Feshbach P-Q partitioning technique and the two-component Dirac equation

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We provide an alternative approach to relativistic dynamics based on the Feshbach projection technique. Instead of directly studying the Dirac equation, we derive a two-component equation for the upper spinor. This approach allows one to investigate the underlying physics in a different perspective. For particles with small mass such as the neutrino, the leading-order equation has a *Hermitian* effective Hamiltonian, implying there is no leakage between the upper and lower spinors. In the weak relativistic regime, the leading order corresponds to a non-Hermitian correction to the Pauli equation, which takes into account the nonzero possibility of finding the lower-spinor state and offers a more precise description.

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I. INTRODUCTION

The Dirac equation [1] offers a quantum-mechanical description of the relativistic dynamics of any spin-$1/2$ particles, and is the first theory that merges these two most important discoveries of modern physics. This elegant equation successfully predicts the existence of the antimatter [2] and offers a theoretical justification for the introduction of electron spin and spin-orbit coupling [3] and the fine-structure of the hydrogenlike atoms [3]. The Dirac equation also predicts a quivering motion of free relativistic quantum particles called Zitterbewegung [4–6], which is attributed to the interference between the positive and negative energy part of the spinor.

Recently, experimental advances allows for the implementation of various proposals to study the relativistic quantum-mechanics phenomena using ion traps [7] as quantum simulators for the Dirac equation, and Zitterbewegung [7,8] as well as the Klein paradox [9,10] have been experimentally observed. While formally simple and elegant, the Dirac equation has some peculiar properties. For example, one needs to change the idea of bare vacuum to an infinite negative energy sea to interpret the negative energy solution for the Dirac equation, which may be quite a hurdle for many. It also employs four components for a relativistic spin-$1/2$ particle, a big departure from the two-component description people are familiar with in the nonrelativistic regime. It has been hitherto unclear what a two-component description of the relativistic dynamics would look like or if it is even possible. In this paper, we ask: can we give a reasonable two-component description for the relativistic dynamics? Indeed, it is often more easy to glean information from the Dirac equation for two-component spinors under some special regime. One interesting regime is for particles with small mass such as neutrinos. Neutrino mass has been experimentally found to be extremely small and theoretically assumed to be zero [11]. There had been various attempts at reducing the four-component spinors of the Dirac equation to arrive at two- and one-component descriptions using various techniques [4,12–17]. Realistically, it is of great importance to study the different-order contribution of nonzero neutrino mass on the relativistic dynamics of the particle in an electromagnetic field, which has been missing in the literature. On the other hand, the Pauli equation is obtained by a heavily approximated lower spinor in the nonrelativistic limit. The Pauli equation provides a good approximation for the gyromagnetic ratio as well as an explanation for the Stern-Gerlach experiment [1,3]. However, for a spin-$1/2$ initially prepared in a state with no lower-spinor component, the effective Hamiltonian in the Pauli equation is Hermitian and produces a unitary evolution for the upper spinor. Therefore, the Pauli equation predicts that there will be no possibility of finding the lower spinor, in contradiction to the prediction of the Dirac equation. High-order correction to the Pauli equation has also been done using the Foldy-Wouthuysen (F-W) transform [16], which eliminates the odd terms from the Hamiltonian through a series of canonical transforms. It is noteworthy that the F-W transform acts as a series of unitary transformation, effectively changing the set of basis and getting a two-component equation in this "dressed basis." Here, we take a different approach and provide an alternative approach to give a non-Hermitian effective Hamiltonian for the upper spinor component in the original, i.e., "bare" basis. By using the Feshbach P-Q partition technique [18–20] for the Dirac equation, we obtain a two-component spinor equation, which may further be cast into a time-convolutionless (TCL) form. Especially, two regimes are investigated, one with small particle mass and the other with weak relativistic effects. It is found that the leading-order equation for the small mass case takes a very compact form and has a Hermitian effective Hamiltonian. In the weak relativistic limit, the leading-order equation gives a non-Hermitian correction to the Pauli equation, and therefore more accurately predicts the nonzero possibility of finding the lower-spinor state for an initial state with no lower-spinor component and offering a much more precise perspective.

