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Motion of a wave packet in the Klein paradox

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Computer simulations for the scattering of a relativistic wave packet by a step potential are performed. Under the condition of the Klein paradox, where the height of the potential barrier becomes supercritical, the scattering induces the creation of electron-positron pairs. The “pair creation” is demonstrated in the present simulation by making use of the hole theory. © 1999 American Association of Physics Teachers.

I. INTRODUCTION

In nonrelativistic quantum mechanics the scattering of an electron by a step potential is known as one of the simplest solvable problems. When we try to solve similar problems for the Dirac equation, on the other hand, we encounter the peculiar situation called the Klein paradox.¹⁻⁴ As shown in Fig. 1, if the height of the potential barrier V_0 is larger than the sum of the initial energy E of an electron and its rest energy m_0c^2 (i.e., the potential is “supercritical”⁴), the positive-energy continuum in region I contacts with the negative-energy continuum in region II at the boundary. In the nonrelativistic case, for $V_0 > E$ there is no oscillatory solution in the potential region and the reflection coefficient is equal to unity. In contrast, in the relativistic case, even when V_0 is much larger than E , we have oscillating waves in region II. Moreover, the reflection current exceeds the initial one.²⁻⁴ The Klein paradox is nowadays known as the simplest model of the decay of the charged vacuum in a supercritical field that creates electron-positron pairs at the potential barrier.⁴

For nonrelativistic electrons, the motion of a wave packet has been presented in many papers and textbooks. On the other hand, to our knowledge, numerical simulations for the motion of a relativistic wave packet have not been demonstrated in the literature. Probably this is because serious difficulties arise when the potential height becomes supercritical. For example, the probability density is not conserved due to the effect of pair creation at the supercritical potential barrier.

The purpose of this paper is to perform numerical simulations for the motion of a relativistic wave packet under the condition of the Klein paradox. Three different approaches will be considered. By making use of the hole theory, pair creation at the supercritical potential barrier is demonstrated.

II. THE KLEIN PARADOX

We start with the 1+1-dimensional Dirac equation for the stationary state

$$\hat{H}\phi_E(x) = E\phi_E(x) \quad (1)$$

with the Hamiltonian (see Appendix A)

$$\hat{H} = c\sigma_x \left(-i\hbar \frac{\partial}{\partial x} \right) + \sigma_z m_0 c^2 + V(x)I, \quad (2)$$

where ϕ_E is a two-component Dirac spinor for the stationary scattering state, σ_x and σ_z are the Pauli matrices, and I is the 2×2 unit matrix. For the step potential

$$V(x) = V_0 \theta(x), \quad (3)$$

where $\theta(x)$ is the Heaviside function, (1) can be solved analytically.^{2,3} The solution depends on the height of the potential V_0 . We obtain

$$\phi_E(x) = \varphi_I(x)\theta(-x) + \varphi_{II}(x)\theta(x), \quad (4)$$

where $\varphi_I(x)$ and $\varphi_{II}(x)$ represent the wave functions in region I and region II in Fig. 1, respectively:

$$\begin{aligned} \varphi_I(x) &= A[u_+ e^{ipx/\hbar} + Ru_- e^{-ipx/\hbar}], \\ \varphi_{II}(x) &= AT\bar{u}e^{i\bar{p}x/\hbar}. \end{aligned} \quad (5)$$

p and $\bar{p}$ are the momentum of electrons in regions I and II, respectively:

$$cp = \sqrt{E^2 - (m_0 c^2)^2}, \quad (6)$$

$$c\bar{p} = \sqrt{(E - V_0)^2 - (m_0 c^2)^2}. \quad (7)$$

The spinors in (5) are given by

$$u_{\pm} = \begin{pmatrix} 1 \\ \pm a \end{pmatrix}, \quad \bar{u} = \begin{pmatrix} 1 \\ b \end{pmatrix}, \quad (8)$$

where

$$a = \frac{cp}{E + m_0 c^2}, \quad b = \frac{c\bar{p}}{E - V_0 + m_0 c^2}. \quad (9)$$

The reflection (transmission) coefficient $R(T)$ is determined as usual by the continuity of the wave function at $x=0$. We obtain

$$R = \frac{a-b}{a+b}, \quad T = \frac{2a}{a+b}. \quad (10)$$

The behavior of the wave function (4) can be classified into three cases.

