Weyl, Dirac, and Maxwell equations on a lattice as unitary cellular automata

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Very simple unitary cellular automata on a cubic lattice are introduced to model a discretized time evolution of the wave functions for spinning particles. In each evolution step the updated value of the wave function at a given site depends only on the values at the nearest sites. The discretized evolution is also unitary and preserves chiral symmetry. The case of the spin-$\frac{1}{2}$ particle is studied in detail, and it is shown that every local and unitary automaton on a cubic lattice, under some natural assumptions, leads in the continuum limit to the Weyl equation. The sum over histories is evaluated and is shown to reproduce the retarded propagator in the continuum limit. Generalizations to include massive particles (Dirac theory), spin-1 particles (Maxwell theory), and higher-spin particles are also described.

I. INTRODUCTION

The aim of this paper is to present a simple lattice algorithm that in the continuum limit reproduces the propagation of massless or massive spinning particles. The discretized time evolution of the wave function satisfies the fundamental physical requirements of locality (the updated value at a given site depends only on the values at the nearest neighboring sites), unitarity (the norm of the wave function is preserved), and chiral symmetry (both helicity components propagate independently). An unexpected result of this study is a discovery that for two-component wave functions on a cubic lattice the Weyl equation necessarily follows in the continuum limit from locality, unitarity, and two additional, natural assumptions: (A) the wave functions that are constant throughout the whole lattice should not change in time and (B) the evolution algorithm must preserve the symmetry of the lattice. Thus, the rotation group, the Lorentz group, and spin emerge automatically in the continuum limit from unitary dynamics on a cubic lattice.

The results presented in this paper are directly related to numerous proposals of path integrals for a Dirac particle since an iteration of a discretized time evolution automatically gives a sum over histories. The path integral for the Dirac particle in one space dimension was found a long time ago by Feynman [1,2] and independently by Riazanov [3], but even this relatively simple problem, where there is no spin to complicate matters, is still attracting attention [4,5]. There is no consensus at all as to the form of path integrals for a Dirac particle in three dimensions. Proposed path integrals fall into three categories. The first category [3,6–13] comprises those approaches that work by "reverse engineering" in-

troducing from the outset the Dirac matrices to describe the spin degrees of freedom. Into the second category [14–16] fall those formulations that derive spin from continuously parametrized space of states related to the rotation group. To the third category [17–21] belong all approaches based on anticommuting Grassmannian variables. The sum over histories that is obtained from my lattice algorithm is distinct from all these path integrals. In the discretized evolution the spin degree of freedom enters only through a multicomponent wave function, and the rotation group emerges in the continuum limit.

There is a connection between this work and theories of fermions on a lattice, but there is also an essential difference in the choice of objects that are being studied. Instead of seeking discretized versions of the Hamiltonian or the Lagrangian, I introduce a discretized version of the *evolution operator*. In this way, common difficulties (breaking of chiral symmetry, doubling of fermion species, special limiting procedures) encountered in formulating the dynamics of a Dirac particle on a lattice [22–31] and the no-go theorem concerning Weyl particles on a lattice [32,33] are avoided.

In a recent paper Kostin [34] has introduced a cellular automaton for the Dirac equation that conserves probability, but his algorithm is nonlinear and it gives a linear equation only in the continuum limit. Following the example set by Kostin, I use the term *cellular automata* despite the fact that one of the eight properties usually required of cellular automata (cf., for example, [35]) does not hold: the states are described by continuous, and not by discrete variables. I shall call a *unitary cellular automaton* a system described by a wave function on a lattice whose discretized time evolution is unitary, synchronous, homogeneous, discrete in space and in time, deterministic, and spatially and temporally local. Genuine Boolean cellular automata were recently introduced by 't Hooft [36–38] to describe quantum systems, but his approach was fully successful only in the case of one spatial dimension.

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II. WEYL EQUATION ON A LATTICE

I shall start with a lattice description of the wave equation for a massless spin-1/2 particle and extend it later to massive particles and to higher spins. In my quantum cellular automaton the two-component wave function $\phi(i,j,k,t)$ is defined on a cubic lattice and it is updated at each time increment Δt according to the local algorithm

$$\phi(i,j,k,t+\Delta t) = W_{+++}\phi(i+1,j+1,k+1,t)$$
$$+W_{++-}\phi(i+1,j+1,k-1,t) + \cdots$$
$$+W_{---}\phi(i-1,j-1,k-1,t), \quad (1)$$

where all eight W's are 2×2 matrices and the integers i, j, and k are the coordinates of the lattice sites, $\mathbf{r} = (i,j,k)a$, in units of the cell size a. Equation (1) can be written in a compact form

$$\phi(\mathbf{r}, t+\Delta t) = \sum_{\mathbf{h}} W(\mathbf{h})\phi(\mathbf{r}+\mathbf{h}, t), \quad (2)$$

where the summation extends over a set of vectors $\mathbf{h}$ pointing from a given site to the eight nearest sites. The components of all vectors $\mathbf{h}$ are equal to $\pm a$,

$$\{\mathbf{h}\} = \{\{1,1,1\}, \{1,1,-1\}, \{1,-1,1\}, \{1,-1,-1\}, \{-1,1,1\}, \{-1,1,-1\}, \{-1,-1,1\}, \{-1,-1,-1\}\}a. \quad (3)$$