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II. FESHBACH *P*-*Q* PARTITION FOR THE TCL DIRAC EQUATION

The Dirac equation merges quantum mechanics with special relativity and has predicted many interesting phenomena, such as spin-orbit coupling. Taking $\hbar = 1$ and assuming minimal coupling for the electromagnetic field, we have

$$i\partial_t \Psi = (\beta mc^2 + e\varphi + c\boldsymbol{\alpha}\cdot\boldsymbol{\pi})\Psi, \tag{1}$$

where e is the charge carried by the particle, $\boldsymbol{\pi} = \boldsymbol{p} - e\boldsymbol{A}/c$ and $(\varphi,\boldsymbol{A})$ is the vector four-potential for the electromagnetic field. A widely used procedure is to partition the state into upper and lower halves, corresponding to normal particle and lower-spinor solutions with positive energies. It can be very illustrative to study the equation of motion for the upper component. For example, in the nonrelativistic approximation, the upper spinor dominates and follows the Pauli equation. Since the effective Hamiltonian of the Pauli equation is Hermitian, the upper spinor evolves unitarily. As a result, this approximation ignores the small but nonzero possibility of finding the negative energy part, i.e., a lower-spinor state. Here we want to derive a time-convolutionless equation for the upper spinor by using a systematic projection technique.

To do that, we first use a Feshbach P-Q partition technique [18–20]. Define the projectors

$$\mathcal{P} \equiv \left(\begin{array}{c|c} \mathbb{1} & \mathbb{0} \\ \hline \mathbb{0} & \mathbb{0} \end{array}\right), \quad \mathcal{Q} \equiv \mathcal{I} - \mathcal{P} = \left(\begin{array}{c|c} \mathbb{0} & \mathbb{0} \\ \hline \mathbb{0} & \mathbb{1} \end{array}\right), \tag{2}$$

where $\mathbb{0}$ and $\mathbb{1}$ are both 2×2 matrices. The wave function $\Psi = [\Psi_1,\Psi_2,\Psi_3,\Psi_4]^T$ can be partitioned as $\mathcal{P}\Psi = [\Psi_1,\Psi_2,0,0]$ and $\mathcal{Q}\Psi = [0,0,\Psi_3,\Psi_4]^T$, where T stands for matrix transpose. Accordingly, the Hamiltonian can be partitioned into four 2-by-2 matrices as

$$H = \left(\begin{array}{c|c} \tilde{h} & \tilde{R} \\ \hline \tilde{W} & \tilde{D} \end{array}\right), \tag{3}$$

where $\tilde{h},\tilde{R},\tilde{W},\tilde{D}$ are nonzero matrix blocks corresponding to $h = \mathcal{P}H\mathcal{P}$, $R = \mathcal{P}H\mathcal{Q}$, $W = \mathcal{Q}H\mathcal{P}$, and $D = \mathcal{Q}H\mathcal{Q}$. The exact integral-differential equation for the upper spinor is then given by

$$\begin{aligned} i\partial_t\mathcal{P}|\psi(t)\rangle &= e\varphi\mathcal{P}|\psi(t)\rangle - ic^2\int_0^t ds\{\phi(t-s)\boldsymbol{\sigma}\cdot \\ &\quad\times[-eA/c - e(t-s)\nabla\varphi]\}\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\mathcal{P}|\psi(s)\rangle \\ &\quad - ic^2\int_0^t ds\phi(t-s)[\boldsymbol{\pi}^2 - e\boldsymbol{\sigma}\cdot\boldsymbol{B}/c]\mathcal{P}|\psi(s)\rangle, \end{aligned} \tag{4}$$

