48)–(50) explicitly show that the "in" vacuum has non-vanishing overlaps with states of outgoing pairs of particle and anti-particle, which implies that it is not stable in the Klein region. In order to explicitly evaluate such probabilities of finding outgoing pairs of particle and anti-particle, it is instructive and helpful to first calculate the following

[1] A formulation of vacuum decay including transverse momentum states can be seen in Ref. [10]. See also, for the scalar case, Ref. [20], and for a review, Ref. [21].

generating functional:

$$G[a] = \langle 0| \exp\left[- \sum_s \int_{E_p < V_0 - m} dp\, a(p,s) d(q,\tilde{s}) b(p,s) \right] \times \exp\left[- \sum_s \int_{E_p < V_0 - m} dp \sqrt{\frac{E_q}{E_p}} \frac{T(p)}{R(p)} b^\dagger(p,s) d^\dagger(q,\tilde{s}) \right] |0\rangle \,, \tag{61}$$

where all the operators and states are understood as "out" ones, though the index "out" is suppressed for simplicity. Following a similar procedure to before, it is not difficult to show that $G[a]$ satisfies the functional differential equation

$$\frac{\delta}{\delta a(p,s)} G[a] = \frac{\sqrt{\frac{E_q}{E_p}} \frac{T(p)}{R(p)}}{1 + \frac{q}{p}\sqrt{\frac{E_p}{E_q}} \frac{T(p)}{R(p)} a(p,s)} \langle 0| d(q,\tilde{s}) d^\dagger(q,\tilde{s}) |0\rangle\, G[a] = \frac{\frac{q}{p}\sqrt{\frac{E_p}{E_q}} \frac{T(p)}{R(p)}}{1 + \frac{q}{p}\sqrt{\frac{E_p}{E_q}} \frac{T(p)}{R(p)} a(p,s)} \langle 0| b(p,s) b^\dagger(p,s) |0\rangle\, G[a]. \tag{62}$$

The solution with the condition $G[0] = 1$ reads

$$G[a] = \exp\left[\sum_s \int_{E_p < V_0 - m} dp \ln\left(1 + \frac{q}{p}\sqrt{\frac{E_p}{E_q}} \frac{T(p)}{R(p)} a(p,s) \right) \langle 0| b(p,s) b^\dagger(p,s) |0\rangle \right]. \tag{63}$$

Successive functional derivatives of G evaluated at $a = 0$ generate amplitudes of finding outgoing particle–anti-particle pairs in the "in" vacuum. For example, the first derivative yields the amplitude finding a single pair,

$$_{\text{out}}\langle 0| d_{\text{out}}(q,\tilde{s}) b_{\text{out}}(p,s) |0\rangle_{\text{in}} = \mathcal{N} \left.\frac{\delta}{\delta a(p,s)} G[a]\right|_{a=0} = \mathcal{N} \frac{q}{p}\sqrt{\frac{E_p}{E_q}} \frac{T(p)}{R(p)}\, _{\text{out}}\langle 0| b_{\text{out}}(p,s) b^\dagger_{\text{out}}(p,s) |0\rangle_{\text{out}}. \tag{64}$$

The second derivative, on the other hand, yields an amplitude of the form

$$_{\text{out}}\langle 0| (db)_1 (db)_2 |0\rangle_{\text{in}} = \mathcal{N} \left.\frac{\delta^2}{\delta a_1 \delta a_2} G[a]\right|_{a=0} = \mathcal{N} \left(-\frac{\beta_1^2 \delta(p_1 - p_2) \delta_{s_1,s_2}}{(1+\beta_1 a_1)^2} + \frac{\beta_1 \beta_2}{(1+\beta_1)(1+\beta_2)}\, _{\text{out}}\langle 0| (bb^\dagger) |0\rangle_{\text{out}} \right) \times\, _{\text{out}}\langle 0| (bb^\dagger) |0\rangle_{\text{out}} \Big|_{a=0}, \tag{65}$$

where we have set $\frac{q}{p}\sqrt{\frac{E_p}{E_q}} \frac{T(p)}{R(p)} = \beta$ and introduced a shorthand notation, $(db)_1 = d_{\text{out}}(q_1,\tilde{s}_1) b_{\text{out}}(p_1,s_1)$, etc. This amplitude vanishes when $p_1 = p_2$, $s_1 = s_2$, as it should, for $_{\text{out}}\langle 0| (bb^\dagger) |0\rangle_{\text{out}} = \delta(p - p)$. We may therefore write