(1) $V_0 < E - m_0 c^2$; the solution (4) in region I is composed of the right-moving incoming wave and the left-moving reflected wave. In region II we have the right-moving transmitted wave. This behavior is similar to the solution of the Schrödinger equation for $V_0 < E$ with the potential of (3).

(2) $E - m_0 c^2 < V_0 < E + m_0 c^2$; the wave propagating into region II disappears. In this case $\bar{p}$ becomes imaginary and

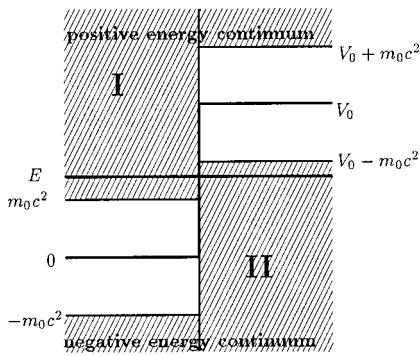


Fig. 1. Energy diagram for the Klein paradox. In region I the energy E of the stationary state $\phi_E(x)$ is in the positive-energy continuum while in region II it is in the negative-energy continuum.

hence we have an evanescent wave in region II. This situation is also similar to the nonrelativistic case for $V_0 > E$.

(3) $V_0 > E + m_0 c^2$; we have oscillatory waves in region II because $\bar{p}$ becomes real again. In the nonrelativistic case for $V_0 > E$ no such solution is obtained. Moreover, since b is now negative, the current of the reflected wave is *larger* than the incoming wave. This situation is called the Klein paradox.

Nowadays the Klein paradox is interpreted in terms of the hole theory.²⁻⁴ At the boundary, incident electrons stimulate the vacuum in region II that is filled by the negative energy electrons (i.e., the Dirac sea). Due to the stimulation, negative-energy electrons are ejected into region I, being observed as positive-energy electrons. Holes remaining in region II are interpreted as positrons. In other words, the incident electrons induce pair creation at the supercritical potential barrier. In this interpretation, the reflected current becomes larger than the incident one because it is composed of totally reflected electrons and created ones. The current in region II is interpreted as the flow of positrons.

III. WAVE PACKET FOR THE KLEIN PARADOX

In this section we construct a wave packet and perform computer simulations in the case of the Klein paradox.

As is well known, there are two ways of approaching this problem.⁵ One is to perform a numerical integration of the time-dependent Dirac equation

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \hat{H} \Psi(x, t). \quad (11)$$

The other approach consists of forming a wave packet as the superposition of the stationary solutions (4):

$$\Psi(x, t) = \int_D dE G(p) \phi_E(x) e^{-iEt/\hbar}. \quad (12)$$

The advantage of the latter approach is that we can freely take the energy domain for the superposition. For the Klein paradox, we take $D = \{E | m_0 c^2 < E < V_0 - m_0 c^2\}$. In principle, taking a finite region for D results in distorting the shape of the initial wave packet $\Phi(x, 0)$. This is not very serious, though. As we will see in Figs. 2–4, we can form an initial wave packet that looks like a Gaussian by giving the coefficient $G(p)$ as

$$G(p) = G_0 \exp \left[-\frac{(p - p_0)^2}{2\sigma^2} - i \frac{pd}{\hbar} \right], \quad (13)$$

where p_0 is the mean value for the momentum distribution of the wave packet and G_0 is the normalization constant. It should be noted that p is a function of E [see (6)]. The center of the wave packet is placed at $d (< 0)$. The momentum dispersion σ^2 takes the value satisfying the condition $[c^2(p_0 + 2\sigma)^2 + (m_0 c^2)^2]^{1/2} < V_0 - m_0 c^2$ and $[c^2(p_0 - 2\sigma)^2 + (m_0 c^2)^2]^{1/2} > m_0 c^2$ so that the major components of the Gaussian distribution are in the overlap region of the positive and negative energy continuum at the boundary (see Fig. 1).