where $\phi(t-s) = \exp[i(2mc^2 - e\varphi)(t-s)]$. Depending on the problem under consideration, we take the dominant part of the Hamiltonian as H_0 and work in the interaction picture with respect to it, i.e., $i\dot{\psi} = H_I(t)\psi$, where $H_I(t) = U_0^\dagger(t)(H - H_0)U_0(t), \psi = U_0^\dagger(t)\Psi$, and $U_0(t)$ is the propagator associated with H_0. Applying the P-Q partition, and assuming we start with a particle state, we can formally solve for $\mathcal{Q}\psi(t)$ and get

$$\partial_t\mathcal{P}\psi(t) = -i\mathcal{P}H_I(t)\mathcal{P}\psi(t) - \int_0^t ds\mathcal{C}(t,s)\mathcal{P}\psi(s), \tag{5}$$

where $\mathcal{C}(t,s) = \mathcal{P}H_I(t)v(t,s)\mathcal{Q}H_I(s)$ is the memory kernel, $v(t,s) = \widehat{T}\{\exp[-i\int_s^t \mathcal{Q}H_I(\tau)d\tau]\}$, and $\widehat{T}$ is the time-ordering operator. This is the exact Nakajima-Zwanzig equation for the state vector $\mathcal{P}\psi$.

We now cast the equation into a time-convolutionless form by using a time local projection [21]. Writing the formal solution for $\mathcal{Q}\psi(t)$ as

$$[1 - \Sigma(t)]\mathcal{Q}\psi(t) = \Sigma(t)\mathcal{P}\psi(t),$$

where

$$\Sigma(t) = -i\int_0^t ds v(t,s)\mathcal{Q}H_I(s)\mathcal{P}u^\dagger(t,s)$$

and $u(t,s) = \hat{T}\exp[-i\int_s^t d\tau H_I(\tau)]$, we get

$$\partial_t\mathcal{P}\psi(t) = \mathcal{K}(t)\mathcal{P}\psi(t), \tag{6}$$

where $\mathcal{K} = -i\{\mathcal{P}H_I(t)\mathcal{P} + \mathcal{P}H_I(t)[1-\Sigma(t)]^{-1}\Sigma(t)\mathcal{P}\}$ is the TCL generator. The invertibility of the operator $1 - \Sigma(t)$ is ensured due to the fact that it is a perturbation of the identity operator since $\lim_{H_I\to 0}\Sigma(t) = 0$. We can now expand $[1-\Sigma(t)]^{-1}\Sigma(t) = \sum_{k=1}\Sigma^k(t)$, up to any order of H_I.

As a first application, we consider a particle with very small mass in a static field, such as the neutrino particle. In this case, $H_0 = e\varphi + c\boldsymbol{\alpha}\cdot\boldsymbol{\pi}$, and $H_I(t) = mh_I(t)$, where $h_I(t)$ is mass independent. At the leading order of mass m, we have

$$\partial_t\mathcal{P}\psi(t) = -im\mathcal{P}h_I(t)\mathcal{P}\psi(t),$$

which, remarkably, has a *Hermitian* effective Hamiltonian, generating a unitary propagator. Therefore, for a state initially prepared in the $\mathcal{P}$ space, i.e., $\mathcal{Q}\psi(0) = 0$, it will stay in the $\mathcal{P}$ space up to the first order. Especially, in absence of external field, we explicitly have $\partial_t\mathcal{P}\psi(t) = -2imc^2\cos^2(c|\boldsymbol{p}|t)\mathcal{P}\psi(t)$ as a first-order approximate equation, where $|\boldsymbol{p}|$ denotes the norm of the momentum $\boldsymbol{p}$. The equation has a plane-wave solution,

$$\int dpc_p(0)e^{ipx - imc^2t[1+\mathrm{sinc}(2cpt)]},$$

where $c_p(0)$ is the initial condition. Up to $O(m^2)$, this is in agreement with the plane-wave solution obtained by directly solving the Dirac equation.