$$\frac{\delta^2}{\delta a_1 \delta a_2} G[a] = \begin{cases} \frac{\beta_1\, _{\text{out}}\langle 0| (bb^\dagger) |0\rangle_{\text{out}}}{1+\beta_1 a_1} \frac{\beta_2\, _{\text{out}}\langle 0| (bb^\dagger) |0\rangle_{\text{out}}}{1+\beta_2 a_2} G[a], & \text{for } 1 \neq 2, \\ 0, & \text{otherwise,} \end{cases} \tag{66}$$

which can be generalized to higher-order derivatives, and we understand that the amplitude of finding n pairs is given by

$$
\begin{aligned}
{}_{\text{out}}\langle 0|(db)_1(db)_2\cdots(db)_n|0\rangle_{\text{in}} &= \mathcal{N}\prod_{k=1}^{n}\beta_k\,{}_{\text{out}}\langle 0|(bb^\dagger)_k|0\rangle_{\text{out}} \\
&= \mathcal{N}\prod_{k=1}^{n}\frac{q_k}{p_k}\sqrt{\frac{E_{p_k}}{E_{q_k}}}\frac{T(p_k)}{R(p_k)}\,{}_{\text{out}}\langle 0|b(p_k,s_k)b^\dagger(p_k,s_k)|0\rangle_{\text{out}}, \quad (67)
\end{aligned}
$$

where all the momenta p_k are different, for otherwise it vanishes.

In order to properly normalize the multi-pair states, so that their inner products are just given by the product of delta functions, each state has to be divided by $\left\{\frac{q}{p}\frac{E_p}{E_q}\,{}_{\text{out}}\langle 0|b(p,s)b^\dagger(p,s)|0\rangle_{\text{out}}\right\}^{1/2}$ because

$$
\begin{aligned}
&{}_{\text{out}}\langle 0|d_{\text{out}}(q,\tilde{s})b_{\text{out}}(p,s)b^\dagger_{\text{out}}(p',s')d^\dagger_{\text{out}}(q',\tilde{s}')|0\rangle_{\text{out}} \\
&\quad = \frac{q}{p}\frac{E_p}{E_q}\,{}_{\text{out}}\langle 0|b_{\text{out}}(p,s)b^\dagger_{\text{out}}(p,s)|0\rangle_{\text{out}}\delta(p-p')\delta_{s,s'}. \quad (68)
\end{aligned}
$$

The probability of finding an outgoing single pair thus reads

$$
P_1 = \mathcal{N}^2\sum_s\int_{E_p<V_0-m}dp\frac{q}{p}\frac{T^2(p)}{R^2(p)}\,{}_{\text{out}}\langle 0|b_{\text{out}}(p,s)b^\dagger_{\text{out}}(p,s)|0\rangle_{\text{out}}. \quad (69)
$$

Generally speaking, however, it is not easy to write down the probability of finding n pairs of outgoing particle and anti-particle, denoted as P_n, because a naive expectation for P_n,

$$
\mathcal{N}^2\frac{1}{n!}\left(\sum_s\int_{E_p<V_0-m}dp\frac{q}{p}\frac{T^2(p)}{R^2(p)}\,{}_{\text{out}}\langle 0|b_{\text{out}}(p,s)b^\dagger_{\text{out}}(p,s)|0\rangle_{\text{out}}\right)^n, \qquad n=0,1,2,\ldots, \quad (70)
$$

is not precise and has to be corrected by properly subtracting all possible coincident contributions where at least two pairs share the same momentum. The explicit form of P_n could instead be read from the power expansion of the generating functional $G[a]$ in Eq. (63).

6. Scattering process seen as transition from single-particle "in" state

Even though the asymptotic "in" state is shown to decay into pairs of particle and anti-particle, and it is not clear whether discussing a stationary scattering process within this framework is meaningful, we can explore what happens to a single-particle state prepared at $t=-\infty$. Such a state would be interpreted as an initial state of the scattering problem. Consider, for definiteness, a state that corresponds to a left-incident particle moving right at $t=-\infty$, which is represented by the state $b^\dagger_{\text{in}}(p,s)\,|0\rangle_{\text{in}}$. This state is shown to contain an outgoing particle and multi-pairs of particle and anti-particle at $t=\infty$. We just rewrite the initial state in terms of the "out" operators and "out" vacuum,

$$
\begin{aligned}
b^\dagger_{\text{in}}(p,s)\,|0\rangle_{\text{in}} &= \left[R(p)b^\dagger_{\text{out}}(p,s)+\sqrt{\frac{E_q}{E_p}}T(p)d_{\text{out}}(q,\tilde{s})\right]\mathcal{N}e^{-B^\dagger_{\text{out}}}\,|0\rangle_{\text{out}} \\
&= \frac{\mathcal{N}}{R(p)}b^\dagger_{\text{out}}(p,s)e^{-B^\dagger_{\text{out}}}\,|0\rangle_{\text{out}}, \quad (71)
\end{aligned}
$$

where the last equality follows if the operators in brackets are moved just next to the vacuum. Since the state contains only those states that contain one more particle than anti-particles, we just concentrate on the transition amplitudes to such states.

