Free-Dirac-particle evolution as a quantum random walk

A. J. Bracken,^{1,*} D. Ellinas,^{2,†} and I. Smyrnakis^{2,‡}

¹Centre for Mathematical Physics, Department of Mathematics, University of Queensland, Brisbane 4072, Australia

²Department of Sciences, Division of Mathematics, Technical University of Crete, GR 731 00, Chania, Crete, Greece (Received 22 May 2006; revised manuscript received 22 October 2006; published 21 February 2007)

Received 22 May 2000, revised manuscript received 22 October 2000, published 21 reordary 2007)

It is known that any positive-energy state of a free Dirac particle that is initially highly localized evolves in time by spreading at speeds close to the speed of light. As recently indicated by Strauch, this general phenomenon, and the resulting "two-horned" distributions of position probability along any axis through the point of initial localization, can be interpreted in terms of a quantum random walk, in which the roles of "coin" and "walker" are naturally associated with the spin and translational degrees of freedom in a discretized version of Dirac's equation. We investigate the relationship between these two evolutions analytically and show how the evolved probability density on the x axis for the Dirac particle at any time t can be obtained from the asymptotic form of the probability distribution for the position of a "quantum walker." The case of a highly localized initial state is discussed as an example.

DOI: 10.1103/PhysRevA.75.022322

PACS number(s): 03.67.-a, 03.65.Ta, 03.65.Pm

I. INTRODUCTION

The concept of a quantum random walk (QRW) has been widely discussed and extended in various directions [1] since its introduction [2-4] and development [5-13]. Much of the interest has derived from an expectation that such a mathematically attractive idea should have important applications in quantum information theory [14], analogous to known applications of classical random walks (CRW's) in classical information science.

On the other hand, CRW's also have many applications outside classical information theory, in a wide variety of areas of science where mathematical modeling is involved, so it should not be surprising if QRW's find applications outside quantum information theory. Here we describe such an application to the evolution of states described by the relativistic Dirac equation. This is closely related to recent work by Strauch [15], who relates that a connection between these two apparently quite different processes was already recognized in somewhat different terms by Feynman [16–19,3]. For another application of QRW's to relativistic quantum mechanics, see [20].

The evolution in time of the state of a free Dirac particle, starting from a highly localized, positive-energy state, is a quantum process that has only recently been described fully [21]. (For earlier related work see [22].) There has long been a widespread misapprehension that no relativistic particle with nonzero rest mass *m* can be localized much within its Compton wavelength $\lambda_c = \hbar/mc$, where *c* is the speed of light. However, it has been shown [23] that there is no such difficulty for the Dirac particle if localization is characterized in terms of the Dirac position operator **x**, by making $\Delta_x = \sqrt{\langle \mathbf{x}^2 \rangle - \langle \mathbf{x} \rangle^2}$ small while keeping the energy positive, and not by unrealistic attempts to restrict the wave function—for example, by requiring its domain to lie within a bounded

region in configuration space or by requiring it to have unphysical decay rates as $|\mathbf{x}| \rightarrow \infty$. Arbitrarily precise localization, with $\Delta_x \ll \lambda_C$, is indeed possible in the case of the free Dirac particle with positive energy. When the particle is localized in such an initial state, it has an associated uncertainty in energy $\Delta_E \gg mc^2$ and the subsequent evolution produces a probability density that spreads outwards in all directions at close to speed c. The graph of the evolving density along any axis through the center of initial localization (see Fig. 1 in [21]) shows a striking resemblance to the two-horned density found for a typical one-dimensional ORW [4]. For the Dirac particle, the horns are close to distance *ct* from the starting point. Our object here is to confirm by a more detailed analysis than those given previously [16,3,15] that this is not a coincidence and that the evolution of any positive-energy state of a free Dirac particle moving in one dimension can be modeled arbitrarily closely as a QRW of the type described in detail by Ambainis *et al.* [4], Konno [12,13], and others.

In addition to providing a somewhat surprising application of a QRW to a real process, this connection provides some insights as to the nature of the quantum walk itself. Until now the various proposed realization schemes for QRW's were typically based on the idea that the coin and walker degrees of freedom of the walk should be associated with two distinct quantum systems. These two systems were to be combined by means of some form of dynamical coupling-decoupling scheme. The present application shows that, alternatively, a single quantum mechanical object such as the free Dirac particle-by its very nature as a relativistic system with translational and spin degrees of freedom-can be identified in the course of its time evolution with a quantum random walk. This natural occurrence of a QRW, instead of some engineered realization, suggests that the question of its ontological status is still an interesting and open one.

The present work draws attention to two other important features of QRW's that have been emphasized by others [6,24]. The first is that a QRW—at least one that is free of classical noise [25]—is a unitary evolution; the associated randomness is of the kind associated with every unitary quantum evolution. In particular, a QRW is typically revers-

^{*}Electronic address: ajb@maths.uq.edu.au

[†]Electronic address: ellinas@science.tuc.gr

[‡]Electronic address: smyrnaki@tem.uoc.gr

ible in time, unlike a CRW. The second feature is that a QRW is typically a ballistic process, associated with spreading at a constant speed, unlike diffusive CRW's, where spreading is proportional to the square root of the time. These two features of a QRW are essential for the application that we describe below to the free-Dirac-particle evolution, which is a time-reversible process characterized by spreading near the speed of light.