On the other hand, in the weak relativistic regime, we have a dominant diagonal Hamiltonian which we take as H_0. In this case, we have $H_0 = \mathcal{P}H\mathcal{P} + \mathcal{Q}H\mathcal{Q} = h + D$ and $H_c = \mathcal{P}H\mathcal{Q} + \mathcal{Q}H\mathcal{P} = R + W$, where h, R, W, D correspond to the blocks in Eq. (3). Here $H_0 \gg H_c$, so H_c can be treated as a correction. In the interaction picture with respect to H_c, we have $H_I(t) = U_0^\dagger(t)H_cU_0(t)$, $|\varphi(t)\rangle = U_0^\dagger(t)|\psi(t)\rangle$, $U_0 = \widehat{T}\exp[-i\int ds H_0(s)] = g_h \oplus g_D$, where g_h and g_D are the propagators associated with the h and D blocks, respectively. Notice here H_c and therefore H_I has no diagonal elements. The lowest order of $\Sigma(t)$ is on the order of H_I with $\Sigma(t) = -i\int ds\mathcal{Q}H_I(s)\mathcal{P}$, and the lowest-order $P|\varphi\rangle$ equation is on the order of H_I^2 and

$$\begin{aligned} \partial_t\mathcal{P}|\varphi\rangle &= -i\mathcal{P}H_I(t)\mathcal{P}|\varphi\rangle - i\mathcal{P}H_I(t)\sum_{k=1}\Sigma^k(t)\mathcal{P}|\varphi\rangle \\ &\approx -i\mathcal{P}H_I(t)\Sigma(t)\mathcal{P}|\varphi\rangle \\ &= -\int ds[\mathcal{P}H_I(t)\mathcal{Q}][\mathcal{Q}H_I(s)\mathcal{P}]\mathcal{P}|\varphi\rangle. \end{aligned}$$

It can be readily shown that $[\mathcal{P}H_I(t)\mathcal{Q}][\mathcal{Q}H_I(s)\mathcal{P}] = \mathcal{P}H_I(t)H_I(s)\mathcal{P}$. Therefore, at the leading order, we have $\partial_t\mathcal{P}\psi(t) = -[\int_0^t ds\mathcal{P}H_I(t)H_I(s)\mathcal{P}]\mathcal{P}\psi(t)$. Going back to the original picture and rotating out a trivial global phase $\exp[-imc^2t]$ for the whole Hamiltonian, we have

$$\partial_t\mathcal{P}\Psi(t) = \left[-ie\varphi - c^2\int_0^t ds(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\exp[-ie\varphi(t-s)](\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\exp[ie\varphi(t-s)]\exp[2imc^2(t-s)]\right]\mathcal{P}\Psi(t). \tag{7}$$

Using $[\boldsymbol{A},\varphi]=0$, $[\boldsymbol{p},f(\boldsymbol{q})] = -i\nabla f(\boldsymbol{q})$, and the BCH formula $\exp[A]B\exp[-A] = B + \sum_{m=1}^{\infty}[_mA,B]/m!$, where $[_mA,B] = [A,[_{m-1}A,B]]$ and $[_1A,B] = [A,B]$, we can simplify the equation and arrive at

$$\begin{aligned}\partial_t\mathcal{P}\Psi(t) = &-i\left[e\varphi + \left(\frac{\boldsymbol{\pi}^2}{2m} - \frac{e\boldsymbol{\sigma}\cdot\boldsymbol{B}}{2mc}\right)[1-\exp(2imc^2t)]\right]\mathcal{P}\Psi(t)\\ &-i\left[\frac{e}{4m^2c^2}[(\nabla\cdot\nabla\varphi) + i(\nabla\varphi)\cdot\boldsymbol{\pi} + \boldsymbol{\sigma}\cdot(\nabla\varphi)\times\boldsymbol{\pi}][1-\exp(2imc^2t)(1-2imc^2t)]\right]\mathcal{P}\Psi(t).\end{aligned} \tag{8}$$

We recognize the first line of the Eq. (8) as a non-Hermitian correction to the Pauli equation with an effective Hamiltonian $H_{\text{eff}} = e\varphi + \boldsymbol{\pi}^2/2m - e\boldsymbol{\sigma}\cdot\boldsymbol{B}/2mc$ since the long-time average of $\exp(2imc^2t) = 0$. The second line is of order $e/4m^2c^2$ and is therefore a higher-order correction. The effective Hamiltonian TCL equation is no longer Hermitian, and tracks the nonzero possibility of finding the lower-spinor state up to the leading order. A higher-order equation can be obtained in the same fashion by including the higher order of $\Sigma^k(t)$.