It is possible to evaluate the following amplitude, which will turn out to be relevant to the current problem, to obtain

$$
\begin{aligned}
&{}_{\text{out}}\langle 0|\exp\left[-\sum_s\int_{E_p<V_0-m} dp\, a(p,s) d_{\text{out}}(q,\tilde{s}) b_{\text{out}}(p,s)\right] b_{\text{out}}(p',s') b^\dagger_{\text{out}}(p,s) e^{-B^\dagger_{\text{out}}}|0\rangle_{\text{out}} \\
&= \frac{\delta(p-p')\delta_{s,s'}}{1+\frac{q}{p}\sqrt{\frac{E_p}{E_q}}\frac{T(p)}{R(p)}a(p,s)} G[a],
\end{aligned} \tag{72}
$$

where $G[a]$ is given in Eq. (63). If we set $a(p,s)=\sqrt{\frac{E_q}{E_p}}\frac{T(p)}{R(p)}$, G becomes ${}_{\text{out}}\langle 0|e^{-B_{\text{out}}}e^{-B^\dagger_{\text{out}}}|0\rangle_{\text{out}} = \mathcal{N}^{-2}$ and the above relation just implies that

$$
{}_{\text{out}}\langle 0|e^{-B_{\text{out}}} b_{\text{out}}(p',s') b^\dagger_{\text{out}}(p,s) e^{-B^\dagger_{\text{out}}}|0\rangle_{\text{out}} = \mathcal{N}^{-2} R^2(p)\delta(p-p')\delta_{s,s'}. \tag{73}
$$

Observe also that

$$
\begin{aligned}
&{}_{\text{out}}\langle 0|\exp\left[-\sum_s\int_{E_p<V_0-m} dp\, a(p,s) d_{\text{out}}(q,\tilde{s}) b_{\text{out}}(p,s)\right] d^\dagger_{\text{out}}(q',\tilde{s}') \\
&= a(p',s')\frac{q'}{p'}\frac{E_{p'}}{E_{q'}}\,{}_{\text{out}}\langle 0|\exp\left[-\sum_s\int_{E_p<V_0-m} dp\, a(p,s) d_{\text{out}}(q,\tilde{s}) b_{\text{out}}(p,s)\right] b_{\text{out}}(p',s'),
\end{aligned} \tag{74}
$$

implying that the states with one less anti-particle than particles are related to those with one more particle than anti-particles.

We expect that the initial state with a single particle moving right with momentum p and spin s, $b^\dagger_{\text{in}}(p,s)|0\rangle_{\text{in}}$, corresponds to a final state with a single particle moving left and multi-pairs of particle and anti-particle because the former is written as in Eq. (71). The probability of finding one outgoing particle with no pairs of particle and anti-particle is simply proportional to the matrix element squared,

$$
\left|{}_{\text{out}}\langle 0|b_{\text{out}}(p',s') b^\dagger_{\text{in}}(p,s)|0\rangle_{\text{in}}\right|^2 = \frac{\mathcal{N}^2}{R^2(p)}\left(\delta(p-p')\delta_{s,s'}\right)^2. \tag{75}
$$

Though the quantity still has to be properly normalized in order to be interpreted as a probability density, we understand that such a probability becomes exponentially small, because the "in" vacuum is not stable and decays out into pairs of particle and anti-particle. If we take into account such decay products of particle–anti-particle pairs, the matrix element squared for a specific final state with a particle and multi-pairs of particle and anti-particle has to be summed over all degrees of freedom, i.e. we have to sum over the spins and integrate over the momenta of the pairs, after properly normalizing the final state. Specifically, we calculate

$$
\sum_{n\geq 0}\frac{1}{n!}\prod_{k=1}^n\sum_{s_k}\int_{E_{p_k}<V_0-m}\frac{dp_k}{\xi_k}\left|{}_{\text{out}}\langle 0|(db)_1\cdots(db)_n b_{\text{out}}(p',s')\frac{\mathcal{N}}{R(p)} b^\dagger_{\text{out}}(p,s) e^{-B^\dagger_{\text{out}}}|0\rangle_{\text{out}}\right|^2, \tag{76}
$$