In what follows, we relate the evolution of Dirac's equation to that of a QRW based on the canonical Heisenberg algebra extended by the Dirac matrices. (For other interesting connections of Dirac's equation with CRW's see [26,27].) Then we construct analytically and discuss the limiting probability distribution describing the translational spreading of an initial state. This provides an independent analytic derivation of the asymptotic behavior in time of an initially well-localized state of a free Dirac particle, which corroborates previous findings [22,23,15]. The work concludes with some speculations about the physical reality of the quantum walk of the Dirac particle and the possibility of detecting it experimentally.

II. QRW AND FREE DIRAC EVOLUTION

The free Dirac Hamiltonian operator for a particle with zero momentum along the y and z directions is

$$H(\hat{p}) = c\,\alpha\hat{p} + mc^2\beta, \quad \hat{p} = -i\,\hbar\,d/dx, \tag{1}$$

acting on four-component spinor wave functions $\Psi(x)$. Here we adopt a representation of the Dirac matrices with

$$\alpha = \sigma_3 \otimes \sigma_3, \quad \beta = \sigma_2 \otimes \mathbf{1}_2, \tag{2}$$

where σ_i , i=1,2,3, are the usual Pauli matrices and $\mathbf{1}_2$ is the 2×2 unit matrix. In this representation the helicity (spin) operator associated with rotations about the *x* axis is $\Sigma = \mathbf{1}_2 \otimes \sigma_3$. From this point onwards we adopt the natural units $\hbar = c = m = 1$. Recalling that only those solutions of Dirac's equation with positive energy describe physical states, we introduce the orthonormal positive-energy spinors in momentum space:

$$u_{\pm}(p) = \frac{1}{2\sqrt{E(p)[E(p)+1]}} \begin{pmatrix} 1+E(p) \pm p\\ i[1+E(p) \mp p] \end{pmatrix} \otimes e_{\pm}, \quad (3)$$

where $e_{+}=(1,0)^{T}$, $e_{-}=(0,1)^{T}$, and $E(p)=\sqrt{p^{2}+1}$. These spinors satisfy the relations

$$u_{\pm}(p)^{\mathsf{T}}u_{\pm}(p) = 1, \quad u_{\pm}(p)^{\mathsf{T}}u_{\mp}(p) = 0,$$
$$H(p)u_{\pm}(p) = E(p)u_{\pm}(p), \quad \Sigma u_{\pm}(p) = \pm \frac{1}{2}u_{\pm}(p). \tag{4}$$

Now we can write an arbitrary positive-energy wave function (with zero y and z components of momentum) $\Psi(x)$ in terms of two arbitrary functions $f_{\pm}(p)$ as

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ipx} \{ f_{+}(p)u_{+}(p) + f_{-}(p)u_{-}(p) \} dp.$$
 (5)

$$\int_{-\infty}^{\infty} \Psi(x)^{\dagger} \Psi(x) dx = 1 \Leftrightarrow \int_{-\infty}^{\infty} \{ |f_+(p)|^2 + |f_-(p)|^2 \} dp = 1.$$
(6)

Suppose now that we choose a normalized positiveenergy state with a definite helicity +1/2 and finite mean energy. Then

$$f_{+}(p) = f(p), \quad f_{-}(p) = 0, \quad \int_{-\infty}^{\infty} |f(p)|^2 dp = 1$$
 (7)

and

$$\langle H(\hat{p})\rangle = \int_{-\infty}^{\infty} E(p)|f(p)|^2 dp = E_0 < \infty .$$
(8)

With $f_{-}(p)=0$, the action of $H(\hat{p})$ in the second factor of the tensor product space in Eqs. (2) and (3) becomes trivial, as the second spinor remains constant at the value e_{+} . Thus the second factor space can be ignored, and we can consider $H(\hat{p})$ to have the *effective* form

$$H(\hat{p}) = \sigma_3 \hat{p} + \sigma_2 \tag{9}$$

acting in the first factor space. In this first space, we write

 $(1 \quad 0)^T = |+\rangle \quad (0 \quad 1)^T = |-\rangle,$ (10)

so that the positive-energy spinor $u_+(p)$ in Eq. (3) takes the (effective) form

$$u_{+}(p) = \frac{1}{2\sqrt{E(p)[E(p)+1]}} \times \{ [1+E(p)+p] | + \rangle + i [1+E(p)-p] | - \rangle \}.$$
(11)

Next we consider a fixed, small time interval $\Delta t \ll 1/E_0$. The (effective) unitary evolution operator for the Dirac particle can then be approximated over the time interval Δt using the relations

$$e^{-iH(\hat{p})\Delta t} = VU + O([E_0\Delta t]^2),$$
$$V = e^{-i\Delta t\sigma_3 \hat{p}}, \quad U = e^{-i\Delta t\sigma_2}.$$
(12)

Here we see the appearance of the evolution operator VU for a one-dimensional QRW [4], with V enacting a step of length Δt to the left or right along the x axis (the "walker space"), depending on the sign of σ_3 , and with the reshuffling matrix U representing the "quantum coin toss" after each time interval of duration Δt . For a longer time $t=n\Delta t$, we have from (12)

$$e^{-iH(\hat{p})t} = (VU)^n + O(E_0\Delta t),$$
(13)

and we see that the evolution of the state of the Dirac particle over any finite time t can be obtained arbitrarily accurately by replacing the exact evolution operator by $(VU)^n$ and letting $n \rightarrow \infty$ and $\Delta t \rightarrow 0$ with $n\Delta t=t$. In other words,