III. EXAMPLES

As an illustrative example, we first consider a free relativistic particle, under zero electromagnetic field. The Dirac equation [Eq. (1)] and the TCL equation [Eq. (8)] are analytically solvable as planar waves. We choose a Gaussian wave packet for the upper spinor as $f(x) = \sqrt[4]{2/x_0\pi}\exp[-x^2/x_0 + ip_0x]$, corresponding to a Gaussian wave packet centered around p_0 in the momentum space. The lower spinor is initially set to zero. Therefore, any nonzero $\mathcal{Q}\Psi(\boldsymbol{q},t)$ means a nonzero probability of finding the lower spinor at position $\boldsymbol{q}$, which is ignored by the Pauli equation. We can use $1 - \int d\boldsymbol{q}\mathcal{P}\Psi(\boldsymbol{q},t)$ to quantify the total possibility of finding the lower spinor at all positions at time t, but a more intricate formula including the positional dependence can be used. To get that, we use the corresponding $\mathcal{Q}$ part of Eq. (8), $\mathcal{Q}\psi(t) \approx -i[\int ds\mathcal{Q}H_I(s)\mathcal{P}]\mathcal{P}\psi(t)$. Going back to the original picture, we have

$$\begin{aligned}\mathcal{Q}\Psi(t) = &-i\{(2imc^2\boldsymbol{\sigma}\cdot\boldsymbol{\pi} - e\boldsymbol{\sigma}\cdot\nabla\varphi)(1-\exp[2imc^2t])\\ &-2imc^2t\exp[2imc^2t]e\boldsymbol{\sigma}\cdot\nabla\varphi\}\mathcal{P}\Psi(t)/(4m^2c^3).\end{aligned} \tag{9}$$

We can study the one-dimensional (1D) equation without loss of generality. In this case, the upper and lower spinor can be described by one component each, and the eigenvector of the Dirac Hamiltonian is

$$U_+ = \sqrt{\frac{\lambda+mc^2}{2\lambda}}\begin{pmatrix}1\\ pc/(\lambda+mc^2)\end{pmatrix},$$

$$U_- = \sqrt{\frac{\lambda+mc^2}{2\lambda}}\begin{pmatrix}-pc/(\lambda+mc^2)\\ 1\end{pmatrix},$$

with eigenvalues $\pm\lambda$, where $\lambda = \sqrt{p^2c^2+m^2c^4}$. The solution of the TCL equation is given by

$$\mathcal{P}\Psi = \int dp\exp[ipx]c_p(0)\times\exp\left[\frac{p^2}{4m^2c^2}[\exp(2imc^2t) - 2imc^2t - 1]\right],$$