where the shorthand notation $(db)_k = d_{\text{out}}(q_k,\tilde{s}_k) b_{\text{out}}(p_k,s_k)$ has again been introduced and ξ_k is the normalization factor,

$$
\begin{aligned}
{}_{\text{out}}\langle 0|(db)_k(b^\dagger d^\dagger)_l|0\rangle_{\text{out}} &= \frac{q_k}{p_k}\frac{E_{p_k}}{E_{q_k}}\,{}_{\text{out}}\langle 0|b_{\text{out}}(p_k,s_k) b^\dagger_{\text{out}}(p_k,s_k)|0\rangle_{\text{out}}\delta(p_k-p_l)\delta_{s_k,s_l} \\
&\equiv \xi_k\delta(p_k-p_l)\delta_{s_k,s_l}.
\end{aligned} \tag{77}
$$

We note that the matrix element can be written as an nth functional derivative of Eq. (72) evaluated at $a = 0$,

$$
\begin{aligned}
&{}_{\text{out}}\langle 0|(db)_1 \cdots (db)_n b_{\text{out}}(p', s') b^\dagger_{\text{out}}(p, s) e^{-B^\dagger_{\text{out}}}|0\rangle_{\text{out}} \\
&= \frac{-\delta}{\delta a_1} \cdots \frac{-\delta}{\delta a_n} \left[\frac{\delta(p - p')\delta_{s,s'}}{1 + \frac{q}{p}\sqrt{\frac{E_p}{E_q}} \frac{T(p)}{R(p)} a(p, s)} G[a] \right]_{a=0}, \qquad (78)
\end{aligned}
$$

where $a_k = a(p_k, s_k)$, and therefore the quantity in Eq. (76), which is now written as

$$
\begin{aligned}
&\frac{\mathcal{N}^2}{R^2(p)} \sum_n \frac{1}{n!} \prod_{k=1}^{n} \sum_{s_k} \int_{E_{p_k} < V_0 - m} dp_k\, {}_{\text{out}}\langle 0|e^{-B_{\text{out}}} b_{\text{out}}(p, s) b^\dagger_{\text{out}}(p', s') \frac{(b^\dagger d^\dagger)_n}{\xi_n} \cdots \frac{(b^\dagger d^\dagger)_1}{\xi_1} |0\rangle_{\text{out}} \\
&\times \frac{-\delta}{\delta a_1} \cdots \frac{-\delta}{\delta a_n} \left[\frac{\delta(p - p')\delta_{s,s'}}{1 + \frac{q}{p}\sqrt{\frac{E_p}{E_q}} \frac{T(p)}{R(p)} a(p, s)} G[a] \right]_{a=0}, \qquad (79)
\end{aligned}
$$

is reduced to

$$
\frac{\mathcal{N}^2}{R^2(p)} {}_{\text{out}}\langle 0|e^{-B_{\text{out}}} b_{\text{out}}(p, s) b^\dagger_{\text{out}}(p', s') \left[\frac{\delta(p - p')\delta_{s,s'}}{1 + \frac{q}{p}\sqrt{\frac{E_p}{E_q}} \frac{T(p)}{R(p)} a(p, s)} G[a] \right]_{a=-\frac{(b^\dagger d^\dagger)}{\xi}} |0\rangle_{\text{out}}. \qquad (80)
$$

Since $b^\dagger_{\text{out}}$ and $d^\dagger_{\text{out}}$ are fermion operators that satisfy $(b^\dagger_{\text{out}}(p, s))^2 = 0 = (d^\dagger_{\text{out}}(q, \tilde{s}))^2$, the operator inserted in the denominator gives no contribution and we have

$$
G[a]\Big|_{a=-\frac{(b^\dagger d^\dagger)}{\xi}} = \exp\left[-\sum_s \int_{E_p < V_0 - m} dp \sqrt{\frac{E_q}{E_p}} \frac{T(p)}{R(p)} b^\dagger_{\text{out}}(p, s) d^\dagger_{\text{out}}(q, \tilde{s}) \right], \qquad (81)
$$

which is nothing but $e^{-B^\dagger_{\text{out}}}$. The quantity in Eq. (76) finally turns out to be

$$
\frac{\mathcal{N}^2}{R^2(p)} {}_{\text{out}}\langle 0|e^{-B_{\text{out}}} b_{\text{out}}(p, s) b^\dagger_{\text{out}}(p', s') e^{-B^\dagger_{\text{out}}}|0\rangle_{\text{out}} \delta(p - p')\delta_{s,s'} = \delta(p - p')\delta_{s,s'}\delta(p - p). \qquad (82)
$$

The last equality follows from the normalization condition in Eq. (73).