In Fig. 2 we show a set of numerical results of the motion of the wave packet. We use atomic units, i.e., $\hbar = m_0 = e^2$

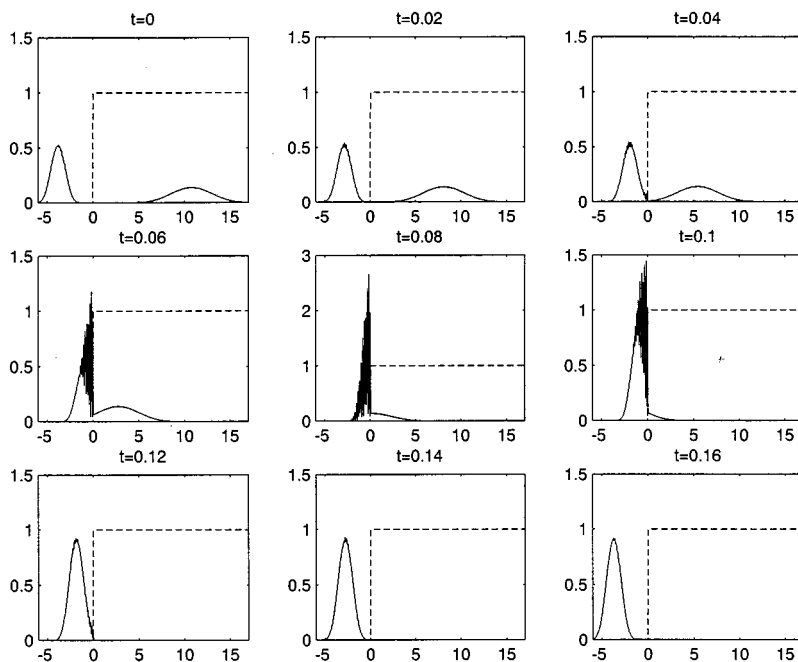


Fig. 2. Numerical simulation of the motion of a Dirac wave packet formed by a superposition of states under the conditions of the Klein paradox. The horizontal and the vertical axes represent the coordinate x and $|\Psi(x, t)|^2$, respectively. The dashed line in each figure represents the step potential. Though we attempt to prepare an initial wave packet on the left, another unexpected wave packet has appeared on the right.

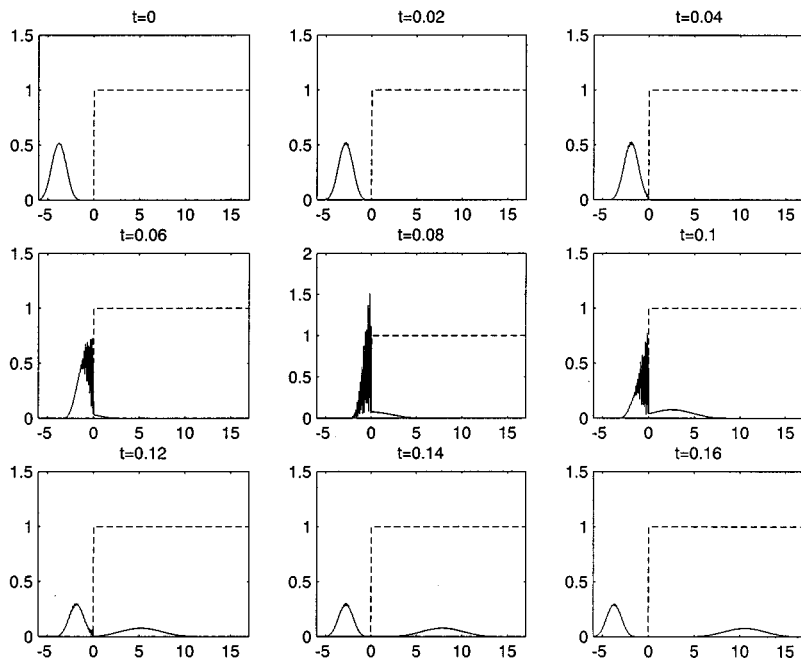


Fig. 3. Motion of a Dirac wave packet after the momentum inversion $\vec{p} \rightarrow -\vec{p}$. Other conditions are the same as that of Fig. 2. As one can see, the probability density is conserved in this case. However, this motion requires the assumption that the negative-energy continuum is not occupied.