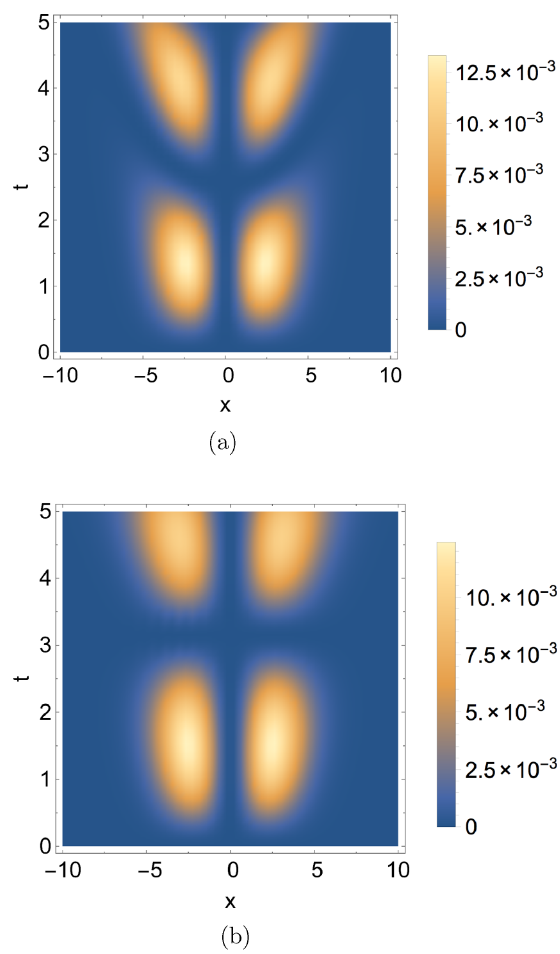

FIG. 1. Density plot for the possibility of finding lower-spinor state as a function of position x and time t with no electromagnetic field, $m=c=1$, $x_0=10$, and $p_0=0$. Panel (a) is obtained from the Dirac equation and panel (b) is obtained from the TCL equations, Eqs. (8) and (9). A good agreement between the two can be observed.

where $c_p(0)$ is determined by a Fourier transform of the initial state in the position space.

In Fig. 1 we plot $|\mathcal{Q}\Psi(x,t)|^2$ as a function of position x and time t using the exact solution via the Dirac equation in panel (a) and via the TCL equation in panel (b), choosing $m = c = 1$, $x_0 = 10$, and $p_0 = 0$. This initial state has an overlap $\int_{-\infty}^{\infty} |c_n(p)|^2 dp \approx 0.0209$ with the negative energy continuum, where $c_n(p) = \langle U_- | \psi_p(0)\rangle$ and $|\psi_p(0)\rangle$ is the initial state in momentum space obtained from a Fourier transform. It can be observed that the TCL equation can approximate the nonzero probability of finding the lower spinor predicted by the Dirac equation, a fact that is completely ignored in the Pauli equation. The slight difference between the upper and lower panels of Fig. 1 is due to the fact that only the leading term is calculated for the TCL equation, where higher orders should be vanishingly small in the weak relativistic regime. This TCL equation here is more accurate than the conventional Pauli equation, where the nonzero lower spinor component is ignored and gives zero probability of finding the lower spinor states, i.e., $|\Psi_3|^2 + |\Psi_4|^2 = 0$.

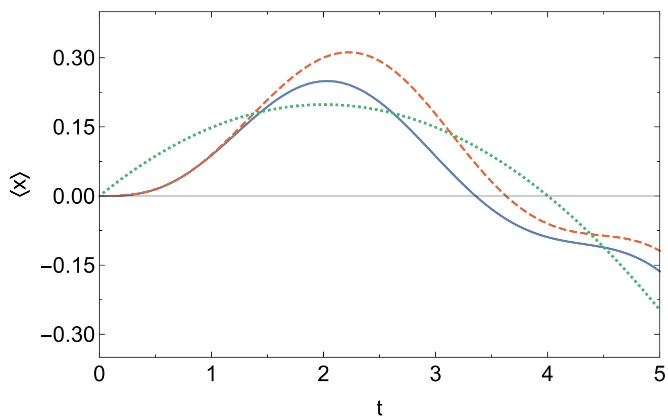

FIG. 3. The expectation value of the position $\langle x\rangle$ as a function of time, with the same parameters as those of Fig. 2. The solid blue line is obtained exactly through the Dirac equation, the dashed red line is obtained from the TCL equations, Eqs. (8) and (9), and the dotted green line is calculated through the conventional Pauli equation. It can be seen that the TCL equation as a weak-relativistic approximation more or less follows the exact dynamics, while the result from the Pauli equation is not very accurate.