Then

FREE-DIRAC-PARTICLE EVOLUTION AS A QUANTUM...

$$\lim_{n \to \infty, \Delta t \to 0, n \Delta t = t} (e^{-i\Delta t\sigma_3 \hat{p}} e^{-i\Delta t\sigma_2})^n = e^{-iH(\hat{p})t},$$
(14)

and we can emulate the Dirac evolution by the evolution of a QRW. This relationship was established implicitly by Meyer [3], building upon observations by Feynman and Hibbs [16], and recently has been studied more explicitly by Strauch [15]. In what follows we investigate the relationship between these two processes analytically, making it more precise. We show how the evolved probability density on the *x* axis for the Dirac particle at any time *t* can be obtained from the asymptotic form of the QRW probability distribution for the "walker" [4,12,13].

It is important to note at this point that whereas the exact Dirac particle evolution operator $e^{-iH(\hat{p})t}$ obviously preserves the positive-energy condition imposed upon physically meaningful initial states, the same is not true of the approximate, QRW evolution $(VU)^n$. However, Eqs. (13) and (14) show that in the asymptotic limit described, the positive-energy condition is respected.

We close this section with the following remark. Rewriting the evolution operators as

$$V = |+\rangle \langle +|e^{-i\Delta t\hat{p}} + |-\rangle \langle -|e^{i\Delta t\hat{p}}, \quad U = e^{-i\Delta t\sigma_2}, \quad (15)$$

we identify the type of quantum walk involved here as a canonical algebra QRW in the classification of [28]. In contrast to the Euclidean QRW, which takes place on the integers and whose evolution operator is constructed from the generators of the Euclidean algebra [28–31], in the present case the generators of the canonical Heisenberg algebra—position and momentum operators—are used in the construction of a discrete walk on the *x*-coordinate axis. The close algebraic relationship between these two walks facilitates the solution of the time evolution in the present case, provided (as is done in next section) that we carefully discretize the coordinate-space (generalized) eigenfunctions which, unlike their Euclidean QRW counterparts, are not orthogonal.

III. ASYMPTOTIC SOLUTIONS AND LOCALIZATION

Let \mathcal{H} denote the Hilbert space spanned by all vectors $|\Phi\rangle \otimes |\pm\rangle$, corresponding in the coordinate representation to normalizable two-component wave functions $\Phi(x) |\pm\rangle$. Introduce a dense subspace $S < \mathcal{H}$ consisting of all finite linear combinations of suitably regular vectors $|\Phi\rangle \otimes |\pm\rangle \in \mathcal{H}$ —say, all those corresponding to $\Phi(x)=P(x)e^{-\alpha x^2}$, where P(x) is an arbitrary polynomial and α is some fixed positive constant. Then denote by S^* the space dual to S and, with the usual abuse of notation, consider \mathcal{H} as a subspace of S^* , so that we obtain the Gelf'and triple (or Rigged Hilbert space [32])

$$\mathcal{S} < \mathcal{H} < \mathcal{S}^*. \tag{16}$$

The space S^* contains in particular the vectors $|x'\rangle \otimes |\pm\rangle$, where $|x'\rangle$ is the generalized eigenvector of the Dirac *x*-coordinate operator \hat{q} ,

$$\hat{q}|x'\rangle = x'|x'\rangle,\tag{17}$$

corresponding in the coordinate representation to $\delta(x-x')$.

The introduction of the time interval Δt as in (12) in turn defines a length interval Δt on the x axis (recall that c=1 now) and a corresponding direct-integral decomposition

$$\mathcal{S}^* = \oplus \int_{-\Delta t/2}^{\Delta t/2} \mathcal{V}_{x_0} dx_0, \qquad (18)$$

where $\mathcal{V}_{x_0} < \mathcal{S}^*$ is spanned by all vectors of the form $|x_0+m\Delta t\rangle \otimes |\pm\rangle$, with $x_0 \in (-\Delta t/2, \Delta t/2]$ fixed and $m \in \mathbb{Z}$. We note at once that each \mathcal{V}_{x_0} is invariant under the action of the QRW evolution operator VU—i.e.,

$$VU\mathcal{V}_{x_0} < \mathcal{V}_{x_0},\tag{19}$$

because

$$V|x_0 + m\Delta t\rangle \otimes |\pm\rangle = |x_0 + (m \mp 1)\Delta t\rangle \otimes |\pm\rangle.$$
(20)

In order to describe the QRW evolution more fully, we now write the initial state with wave function as in Eqs. (5) and (7), as an entangled state of the walker and coin subsystems,

$$|\Psi\rangle\rangle = \int_{-\infty}^{\infty} \{c_{+}(x)|x\rangle \otimes |+\rangle + c_{-}(x)|x\rangle \otimes |-\rangle\}dx, \quad (21)$$

where

$$c_{+}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1 + E(p) + p}{2\sqrt{E(p)[E(p) + 1]}} f(p)e^{ipx}dp,$$
$$c_{-}(x) = \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1 + E(p) - p}{2\sqrt{E(p)[E(p) + 1]}} f(p)e^{ipx}dp.$$
(22)

Normalization of $|\Psi\rangle\rangle$ is satisfied because

$$\int_{-\infty}^{\infty} \{ |c_{+}(x)|^{2} + |c_{-}(x)|^{2} \} dx = 1,$$
(23)

as a consequence of Eqs. (4) and (6). At this point we emphasize again that although, as is well known [33], $|x\rangle \otimes |\pm\rangle$ is *not* a positive-energy (generalized) state, $|\Psi\rangle$ is a positive-energy state, as a consequence of the particular form of the coefficients in Eqs. (22).