In order to properly reproduce the probabilities or "cross section" in the scattering problem, the result in Eq. (82) has to be devided by the incident flux and the total scattering time. The incident flux $j_{\text{inc}} = \psi^\dagger_s(p)\alpha_z\psi_s(p)$ is calculated from the incident wave function,

$$
\psi_s(p) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{m}{E_p}} u(p, s), \qquad (83)
$$

and we obtain

$$
j_{\text{inc}} = \frac{1}{2\pi} \frac{m}{E_p} \frac{E_p + m}{2m} \frac{2p}{E_p + m} = \frac{1}{2\pi} \frac{p}{E_p}. \qquad (84)
$$

Observe that we can replace the diverging factor $\delta(p - p)$ by the infinite time interval T_{total} that is defined as

$$
T_{\text{total}} = \int_{-\infty}^{\infty} dt = \int_{-\infty}^{\infty} dt e^{i(E_p - E_p)t} = 2\pi\delta(E_p - E_p) = 2\pi\delta(p - p)\frac{E_p}{p}. \qquad (85)
$$

This means that the amplitude squared has to be multiplied by

$$
\frac{1}{T_{\text{total}}\, j_{\text{inc}}} = \frac{1}{\delta(p - p)} \qquad (86)
$$

to yield a probability density. Notice that the same result could be attained if the initial state is normalized just by formally dividing it by ${}_{\text{in}}\langle 0|b_{\text{in}}(p, s) b^\dagger_{\text{in}}(p, s)|0\rangle_{\text{in}} = \delta(p - p)$.

We arrive at the conclusion that when a particle with momentum $p > 0$ and spin s is injected, the probability of finding an outgoing particle moving left asymptotically is just one, when one does not care about the number of particle–anti-particle pairs produced:

$$\text{Prob.}\left(\begin{array}{c}\text{particle moving right with } p, s \\ \rightarrow \text{particle moving left with arbitrary numbers of pairs}\end{array}\right) = 1. \tag{87}$$

Since the outgoing particle moves left, this is considered to be the reflection probability, i.e. total reflection, and states that this is all that happens.

7. Summary and discussions

The Klein tunneling process in relativistic quantum mechanics has been examined on the basis of quantum field theory, where the field operator Ψ, which is assumed to have all the information on the physical process, plays a crucial and central role. It is constructed on the basis of the solutions of the Dirac equation that satisfy boundary conditions for the stationary scattering problem. It is stressed that the condition that they constitute a complete orthonormal set is crucial in order for operators introduced as the expansion coefficients to satisfy the standard anti-commutation relations. In contrast to most cases where the completeness of the basis functions has just been assumed on physical grounds, the stationary solutions of the Dirac equation on which the field quantization of this paper is based have been shown explicitly to satisfy the completeness condition [15]. This guarantees the standard anti-commutation relations among creation/annihilation operators introduced in the field operator. Other choices of basis functions, of course, would be possible, but only when they are shown (not simply assumed) to be complete and orthonormal.

In this respect, it should be remarked that the orthogonality of the stationary solutions belonging to the same energy eigenvalue is closely connected to the choice of proper boundary conditions. As stated above and can be shown explicitly in simple cases, the usual boundary condition for the scattering process, i.e. the existence of incident and reflected plane waves on one far side of the interaction region and the transmitted plane wave on the other far side, entails, in general, orthogonality between the left-incident and right-incident solutions. The result can be derived in connection with a position-independent current formed from these solutions. It should be observed that the other solutions that satisfy, say, spatially asymptotic plane wave conditions, i.e. solutions that have either outgoing or incoming plane waves on the same far side of the interaction region, are not orthogonal to each other. See Appendix B for details.

Next, the asymptotic operators were introduced as the appropriate $t = \pm\infty$ limits of the field operator Ψ. At $t = -\infty$, only the right-moving wave existing at the left of the step ($z < 0$) and left-moving wave in the potential region ($z > 0$) survive in Ψ, which are supposed to represent incident waves. On the other hand, only the left-moving and right-moving waves are extracted for $z < 0$ and $z > 0$, respectively, at $t = \infty$, representing outgoing scattered ones. The asymptotic operators are just defined as the coefficients of these waves in Ψ. The asymptotic vacuum states are then defined to be those annihilated by the asymptotic annihilation operators. Two sets of asymptotic operators are related by a Bogoliubov-like transformation in the Klein energy range, on which we have exclusively focused in this paper, resulting in an unstable "in" vacuum.