$=1$ and hence $c=137$ in numerical calculations. In these units we take $p_0=50$, $\sigma=1$, $V_0=5[(p_0c)^2+m_0c^2]^{1/2}$, and $d=-3.8$ for all simulations presented in this paper. It is interesting to observe that, besides the wave packet we prepared as incoming electrons at $t=0$ in region I, another wave packet has appeared in region II. The wave packet in region II travels to the left because its group velocity

$$v_g = \frac{c^2}{E - V_0} \bar{p} \quad (14)$$

is negative. The left-going wave packet collides with the incoming one at the boundary. After their collision, the reflected wave packet becomes larger than the incident one as a result of the superposition of two wave packets. By defin-

ing the integrated distribution for each region as

$$P_I(t) = \int_{-\infty}^0 dx \Psi^\dagger(x,t) \Psi(x,t), \quad (15)$$

$$P_{II}(t) = \int_0^{\infty} dx \Psi^\dagger(x,t) \Psi(x,t), \quad (16)$$

we may numerically confirm the conservation of $P_I(t) + P_{II}(t)$. For example, initially we have $P_I(0)=1.00$ and $P_{II}(0)=0.75$ while for the last picture $P_I(0.16)=1.75$.

The motion given in Fig. 2 is rather unphysical because we want as the initial condition that there be only the incom-

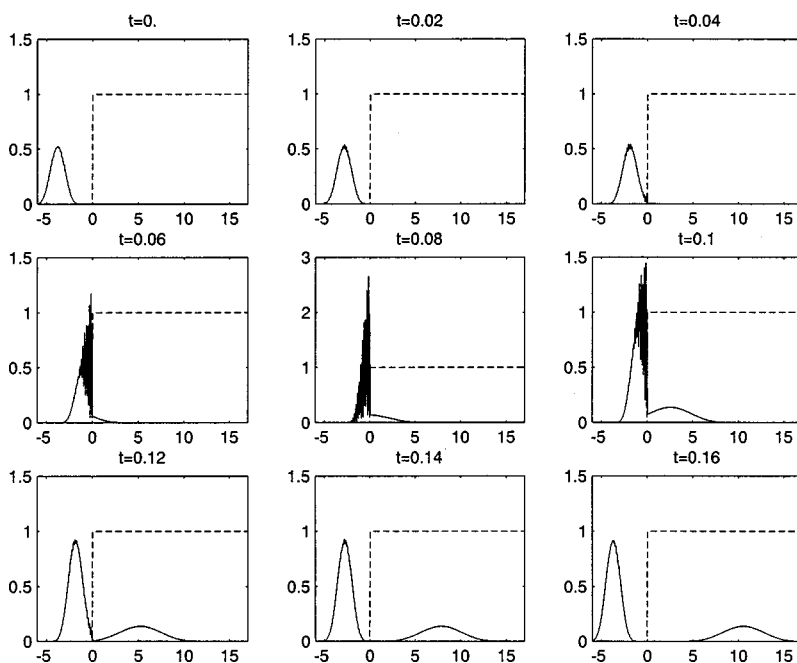


Fig. 4. Numerical simulation of the motion of a Dirac wave packet by taking into account the hole theory. At $x=0$, the initial wave packet stimulates the “charged vacuum” and electrons are ejected from it. Their holes are left in the negative-energy continuum, being interpreted as positrons. After scattering by the potential barrier, the wave packet becomes larger than the initial one and another wave packet appears representing positrons moving to the right. The total electric charge is conserved throughout the figures.

ing wave packet in region I. How can we then obtain a physically allowed motion with one wave packet at $t=0$?

One possible way is to take $\bar{p}' = -\bar{p} < 0$ as the momentum in region II instead of the positive value (7).^{1,3} Let us denote the wave function given by the substitution $\bar{p} \rightarrow -\bar{p}$ as $\phi'_E(x)$. It should be noted that $\phi'_E(x)$ also satisfies the Dirac equation of (1).

A typical motion of the wave packet using (12) with substitution of $\phi'_E(x)$ is given in Fig. 3. In this case we have only one incoming wave packet at $t=0$. Though the momentum is negative, the transmitted wave packet in region II moves to the right. This is because the group velocity in region II is now positive, $v'_g = c^2|p|/(V_0 - E) > 0$ [cf. (14)]. The probability distribution is conserved in this case. For example, $P_I(0) = 1.00$ while $P_I(0.16) = 0.43$ and $P_{II}(0.16) = 0.57$.