The expansion in Eq. (21) can be rewritten as

$$\begin{split} |\Psi\rangle\rangle &= \sum_{m \in \mathbb{Z}} \int_{-\Delta t/2}^{\Delta t/2} \{ c_+(x_0 + m\Delta t) | x_0 + m\Delta t\rangle \otimes | + \rangle \\ &+ c_-(x_0 + m\Delta t) | x_0 + m\Delta t\rangle \otimes | - \rangle \} dx_0, \end{split}$$
(24)

which is to be compared with Eq. (18). In view of the invariance of each V_{x_0} under the action of the QRW evolution, we can restrict our attention to that action on each substate:

$$\begin{split} |\Phi_{x_0}\rangle\rangle &= \sum_{m \in \mathbb{Z}} \left\{ c_+(x_0 + m\Delta t) | x_0 + m\Delta t\rangle \otimes | + \right. \\ &+ c_-(x_0 + m\Delta t) | x_0 + m\Delta t\rangle \otimes | - \rangle \right\} \sqrt{\Delta t}, \end{split} \tag{25}$$

with x_0 fixed, even though these substates are not normalizable and are not positive-energy states. The point is that the general form of any such substate is preserved under the action of the QRW evolution *VU*, with no change in the value of x_0 . The inclusion of the multiplicative factor $\sqrt{\Delta t}$ in Eq. (25) is for later convenience with the normalization.

Consider first the action of V on a general substate $|\Phi_0\rangle\rangle \in \mathcal{V}_{x_0}$ —say, one with $x_0=0$ for definiteness. We have

$$V|\Phi_{0}\rangle\rangle = \sum_{m\in\mathbb{Z}} |m\Delta t\rangle \otimes \{c_{+}((m-1)\Delta t)| + \rangle$$
$$+ c_{-}((m+1)\Delta t)| - \rangle\}\sqrt{\Delta t}$$
$$= \sum_{m\in\mathbb{Z}} \sum_{\alpha=\pm} [c_{\alpha}(m\Delta t)|(m+\alpha)\Delta t\rangle \otimes |\alpha\rangle]\sqrt{\Delta t}$$
$$\equiv (E_{+} \otimes P_{+} + E_{-} \otimes P_{-})|\Phi_{0}\rangle\rangle, \qquad (26)$$

where

$$E_{\pm}|m\Delta t\rangle = |(m\pm 1)\Delta t\rangle, \quad P_{\pm}|\pm\rangle = |\pm\rangle, \quad P_{\pm}|\pm\rangle = 0.$$
(27)

The action of U on $|\Phi_0\rangle\rangle$ is easily seen from (12), which implies that

$$U|+\rangle = \cos(\Delta t)|+\rangle + \sin(\Delta t)|-\rangle,$$

$$U|-\rangle = \cos(\Delta t)|-\rangle - \sin(\Delta t)|+\rangle.$$
 (28)

Combining Eqs. (26) and (28), we see that

$$VU|\Phi_0\rangle\rangle = (E_+ \otimes P_+U + E_- \otimes P_-U)|\Phi_0\rangle\rangle.$$
(29)

If we had taken $f_+(p)=0$, $f_-(p)=f(p)$ in Eq. (7), we would have written instead

$$u_{-}(p) = \frac{1 + E(p) - p}{2\sqrt{E(p)[E(p) + 1]}} |+\rangle + i\frac{1 + E(p) + p}{2\sqrt{E(p)[E(p) + 1]}} |-\rangle,$$
(30)

and we would have obtained

$$|\Psi\rangle\rangle = \int_{-\infty}^{\infty} \{c_{+}(x)|x\rangle \otimes |+\rangle + c_{-}(x)|x\rangle \otimes |-\rangle\}dx, \quad (31)$$

where now

$$c_{+}(x) = \frac{1}{\sqrt{2\pi}} \int \frac{1 + E(p) - p}{2\sqrt{E(p)[E(p) + 1]}} f(p)e^{ipx}dp,$$
$$c_{-}(x) = \frac{i}{\sqrt{2\pi}} \int \frac{1 + E(p) + p}{2\sqrt{E(p)[E(p) + 1]}} f(p)e^{ipx}dp.$$
(32)

Then, decomposing $|\Psi\rangle\rangle$ into substates $|\Phi_{x_0}\rangle\rangle$ as before, we would have obtained on a state of this general form—say, one with $x_0=0$ —that

$$VU|\Phi_0\rangle\rangle = \{E_- \otimes P_+U + E_+ \otimes P_-U\}|\Phi_0\rangle\rangle.$$
(33)

We will treat here the first case, as the second one can be treated similarly.