In this way we arrive at the following view on Klein tunneling on the basis of quantum field theory. When the step potential is higher than $2m$, not only is the "in" vacuum unstable, but also a particle injected into such a potential is totally reflected and is accompanied by pair-produced particles moving left and anti-particles moving right. No transmitted particles moving right exist. This view would have been somewhat expected when the field operator Ψ is expanded in terms of b_{out} and $d^{\dagger}_{\text{out}}$; however, the explicit calculations presented in the previous sections show consistently that this is indeed the case.

Even though in this paper we have exclusively considered operators relevant to the Klein region, the framework developed here surely admits the presence of other particle and anti-particle modes, for which both asymptotic vacua are the same. This is because, in each energy range outside the Klein region, particle and anti-particle modes do not coexist and thus, e.g. an "out" annihilation operator is expressed as a linear combination of "in" annihilation operators, implying there is no mixing among annihilation and creation operators. This means that the vacuum structure is trivial (the "in" vacuum is the same as the "out" vacuum, or the latter is annihilated by the "in" annihilation operators) for such modes outside the Klein region, and nothing peculiar would happen for such modes.

Finally, we remark that since the normalization factor is nothing but the transition amplitude $\mathcal{N} = {}_{\text{out}}\langle 0|0\rangle_{\text{in}}$, it can provide information on the effective action ${}_{\text{out}}\langle 0|0\rangle_{\text{in}} = e^{iS_{\text{eff}}}$. Our result in Eq. (60) is consistent with a subset of the momentum states contributing to the known decay rate that appears in the imaginary part of S_{eff} [8,9,16], where more than one spatial dimension is considered. Notice that the full rate in three spatial dimensions includes integration over transverse momenta, producing a vacuum decay per unit cross-sectional area and time. We also comment that the result for the Klein step in Eq. (60) only has an exponential decay factor for the reflection amplitude $R(p)$ is real. This formula can be applied to the case of, say, the Sauter step [11] just by replacing $R(p)$ with the counterpart for the Sauter step, which is complex, because the Bogoliubov coefficients in Eq. (42) are determined by the orthogonal structure of the mode functions and it depends only on their asymptotic behavior at spatial infinity; see Appendix B. It is possible to derive the imaginary part of the effective action from $\mathcal{N}$ [16]; however, to extract the real part of the effective action on the basis of the present framework, one may have to know how to fix the relative phase between the two vacua, which would require additional considerations.

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Appendix A. Dirac spinors

We fix the notations and normalizations of four-component spinors. The stationary plane-wave solutions for the free Dirac Hamiltonian

$$H_0 = -i\alpha_z\partial_z + \beta m, \qquad \alpha_z = \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \tag{A1}$$

are

$$u(p,s)e^{-ip\cdot z} = \sqrt{\frac{E_p+m}{2m}}\begin{pmatrix} \mathbb{1} \\ \frac{\sigma_z p}{E_p+m} \end{pmatrix}\boldsymbol{\xi}(s)e^{ipz-iE_pt} \tag{A2}$$

for a positive frequency $E_p = \sqrt{p^2 + m^2}$ and

$$v(p,s)e^{ip\cdot z} = \sqrt{\frac{E_p + m}{2m}} \begin{pmatrix} \frac{\sigma_z p}{E_p+m} \\ \mathbb{1} \end{pmatrix} \boldsymbol{\xi}(s) e^{-ipz+iE_pt} \tag{A3}$$

for a negative frequency $-E_p$, where σ_z is the third Pauli matrix, $\mathbb{1}$ the 2×2 unit matrix, and $\boldsymbol{\xi}(s)$ a two-component spinor. They are normalized and form a complete orthonormal set:

$$\bar{u}(p,s)u(p,s') = \delta_{s,s'}, \qquad \bar{v}(p,s)v(p,s') = -\delta_{s,s'}, \tag{A4}$$

$$u^\dagger(p,s)u(p,s') = v^\dagger(p,s)v(p,s') = \frac{E_p}{m}\delta_{s,s'}, \tag{A5}$$

$$\sum_s [u(p,s)\bar{u}(p,s) - v(p,s)\bar{v}(p,s)] = \mathbb{1}_{4\times 4}. \tag{A6}$$