Unfortunately, again the motion in Fig. 3 is not physically allowed because this solution assumes that the negative-energy states in region II are empty. As is well known in the hole theory, the negative-energy continuum must be filled by electrons; otherwise no ground state would be stable due to the radiation catastrophe.³

An alternative way to obtain a more realistic motion of a wave packet in region II consists in the use of the hole theory. As explained in Sec. II, the Klein paradox is now considered as the simplest case of the decay of charged vacuum. From this point of view, the reflected wave packet in Fig. 2 is interpreted as the superposition of the wave representing the totally reflected incoming electrons and that of electrons ejected from the fully occupied negative-energy continuum. According to the hole theory, the ejected electrons leave their holes in the negative-energy continuum. The probability density for holes, $\tilde{\rho}_{II}(x, t)$, should have a specular-reflected distribution of ejected electrons (see Appendix B). We may form such a wave packet for holes as the superposition of the charge-conjugate state to $\varphi_{II}(x)$:

$$\tilde{\varphi}_{II}(x) = A T v e^{-i\bar{p}x/\hbar}, \quad (17)$$

with

$$\bar{v} = \begin{pmatrix} b \\ 1 \end{pmatrix}, \quad (18)$$

which may be considered as the wave function for positrons (cf. Appendix C). Using $\tilde{\varphi}_{II}(x)$, we obtain

$$\tilde{\Psi}_{II}(x, t) = \int_D dE G(p) \tilde{\varphi}_{II}(x) e^{-iEt/\hbar}. \quad (19)$$

In Fig. 4 we show a numerical simulation using (19) for $x > 0$. Again, we have initially only the incoming wave packet. When the wave packet collides with the potential barrier, a new packet appears in region II. This represents *positrons* created at the boundary due to the decay of the charged vacuum.⁴ The reflected wave packet is greater than the incoming one because it includes the contribution of electrons created at the supercritical potential barrier.

In this case we have the conservation of the total charge instead of the total probability. Denoting the total charge for each region as $Q_I(t) = -eP_I(t)$ and $Q_{II}(t) = +e\tilde{P}_{II}(t)$, where $\tilde{P}_{II}(t)$ represents (16) substituted by (19), we obtain (see Appendix B)

$$\frac{d}{dt} [Q_I(t) + Q_{II}(t)] = 0, \quad (20)$$

which represents the charge conservation. We may observe this numerically in Fig. 4: $Q_I(0) = -1.00e$, and, for example, $Q_I(0.1) = -1.66e$ and $Q_{II}(0.1) = 0.66e$ so we have $Q_I(0.08) + Q_{II}(0.08) = -1.00e$.

IV. CONCLUDING REMARKS

In this paper, we have presented the motion of a Dirac wave packet under the conditions of the Klein paradox. To obtain the motion that has a consistent interpretation, we have followed the hole theory for constructing the wave packet in region II. By this procedure, we obtain a motion representing pair creation due to the decay of the vacuum in a supercritical potential. In this case, of course, the probability density is not conserved. The wave packet in Fig. 4 should be regarded as representing the charge density distribution. The total charge is conserved even in the case of the supercritical potential, as is expected.

Finally, it is worthwhile to mention that by using our present method, it is easy to perform simulations for the normal scattering under the condition 1 or 2 classified in Sec. II, if one does not care very much about the detailed shape of the initial wave packet.

APPENDIX A: DERIVATION OF 1+1-DIMENSIONAL DIRAC EQUATION

As clearly pointed out by Glass and Mendlowitz,⁶ spin-flip occurs only when there is more than one dimension in space. Repeating the discussion of deriving the Dirac equation² for the case of one spatial dimension, one easily finds that the Dirac matrices α and β are reduced to 2×2 matrices that can be represented by the Pauli matrices. This fact simply implies that if there is only one spatial dimension, there is no spin. It should be instructive to show explicitly how to derive the 1+1-dimensional Dirac equation.