To proceed we choose $-\pi \leq \phi < \pi$ and set

$$|\phi/\Delta t\rangle = \frac{1}{2\pi} \sum_{m \in \mathbb{Z}} e^{-im\phi} |m\Delta t\rangle, \qquad (34)$$

$$E_{\pm}|\phi/\Delta t\rangle = e^{\pm i\phi}|\phi/\Delta t\rangle, \quad |m\Delta t\rangle = \int_{-\pi}^{\pi} e^{im\phi}|\phi/\Delta t\rangle d\phi.$$
(35)

Considering the evolution operator VU acting as in Eq. (33), but now with E_{\pm} diagonalized, we have

$$VU(\phi) = (e^{i\phi}P_{+} + e^{-i\phi}P_{-})U.$$
 (36)

The eigenvalues of this 2×2 matrix with parameter ϕ are

$$\lambda_{\pm}(\phi) = \cos \phi \cos \Delta t \pm i \sqrt{1 - \cos^2 \phi \cos^2 \Delta t}.$$
 (37)

Suppose that the corresponding eigenvectors are

$$|v_{+}(\phi)\rangle = f_{++}(\phi)|+\rangle + f_{+-}(\phi)|-\rangle,$$

$$|v_{-}(\phi)\rangle = f_{-+}(\phi)|+\rangle + f_{--}(\phi)|-\rangle.$$
 (38)

Then the eigenvectors of VU are of the form $|\phi/\Delta t\rangle \otimes |v_{\pm}(\phi)\rangle$, with eigenvalues $\lambda_{\pm}(\phi)$. Expanding $|\Phi_0\rangle\rangle$ in terms of these eigenvectors of VU we get

$$\begin{split} |\Phi_{0}\rangle\rangle &= \int_{-\pi}^{\pi} \{g_{+}(\phi) | \phi/\Delta t\rangle \otimes | v_{+}(\phi)\rangle \\ &+ g_{-}(\phi) | \phi/\Delta t\rangle \otimes | v_{-}(\phi)\rangle\} \sqrt{\Delta t} d\phi, \end{split} \tag{39}$$

where

$$g_{\pm}(\phi) = \sum_{m \in \mathbb{Z}} \{ c_{+}(m\Delta t) f_{\pm +}^{*}(\phi) + c_{-}(m\Delta t) f_{\pm -}^{*}(\phi) \} e^{im\phi}.$$
(40)

Hence

$$\begin{split} |\Phi_n\rangle &\equiv (VU)^n |\Phi_0\rangle \\ &= \int_{-\pi}^{\pi} \left\{ g_+(\phi)\lambda_+(\phi)^n |\phi/\Delta t\rangle \otimes |v_+(\phi)\rangle \right. \\ &\quad + g_-(\phi)\lambda_-(\phi)^n |\phi/\Delta t\rangle \otimes |v_-(\phi)\rangle \right\} \sqrt{\Delta t} d\phi. \quad (41) \end{split}$$

If we now denote by X_n the random variable defining the "walker position" after *n* evolution steps, then we obtain for the "quantum statistical moment"

$$\langle (X_n)^k \rangle \equiv \langle \langle \Phi_n | \hat{q}^k \otimes \mathbf{1} | \Phi_n \rangle \rangle = \operatorname{Tr}_{S+T}(|\Phi_n \rangle) \langle \langle \Phi_n | \hat{q}^k \otimes \mathbf{1})$$
$$= \operatorname{Tr}_T((\operatorname{Tr}_S | \Phi_n \rangle) \langle \langle \Phi_n |) \hat{q}^k) = \operatorname{Tr}_T(\rho_T^{(n)} \hat{q}^k), \tag{42}$$

where the expectation value has been expressed in terms of traces over the translational degree of freedom (*T*) of the Dirac particle—the walker system in the parlance of QRW and its spin (*S*)—the coin system for the QRW. This has allowed us to cast the "quantum statistical moment" in terms of the reduced density operator $\rho_T^{(n)} = (\text{Tr}_S | \Phi_n \rangle) \langle \langle \Phi_n | \rangle$ which, as it provides all the necessary statistical information about the position of the Dirac particle, could have also been the main object of our mathematical investigation, as in most studies of QRW's.

We proceed to determine the statistical moment of the position variable, which takes the form

so that

$$\langle (X_n)^k \rangle = \int_{-\pi}^{\pi} [g_+^*(\phi) \lambda_+^*(\phi)^n (-i\partial_{\phi})^k \{g_+(\phi) \lambda_+(\phi)^n\} + g_-^*(\phi) \lambda_-^*(\phi)^n (-i\partial_{\phi})^k \{g_-(\phi) \lambda_-(\phi)^n\}] \frac{d\phi}{2\pi} (\Delta t)^{k+1}$$

$$(43)$$

or, equivalently,

$$\begin{split} \langle (X_n)^k \rangle &= (n\Delta t)^k \int_{-\pi}^{\pi} \left\{ |g_+(\phi)|^2 [-i\lambda'_+(\phi)/\lambda_+(\phi)]^k + |g_-(\phi)|^2 [-i\lambda'_-(\phi)/\lambda_-(\phi)]^k \right\} \frac{d\phi}{2\pi} \Delta t + O(n\Delta t)^{k-1}. \end{split}$$

$$\end{split}$$
(44)

Hence, as $n \rightarrow \infty$, $\Delta t \rightarrow 0$, with $t = n\Delta t$ large, we have that

$$\langle (X_n/n\Delta t)^k \rangle \sim \int_{-\pi}^{\pi} \left\{ |g_+(\phi)|^2 [-i\lambda'_+(\phi)/\lambda_+(\phi)]^k + |g_-(\phi)|^2 [-i\lambda'_-(\phi)/\lambda_-(\phi)]^k \right\} \frac{d\phi}{2\pi} \Delta t.$$
(45)