Now, if a constant potential is added to the above Hamiltonian,

$$H_0' = H_0 + V_0 = -i\alpha_z\partial_z + \beta m + V_0 \qquad (-\infty < z < \infty), \tag{A4}$$

the corresponding plane-wave solutions are ($E_q = \sqrt{q^2 + m^2}$)

$$u(q,s)e^{-iq\cdot z} = \sqrt{\frac{E_q + m}{2m}} \begin{pmatrix} \mathbb{1} \\ \frac{\sigma_z q}{E_q+m} \end{pmatrix} \boldsymbol{\xi}(s) e^{iqz-i(E_q+V_0)t} \tag{A8}$$

for a "positive" frequency $E_q + V_0 \geq V_0$ and

$$v(q,s)e^{iq\cdot z} = \sqrt{\frac{E_q + m}{2m}} \begin{pmatrix} \frac{\sigma_z q}{E_q+m} \\ \mathbb{1} \end{pmatrix} \boldsymbol{\xi}(s) e^{-iqz-i(-E_q+V_0)t} \tag{A9}$$

for a "negative" frequency $-E_q + V_0 \leq V_0$. They are again normalized and form a complete orthonormal set in spinor space, just like Eqs. (A4)–(A6), with E_p replaced with E_q. Notice that the frequency $-E_q + V_0$ can be positive for small momenta $|q| < \sqrt{V_0^2 - m^2}$, even though it is to be associated with the spinor v. Note also that the above explicit forms of spinors are not unique since σ_z is commutable with the above H_0 and H_0', and therefore, e.g., $\sigma_z u(p,s)$ can be used instead of $u(p,s)$.

Incidentally, the current conservation $\partial_0 j^0 + \partial_z j^z = 0$ resulting from the invariance under the global phase transformation implies a z-independent current $j^z = \psi^\dagger\alpha_z\psi$ for stationary states, and the above positive- and negative-frequency solutions both give positive currents,

$$u^\dagger(q,s)\sigma_z u(q,s) = \frac{q}{m} = v^\dagger(q,s)\sigma_z v(q,s), \tag{A10}$$

for positive $q > 0$, irrespective of the value of V_0. In this respect, both $u(q,s)$ and $v(q,s)$ are considered to express positive flows of current with positive and negative frequencies.

Appendix B. Orthogonality and boundary conditions of stationary solutions

We show here that the orthogonality of stationary solutions of the Dirac equation that belong to the same energy eigenvelue is closely connected to the boundary conditions they satisfy and the existence of spatially constant quantities. First, under the standard boundary conditions for scattering problems, a left-incident solution ψ is characterized by its asymptotic behavior,

$$z \to -\infty: \quad \psi \sim e^{\pm ipz}\chi_p + R_\leftarrow \chi_{-p} e^{\mp ipz}, \qquad z \to \infty: \quad \psi \sim T_\rightarrow \chi_{p'} e^{\pm ip'z}, \tag{B1}$$

and a right-incident solution ϕ by

$$z \to -\infty: \quad \phi \sim T_\leftarrow e^{\mp ipz}\chi_{-p}, \qquad z \to \infty: \quad \phi \sim e^{\mp ip'z}\chi_{-p'} + R_\rightarrow \chi_{p'} e^{\pm ip'z}, \tag{B2}$$

where χ represents either spinor u (positive frequency solution) or v (negative frequency solution), upper and lower signs in the exponent are to be associated with u and v, respectively (spin degrees of freedom is neglected), and $p > 0$ and $p^{'} > 0$ are the magnitudes of asymptotic momenta at $z = -\infty$ and $z = \infty$ where the potential takes constant values. Since both ψ and ϕ satisfy the same Dirac equation with the same energy, the quantity $\psi^\dagger\alpha_z\phi$ is shown to be z-independent $\partial_z(\psi^\dagger\alpha_z\phi) = 0$, and in particular its values at $z = \pm\infty$ are the same. Inserting their spatially asymptotic forms in Eqs. (B1) and (B2), we have

$$\psi^\dagger\alpha_z\phi \sim \left(e^{\mp ipz}\chi_p^\dagger + R_\leftarrow^* e^{\pm ipz}\chi_{-p}^\dagger\right)\alpha_z T_\leftarrow e^{\mp ipz}\chi_{-p} = -\frac{p}{m}R_\leftarrow^* T_\leftarrow \tag{B3}$$

at $z = -\infty$ and

$$\psi^\dagger\alpha_z\phi \sim T_\rightarrow^* e^{\mp ip'z}\chi_{p'}^\dagger\alpha_z\left(e^{\mp ip'z}\chi_{-p'} + R_\rightarrow e^{\pm ip'z}\chi_{p'}\right) = \frac{p'}{m}T_\rightarrow^* R_\rightarrow \tag{B4}$$

at $z = \infty$, resulting in the equality (reciprocity)

$$-\frac{p}{m}R_\leftarrow^* T_\leftarrow = \frac{p'}{m}T_\rightarrow^* R_\rightarrow. \tag{B5}$$