As discussed in textbooks,^{2,3} a wave equation that satisfies relativistic covariance in space-time as well as the probabilistic interpretation should have the form

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \left[c\alpha \left(-i\hbar \frac{\partial}{\partial x} \right) + \beta m_0 c^2 \right] \Psi(x, t). \quad (21)$$

To obtain the relativistic energy-momentum relation $E^2 = (pc)^2 + (m_0 c^2)^2$, we postulate that (21) coincides with the Klein-Gordon equation

$$\left[\frac{\partial^2}{(\partial ct)^2} - \frac{\partial^2}{\partial x^2} + \left(\frac{m_0 c}{\hbar} \right)^2 \right] \Psi(x, t) = 0. \quad (22)$$

By comparing (21) and (22) it is easily seen that α and β must satisfy

$$\alpha^2 = \beta^2 = 1, \quad \alpha\beta + \beta\alpha = 0. \quad (23)$$

Any two of the Pauli matrices can satisfy these relations. Therefore, we may choose $\alpha = \sigma_x$ and $\beta = \sigma_z$. Then we obtain

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \left[c\sigma_x \left(-i\hbar \frac{\partial}{\partial x} \right) + \sigma_z m_0 c^2 \right] \Psi(x, t), \quad (24)$$

where $\Psi(x, t)$ is a 2-component spinor

$$\Psi(x,t) = \begin{pmatrix} \phi_+(x,t) \\ \phi_-(x,t) \end{pmatrix}, \quad (25)$$

and $\phi_{\pm}(x,t)$ satisfy

$$i\hbar \frac{\partial}{\partial t} \phi_{\pm}(x,t) = c\sigma_x \left(-i\hbar \frac{\partial}{\partial x} \right) \phi_{\mp}(x,t) \pm \sigma_z m_0 c^2 \phi_{\pm}(x,t). \quad (26)$$

In the presence of the scalar potential $V(x)$, the 1+1-dimensional Dirac equation is extended to the form

$$\begin{aligned} \left[i\hbar \frac{\partial}{\partial t} - V(x) \right] \Psi(x,t) \\ = \left[c\sigma_x \left(-i\hbar \frac{\partial}{\partial x} \right) + \sigma_z m_0 c^2 \right] \Psi(x,t). \end{aligned} \quad (27)$$

If we consider the stationary states, (27) reduces to (1) in Sec. II.

The use of the 2-component spinor for the 1+1-dimensional Dirac equation makes calculations much simpler. This simplification is only possible for the 1+1-dimensional case because there is no degree of freedom for rotation. For the case of 2 or 3 dimensions, we have to use the Dirac equation with ordinary 4×4 Dirac matrices and 4-component spinors because there appears the spin degree of freedom.

APPENDIX B: WAVE PACKET FOR HOLES AND CHARGE CONSERVATION

We define the solution of the negative energy continuum (region II) as $\Psi_{\text{II}}(x,t)$:

$$\Psi_{\text{II}}(x,t) = \int_D dE G(p) \varphi_{\text{II}}(x) e^{-iEt/\hbar}. \quad (28)$$

Let us suppose that $\Psi_{\text{II}}(x,t)$ goes into region I as though there were no potential barrier. Then the left-moving wave packet in region II, such as shown in Fig. 2, would continue to move into region I with the same group velocity. The distribution of electrons $\rho_{\text{II}}(x,t)$ represented by this fictitious wave packet must be in mirror symmetric to that of their holes. Therefore, we assume

$$\tilde{\rho}_{\text{II}}(x,t) = \rho_{\text{II}}(-x,t) \quad (29)$$

for $x > 0$, where $\tilde{\rho}_{\text{II}}(x,t)$ represents the distribution of the holes. Indeed, the wave function (19) formed by the positron waves of $\tilde{\varphi}_{\text{II}}(x)$ gives

$$\tilde{\rho}_{\text{II}}(x,t) = \tilde{\Psi}_{\text{II}}^{\dagger}(x,t) \tilde{\Psi}_{\text{II}}(x,t), \quad (30)$$

which coincides with (29).