This has the following important consequence [34] (see also [35] and [12]): we can take as a random variable a function Y from $\Omega = S^1 \times \{+, -\}$ to the real numbers, with Y $=-i\lambda'_+(\Phi)/\lambda_+(\Phi)$ on $S^1 \times \{+\}$ and $Y = -i\lambda'_-(\Phi)/\lambda_-(\Phi)$ on S^1 $\times \{-\}$. Here $\Phi: \Omega \to R$ is a random variable which projects on the circle S^1 with measure $|g_+(\phi)|^2 \Delta t(d\phi/2\pi)$ on $S^1 \times \{+\}$ and measure $|g_-(\phi)|^2 \Delta t(d\phi/2\pi)$ on $S^1 \times \{-\}$. Since in the above limit all the moments of $X_n/n\Delta t$ agree with all the moments of Y and the support of $X_n/n\Delta t$ is compact, it follows that $X_n/n\Delta t$ converges weakly to Y. Hence we have that

$$\lim_{n\Delta t=t\to\infty} P(y_1 \le X_n/n\Delta t \le y_2)$$

= $P(y_1 \le Y \le y_2)$
= $\int_{T_+} |g_+(\phi)|^2 \Delta t \frac{d\phi}{2\pi} + \int_{T_-} |g_-(\phi)|^2 \Delta t \frac{d\phi}{2\pi},$ (46)

where the intervals of integration are $T_{\pm}=y_1 \leq [-i\lambda'_{\pm}(\Phi)/\lambda_{\pm}(\Phi)] \leq y_2$. It follows that in order to determine the long-time position distribution we need only determine $g_{\pm}(\phi)$ and $\lambda_{\pm}(\phi)$.

In addition to calculating the asymptotic position distribution of the discretized model in this way, it is possible for the purposes of comparison to derive the asymptotic form of the wave function solution of the Dirac equation by the method of stationary phase (see the Appendix) and to construct the density from the wave function in the usual way. We shall show in the case of a highly localized initial state that this leads to the same expression for the density at large times. It is satisfying if not entirely surprising that the same result can be obtained by these apparently quite different asymptotic methods, which point to possibly new ways of obtaining the asymptotic form of densities associated with other wave equations.

To construct a highly localized initial state, we take [21]

$$f(p) = f_{\nu}(p) = \frac{1}{\sqrt{\nu\sqrt{\pi}}} e^{-p^2/2\nu^2},$$
(47)

where ν is large and positive and quantifies the extent of the localization of the Dirac particle's initial state—the larger is ν , the sharper is the initial localization. As ν approaches infinity we have

$$c_{+}(x) \sim \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\nu}{\sqrt{\pi}}} \int_{0}^{\infty} e^{i\nu px} e^{-p^{2}/2} dp,$$
 (48)

$$c_{-}(x) \sim \frac{i}{\sqrt{2\pi}} \sqrt{\frac{\nu}{\sqrt{\pi}}} \int_{-\infty}^{0} e^{i\nu px} e^{-p^{2}/2} dp.$$
 (49)

Note that in the limit $\nu \to \infty$, $\int_{-\infty}^{\infty} |c_+(x)|^2 dx = \int_{-\infty}^{\infty} |c_-(x)|^2 dx = 1/2$. If we now make $\nu \Delta t$ small by taking Δt small enough, then

$$g_{\pm}(\phi) \sim i \sqrt{2\sqrt{\pi}/(\nu \Delta t^{2})} e^{-\phi^{2}/(2\nu^{2}\Delta t^{2})} f_{\pm+}^{*}(\phi) \quad \text{(if } \phi > 0)$$
$$\sim \sqrt{2\sqrt{\pi}/(\nu \Delta t^{2})} e^{-\phi^{2}/(2\nu^{2}\Delta t^{2})} f_{\pm-}^{*}(\phi) \quad \text{(if } \phi < 0).$$
(50)

We note that

$$-i\lambda'_{\pm}(\phi)/\lambda_{\pm}(\phi) = \pm \frac{\sin\phi\cos\Delta t}{\sqrt{1-\cos^{2}\Delta t\cos^{2}\phi}} \equiv \pm h(\phi),$$
(51)

say, and also that $|g_+(\phi)|^2 + |g_-(\phi)|^2 = 2\sqrt{\pi}e^{-\phi^2/\nu^2\Delta t^2}/(\nu\Delta t^2)$. To compute the asymptotic distribution we need to compute the integrals

$$I_{1} = \sum_{i} \int_{h_{i}^{-1}[y_{1}, y_{2}]} |g_{+}(\phi)|^{2} \Delta t \frac{d\phi}{2\pi}$$
$$= \frac{1}{2\pi} \sum_{i} \int_{y_{1}}^{y_{2}} \frac{1}{|h_{+}'(h_{i}^{-1}(y))|} |g_{+}(h_{i}^{-1}(y))|^{2} \Delta t dy \qquad (52)$$

and

$$I_{2} = \sum_{i} \int_{h_{i}^{-1}[-y_{2},-y_{1}]} |g_{-}(\phi)|^{2} \Delta t \frac{d\phi}{2\pi}$$
$$= \frac{1}{2\pi} \sum_{i} \int_{y_{1}}^{y_{2}} \frac{1}{|h_{-}'(h_{i}^{-1}(-y))|} |g_{-}(h_{i}^{-1}(-y))|^{2} \Delta t dy, \quad (53)$$

where the index *i* labels the local inverses of the function *h*. Because of (50), the only inverse relevant to leading order is the one that keeps ϕ close to zero. For this inverse, $h_i^{-1}(-y) = -h_i^{-1}(y)$. Furthermore, and realizing that $|v_{\pm}(\phi)\rangle^* = |v_{\mp}(-\phi)\rangle$, we can show that $|g_{\pm}(-\phi)|^2 = |g_{\pm}(\phi)|^2$. A direct computation then gives