Here we have used the relations $\chi_p^\dagger\alpha_z\chi_p = \frac{p}{m}$ and $\chi_p^\dagger\alpha_z\chi_{-p} = 0$ that hold for any choice of χ.

Now consider an inner product between ψ_1 with left-incident momentum p_1 and ϕ_2 with right-incident momentum p_2'. If $p_1 \neq p_2$, where p_2 is the asymptotic momentum corresponding to p_2', two solutions belong to different energy eigenvalues and are thus orthogonal to each other. We therefore anticipate that if two momenta become identical, only singular contributions proportional to delta functions would appear in the inner product (for any finite contributions are absent if the momenta are different). Such contributions only appear from the spatially asymptotic regions $z \sim \infty$ and $z \sim -\infty$, and can be estimated as

$$\begin{aligned}\int_{-\infty}^{\infty} dz\psi_1^\dagger\phi_2 &= \text{divergent parts of}\left[\int_{-\infty}^{z_-} dz\left(e^{\mp ip_1z}\chi_{p_1}^\dagger + R_\leftarrow^* e^{\pm ip_1z}\chi_{-p_1}^\dagger\right)T_\leftarrow e^{\mp ip_2z}\chi_{-p_2}\right.\\ &\quad\left.+\int_{z_+}^{\infty} dz\, T_\rightarrow^* e^{\mp ip_1'z}\chi_{p_1'}^\dagger\left(e^{\mp ip_2'z}\chi_{-p_2'} + R_\rightarrow e^{\pm ip_2'z}\chi_{p_2'}\right)\right]\\ &= \pi R_\leftarrow^* T_\leftarrow\frac{E_{p_1}}{m}\delta(p_1 - p_2) + \pi T_\rightarrow^* R_\rightarrow\frac{E_{p_1'}}{m}\delta(p_1' - p_2') = 0,\end{aligned} \tag{B6}$$

where $z_+ > 0$ and $z_- < 0$ are arbitrary (but finite) large and small numbers. In this estimation, rapidly oscillating terms give no contributions owing to the Riemann–Lebesgue lemma, and use has been made of $p_1'E_{p_1}\delta(p_1 - p_2) = p_1E_{p_1'}\delta(p_1' - p_2')$, which follows from the equality $E_{p_1} - E_{p_2} = E_{p_1'} - E_{p_2'}$ and Eq. (B5). The orthogonality between left-incident and right-incident degenerate solutions of the stationary Dirac equation is thus proved.

Consider next another degenerate solution of the same Dirac equation but with different boundary condition $\tilde{\phi}$ that has only a left-moving component at the far right end $z \sim \infty$. It should behave asymptotically like

$$z \to -\infty: \quad \tilde{\phi} \sim Ae^{\pm ipz}\chi_p + Be^{\mp ipz}\chi_{-p}, \qquad z \to \infty: \quad \tilde{\phi} \sim e^{\mp ip'z}\chi_{-p'}. \tag{B7}$$

Following the same line of thought, a spatially conserved quantity $\psi^\dagger\alpha_z\tilde{\phi}$ derives the equality

$$\frac{p}{m}(A - R_\leftarrow^* B) = 0. \tag{B8}$$

The inner product between ψ_1 and $\tilde{\phi}_2$ is similarly evaluated as

$$\int_{-\infty}^{\infty} dz\psi_1^\dagger\tilde{\phi}_2 \propto \pi(A + R_\leftarrow^* B)\frac{E_{p_1}}{m}\delta(p_1 - p_2) = 2\pi A\frac{E_{p_1}}{m}\delta(p_1 - p_2), \tag{B9}$$

which does not vanish because neither A nor B are allowed to vanish. A similar argument is also applied to cases with two solutions that have a single component in the other asymptotic region $z \to -\infty$, and we can show that such solutions are not orthogonal to each other. We thus conclude that the degenerate solutions of the stationary Dirac equation, one with only a right-moving component and the other with only a left-moving component in the same spatial asymptotic region, are never orthogonal to each other.

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