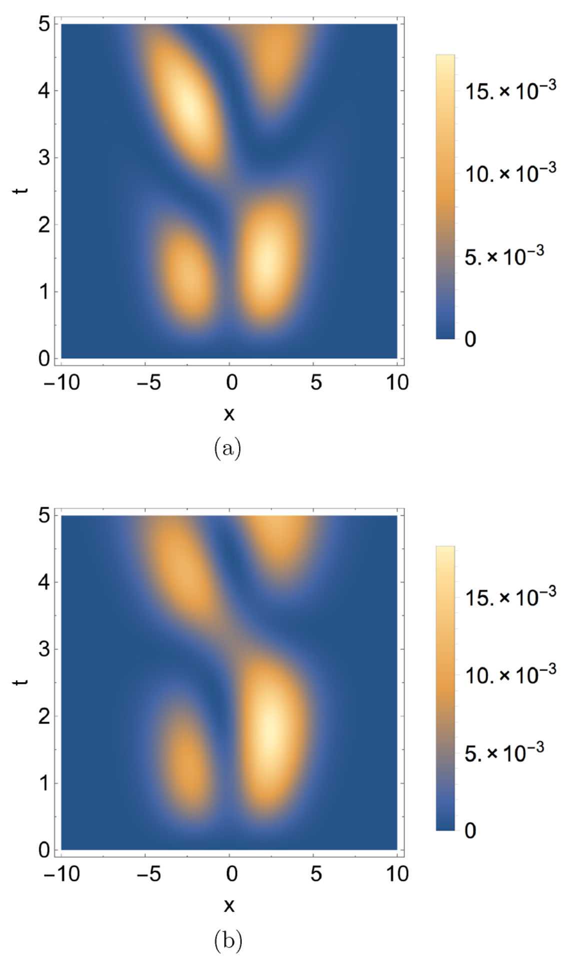

FIG. 2. Density plot for the possibility of finding lower-spinor state as a function of position x and time t with a static potential $e\varphi = ax$. Parameters used are $m = c = 1$, $a = 0.1$, $x_0 = 10$, and $p_0 = 0.2$. Panel (a) is obtained from the Dirac equation and panel (b) is obtained from the TCL equation, which is shown to offer a good approximation of the exact dynamics.

As a second example, we choose a linear static linear field $e\varphi = ax$ and numerically solve the exact equation and the TCL equation. Choosing $m = c = 1$, $a = 0.1$, $x_0 = 10$, and $p_0 = 0.2, |\mathcal{Q}\Psi(x,t)|^2$ as a function of position x and time t is shown in Fig. 2, where panel (a) is obtained using the exact Dirac equation and panel (b) is obtained via the TCL equations, where a good agreement between the two is also observed. Therefore, the TCL equation can give us a more precise two-component description for the relativistic particle than the Pauli equation. We also numerically calculate the expectation value of the particle's position as a function of time by means of exact solution, TCL solution and the conventional Pauli equation solution (see Fig. 3). The TCL equation as a weak-relativistic approximation matches the exact dynamics better than the Pauli equation where the nonzero lower spinor state is ignored.

IV. CONCLUSION

In conclusion, by using a Feshbach P-Q partition and a time-local projection with the Dirac equation, we obtain a two-component equation for the upper spinor, which can be further be cast into a TCL form. This alternative approach allows for a different perspective to study the relativistic dynamics for spin-1/2 particles. Both the small mass regime and the weak relativistic regimes are investigated. The leading-order equation in the small mass regime takes a compact form. Remarkably, the effective Hamiltonian for the upper spinor is Hermitian at the leading order, predicting that the particle will stay in the $\mathcal{P}$ space as a first-order approximation. For the weak relativistic regime, unlike the Pauli equation whose effective Hamiltonian for the upper spinor is Hermitian, the TCL equation obtained here is non-Hermitian and correctly takes into account the nonzero probability of finding the lower-spinor state.

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