FIG. 1. The asymptotic position probability density function, with localization parameter ν =1.9, 2.5, and 2.9. As ν increases, the plots become more sharply peaked near the ends of the interval. Note that $y=\pm 1$ corresponds to $x=\pm t$, labeling points moving apart, each at the speed of light.

$$I_{1} + I_{2} \sim \frac{\Delta t \sin \Delta t}{2\pi} \int_{y_{1}}^{y_{2}} \frac{1}{(1 - y^{2})\sqrt{\cos^{2}\Delta t - y^{2}}} \\ \times \frac{2\sqrt{\pi}}{\nu\Delta t^{2}} e^{-[h_{i}^{-1}(y)]^{2}/\nu^{2}\Delta t^{2}} dy.$$
(54)

If we set $y = h(\phi)$, then for all inverses ϕ_i we have $\cos^2 \phi_i = (\cos^2 \Delta t - y^2)/\cos^2 \Delta t (1 - y^2)$. Since for our inverse the value of ϕ_i is small, we have

$$[h_i^{-1}(y)]^2 = \phi_i^2 \simeq \sin^2 \phi_i = 1 - (\cos^2 \Delta t - y^2)/(\cos^2 \Delta t)(1 - y^2)$$

= $y^2 \sin^2 \Delta t / \cos^2 \Delta t (1 - y^2).$ (55)

Taking the limit $\Delta t \rightarrow 0$ we arrive at the asymptotic distribution function associated with the random variable $X_n/n\Delta t \sim Y$,

$$P(y_1 \le Y \le y_2) = \lim_{\Delta t \to 0} (I_1 + I_2) = \int_{y_1}^{y_2} F(y) dy,$$
$$F(y) = \frac{1}{\nu \sqrt{\pi}} \frac{1}{(1 - y^2)^{3/2}} e^{-y^2/\nu^2 (1 - y^2)}.$$
(56)

In Fig. 1, for three values of the localization parameter ν , we plot this two-horned probability distribution which we recognize as the one-dimensional analog of the result obtained for the Dirac particle in three dimensions in [21], Eq (3.1) (see the Appendix below).

Note that there are two sources of error in taking the above continuum limit: one is associated with the approximation (45) and is expected to be $O(\Delta t/t)$, and the other is associated with the approximation (54) and is expected to be $O([E_0\Delta t]^2)$.

IV. DISCUSSION

It has been shown that the one-dimensional Dirac evolution of a state with positive energy and definite spin is equivalent to a QRW in the limit of small positional steps and a large number of iterations. An initial state that is highly localized, with all but one momentum component set to zero, spreads in the remaining direction at a speed that almost surely approaches the speed of light as the initial localization increases.

This relationship between the Dirac particle evolution and a QRW leads to the intriguing speculation that at some small space-time scale, there may really be a QRW defining the evolution of states of the relativistic electron and that it is the Dirac evolution that is only a large-scale approximation. One way to test this would be to make very precise measurements of the spreading characteristics of initially highly localized electron states over short distances. Comparison with the characteristics that are typical for a QRW, in particular the shape of the position probability distribution at early times, may reveal whether or not there is indeed a QRW underlying an approximate Dirac particle evolution. Note, however, that the requirement $\Delta t \ll 1/E_0$ requires that $\Delta t \ll \hbar/mc^2$. For the electron, $\hbar/mc^2 \approx 10^{-21}$ sec, so that the implied discretization is extremely small on observable time scales.

It is tempting to speculate further that there may be some deep relationship between such an underlying QRW and the *Zitterbewegung* of the relativistic electron, as first discussed by Schrödinger [36]. This awaits further study.

ACKNOWLEDGMENTS

A.J.B. acknowledges the support of Australian Research Council Grant No. DP0450778. The work of D.E. and I.S. was supported by the EPEAEK research programme "Pythagoras II."

APPENDIX

It is possible to derive the asymptotic form (56) of the probability density by directly solving the Dirac equation and then carrying out a stationary phase approximation on the solution. If the initial positive-energy wave function has the form, from Eqs. (5) and (6),

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int e^{ipx} \Phi(p) dp,$$

with $\Phi(p)=f(p)[d_+u_+(p)+d_-u_-(p)]$ and $|d_+|^2+|d_-|^2=1$, then the time-dependent solution reads (with y=x/t)

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int \Phi(p) e^{i[px - E(p)t]} dp$$
$$= \frac{1}{\sqrt{2\pi}} \int \Phi(p) e^{it[py - E(p)]} dp.$$
(A1)