We may also introduce the current for $\tilde{\Psi}_{\text{II}}(x,t)$ by

$$\tilde{j}_{\text{II}}(x,t) = c \tilde{\Psi}_{\text{II}}^{\dagger}(x,t) \sigma_x \tilde{\Psi}_{\text{II}}(x,t) \quad (31)$$

and that for $\Psi_{\text{II}}(x,t)$ by $j_{\text{II}}(x,t)$. We find

$$\tilde{j}_{\text{II}}(0,t) = j_{\text{II}}(0,t). \quad (32)$$

By straightforward calculations we have the “continuity equation” for holes,

$$\frac{\partial \tilde{\rho}_{\text{II}}(x,t)}{\partial(-t)} + \frac{\partial \tilde{j}_{\text{II}}(x,t)}{\partial x} = 0. \quad (33)$$

It should be noted that (33) implies that the direction of time for positrons in region II is opposite to region I. Using (32) and (33), we have

$$\begin{aligned} \frac{d\tilde{P}_{\text{II}}(t)}{dt} &= \int_0^{\infty} dx \frac{\partial \tilde{\rho}_{\text{II}}(x,t)}{\partial t} \\ &= \int_0^{\infty} dx \frac{\partial \tilde{j}_{\text{II}}(x,t)}{\partial x} \\ &= [\tilde{j}_{\text{II}}(\infty,t) - \tilde{j}_{\text{II}}(0,t)] = -j_{\text{II}}(0,t). \end{aligned} \quad (34)$$

On the other hand, we have

$$\frac{dP_{\text{I}}(t)}{dt} = -j_{\text{I}}(0,t). \quad (35)$$

Since $j_{\text{I}}(0,t) = j_{\text{II}}(0,t)$ holds as the boundary condition, we obtain

$$\frac{dP_{\text{I}}(t)}{dt} - \frac{d\tilde{P}_{\text{I}}(t)}{dt} = 0, \quad (36)$$

which corresponds to the charge conservation (20).

APPENDIX C: CHARGE CONJUGATION

Using the 1+1-dimensional Dirac equation, we may discuss many fundamental properties, such as symmetry, etc., of the Dirac equation in a way that is much easier than the approaches generally given in textbooks.^{2,3} For example, here we discuss charge conjugation in connection with Sec. III. If the potential $V(x)$ in the Dirac equation (27) represents the scalar potential for electrons, the Dirac equation for positrons is given by replacing $V(x)$ by $-V(x)$:

$$\begin{aligned} \left[i\hbar \frac{\partial}{\partial t} + V(x) \right] \Psi_{\text{C}}(x,t) \\ = \left[c\sigma_x \left(-i\hbar \frac{\partial}{\partial x} \right) + \sigma_z m_0 c^2 \right] \Psi_{\text{C}}(x,t). \end{aligned} \quad (37)$$

Let us try to find the operator $\hat{C}$ defined by

$$\Psi_{\text{C}}(x,t) = \hat{C} \Psi(x,t). \quad (38)$$

Taking into account the sign of the potential and the energy operator, we may assume that

$$\hat{C} \Psi(x,t) = \mathbf{C} \Psi^*(x,t), \quad (39)$$

where $\mathbf{C}$ is a 2×2 matrix. Multiplying the complex conjugate of (27) from the left by $\mathbf{C}$ and then comparing it with (37), we get the relations

$$\mathbf{C} \sigma_x \mathbf{C}^{-1} = \sigma_x, \quad (40)$$

$$-\mathbf{C} \sigma_z \mathbf{C}^{-1} = \sigma_z. \quad (41)$$

Therefore, we obtain

$$\mathbf{C} = \sigma_x. \quad (42)$$

By making use of the charge conjugation operator, we obtain

$$\tilde{\varphi}_{\text{II}}(x) = \hat{C} \varphi_{\text{II}}(x) = \sigma_x [A T u e^{-i \bar{p} x / \hbar}]^*, \quad (43)$$

which reduces to (17).

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THE THREAT OF THE FIRST CLASS

A worthwhile university or college is quite simply one in which the student is brought into personal contact with, is made vulnerable to, the aura and the threat of the first class. In the most direct sense, this is a matter of proximity, of sight and hearing. The institution, particularly in the humanities, should not be too large. The scholar, the significant teacher ought to be readily visible. We cross his or her daily path. The consequence, as in the Periclean *polis*, in medieval Bologna or 19th-century Tübingen, is one of implosive and cumulative contamination. The whole is energized beyond its eminent parts. By unforced contiguity, the student, the young researcher, will (or should be) infected. He will catch the scent of the real thing. I resort to sensory terms because the impact can be physical. Thinkers, the erudite, mathematicians or theoretical and natural scientists, are beings possessed. They are in the grip of a mastering unreason.

George Steiner, "An Academic Comes of Age in 'the Sleepless City'," *The Chronicle of Higher Education*, 6 February 1998.