The phase t[py-E(p)] in this integral is stationary for variable *p* at just the one point $p=y/\sqrt{1-y^2}=k$, say, and a stationary phase approximation [37] (with |x| and *t* large, and *y*

finite) then leads to the asymptotic form of the solution [21],

$$\Psi(x,t) \sim \frac{1}{\sqrt{t}} \Phi(k) e^{it[k\xi - E(k)]} E(k)^{3/2} e^{-i\pi/4}, \qquad (A2)$$

and hence to the asymptotic form of the position density,

- [1] J. Kempe, Contemp. Phys. 44, 307 (2003).
- [2] Y. Aharonov, L. Davidovich, and N. Zagury, Phys. Rev. A 48, 1687 (1993).
- [3] D. A. Meyer, J. Stat. Phys. 85, 551 (1996).
- [4] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath, and J. Watrous, in *Proceedings of the 33rd Annual ACM Symposium on Theory of Computing (STOC'01)* (ACM Press, New York, 2001), pp. 37–49.
- [5] N. Shenvi, J. Kempe, and K. Birgitta Whaley, Phys. Rev. A 67, 052307 (2003).
- [6] A. Childs, E. Fahri, and S. Gutmann, Quantum Inf. Process. 1, 35 (2002).
- [7] D. Aharonov, A. Ambainis, J. Kempe, and U. Vazirani, Proceedings of the 33rd Annual ACM Symposium on Theory of Computing (STOC'01) [4], pp. 50–59.
- [8] N. Konno, Quantum Inf. Process. 1, 345 (2002).
- [9] B. C. Travaglione and G. J. Milburn, Phys. Rev. A 65, 032310 (2002).
- [10] T. D. Mackay, S. D. Bartlett, L. T. Stephenson, and B. C. Sanders, J. Phys. A 35, 2745 (2002).
- [11] W. Dür, R. Raussendorf, V. M. Kendon, and H.-J. Briegel, Phys. Rev. A **66**, 052319 (2002).
- [12] N. Konno, J. Math. Soc. Jpn. 57, 1179 (2005).
- [13] N. Konno, Phys. Rev. E 72, 026113 (2005).
- [14] M. A. Nielsen and I. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).
- [15] F. W. Strauch, Phys. Rev. A 73, 054302 (2006).
- [16] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
- [17] G. V. Riazanov, Sov. Phys. JETP 6, 1107 (1958).
- [18] T. Jacobson and L. S. Schulman, J. Phys. A 17, 375 (1984).
- [19] S. S. Schweber, Rev. Mod. Phys. 58, 449 (1986).
- [20] M. Katori, S. Fujino, and N. Konno, Phys. Rev. A 72, 012316 (2005).

$$\rho(x,t) = \Psi(x,t)^{\dagger} \Psi(x,t) \sim \frac{1}{t} \Phi(k)^{\dagger} \Phi(k) E(k)^3.$$
 (A3)

In the special case of a highly localized initial state, with f(p) as in Eq. (47), this gives

$$\rho(x,t)dx \sim \frac{1}{\nu\sqrt{\pi}} \frac{1}{(1-y^2)^{3/2}} e^{-y^2/\nu^2(1-y^2)} dy,$$
(A4)

where y = x/t, which is the same as in Eq. (56).

- [21] A. J. Bracken, J. A. Flohr, and G. F. Melloy, Proc. R. Soc. London, Ser. A 461, 3633 (2005).
- [22] F. Bakke and H. Wergeland, Physica (Amsterdam) **69**, 5 (1973).
- [23] A. J. Bracken and G. F. Melloy, J. Phys. A 32, 6127 (1999).
- [24] A. M. Childs and J. Goldstone, Phys. Rev. A 70, 022314 (2004).
- [25] D. Shapira, O. Biham, A. J. Bracken, and M. Hackett, Phys. Rev. A 68, 062315 (2003).
- [26] B. Gaveau, T. Jacobson, M. Kac, and L. S. Schulman, Phys. Rev. Lett. 53, 419 (1984).
- [27] D. G. C. McKeon and G. N. Ord, Phys. Rev. Lett. **69**, 3 (1992).
- [28] D. Ellinas, in *Quantum Probability and Infinite Dimensional Analysis: From Foundations to Applications*, edited by M. Schurmann and U. Franz (World Scientific, Singapore, 2005), pp. 174–200.
- [29] A. J. Bracken, D. Ellinas, and I. Tsohantjis, J. Phys. A 37, L91 (2004).
- [30] D. Ellinas and I. Smyrnakis, J. Opt. B: Quantum Semiclassical Opt. 7, S152 (2005).
- [31] D. Ellinas and I. Smyrnakis, Physica A 365, 222 (2006).
- [32] A. Bohm, The Rigged Hilbert Space and Quantum Mechanics (Springer-Verlag, New York, 1978).
- [33] T. D. Newton and E. P. Wigner, Rev. Mod. Phys. 21, 400 (1949).
- [34] G. Grimmett, S. Janson, and P. F. Scudo, Phys. Rev. E **69**, 026119 (2004).
- [35] A. D. Gottlieb, S. Janson, and P. F. Scudo, Infinite Dimen. Anal., Quantum Probab., Relat. Top. 8, 129 (2005).
- [36] E. Schrödinger, Sitzungsber. Preuss. Akad. Wiss., Phys. Math. Kl. 24, 418 (1930).
- [37] C. M. Bender and S. A. Orszag, Advanced Mathematical Methods for Scientists and Engineers (McGraw-Hill, New York, 1978).