The unitary operator U_Δ acting on the wave functions at each iteration,

$$\phi(t+\Delta t) = U_\Delta \phi(t), \quad (4)$$

can be expressed explicitly as a sum of eight shift operators along the vectors $\mathbf{h}$

$$U_\Delta = \sum_{\mathbf{h}} W(\mathbf{h}) \exp(\mathbf{h}\cdot\nabla). \quad (5)$$

Upon evaluating the norm of the updated wave function, one finds that in order to guarantee the unitarity of the transformation (2), the matrices $W(\mathbf{h})$ must satisfy the algebraic relations

$$\sum_{\mathbf{h}} W^\dagger(\mathbf{h})W(\mathbf{h}) = 1, \quad (6)$$

$$\sum_{\mathbf{h}} W^\dagger(\mathbf{h})W(\mathbf{h}+\mathbf{h}'-\mathbf{h}'') = 0, \quad (7)$$

where $\mathbf{h}'$ and $\mathbf{h}'' \neq \mathbf{h}'$ are arbitrarily chosen vectors belonging to the set (3). The sum in Eq. (7) extends only over those vectors $\mathbf{h}$ that the vectors $\mathbf{h}+\mathbf{h}'-\mathbf{h}''$ are also members of the set (3). It follows from these unitarity conditions that the inverse of (2) has a similar local form so that my automaton is fully reversible,

$$\phi(\mathbf{r}, t) = \sum_{\mathbf{h}} W^\dagger(\mathbf{h})\phi(\mathbf{r}-\mathbf{h}, t+\Delta t). \quad (8)$$

Since the inverse of a unitary transformation is also unitary, the Hermitian conjugate matrices $W^\dagger$ must obey the same conditions as do the matrices W,

$$\sum_{\mathbf{h}} W(\mathbf{h})W^\dagger(\mathbf{h}) = 1, \quad (9)$$

$$\sum_{\mathbf{h}} W(\mathbf{h})W^\dagger(\mathbf{h}+\mathbf{h}'-\mathbf{h}'') = 0. \quad (10)$$

Depending on the mutual orientation of the vectors $\mathbf{h}'$ and $\mathbf{h}''$, the conditions (7) and (10) have one, two, or four terms, as exemplified below

$$W^\dagger_{+++}W_{---} = 0, \quad (11a)$$

$$W^\dagger_{+++}W_{+--} + W^\dagger_{-++}W_{---} = 0, \quad (11b)$$

$$W^\dagger_{+++}W_{++-} + W^\dagger_{+-+}W_{+--}$$
$$+W^\dagger_{-++}W_{-+-} + W^\dagger_{--+}W_{---} = 0. \quad (11c)$$

In total there are 8 conditions of the type (11a), 12 conditions of the type (11b), 6 conditions of the type (11c), one condition (6), and then the same number of conditions with W and $W^\dagger$ interchanged. Nonetheless they can all be met by the following simple choice of the matrices W

$$W_{+++} = q_+P_1, \quad W_{++-} = q_-P_2, \quad W_{+-+} = q_-P_1, \quad (12a)$$
$$W_{+--} = q_+P_2, \quad W_{-++} = q_-P_3, \quad W_{-+-} = q_+P_4, \quad (12b)$$
$$W_{--+} = q_+P_3, \quad W_{---} = q_-P_4, \quad (12c)$$

where

$$q_+ = (1+i)/4, \quad q_- = (1-i)/4, \quad (13)$$

and

$$P_1 = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad P_2 = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \quad (14a)$$

$$P_3 = \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, \quad P_4 = \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}. \quad (14b)$$

I have obtained this representation of the matrices W by choosing an approximation to the exact evolution operator for the Weyl particle in the continuum case in the form of a product T_a of three unitary operators,

$$\exp(c\,\boldsymbol{\sigma}\cdot\nabla\,\Delta t) \approx T_a \equiv \exp(a\sigma_x\partial_x)\exp(a\sigma_y\partial_y)\exp(a\sigma_z\partial_z), \quad (15)$$

where $a = c\Delta t$. Each factor on the right-hand side can be written as a sum of two shift operators. For example,

$$\exp(a\sigma_x\partial_x) = \tfrac{1}{2}[1 + \epsilon(h_x)\sigma_x]\exp(h_x\partial_x) \\ + \tfrac{1}{2}[1 - \epsilon(h_x)\sigma_x]\exp(-h_x\partial_x), \qquad (16)$$

where $\epsilon(h_x)$ denotes the sign function. I have determined all matrices $W(\mathbf{h})$ by multiplying out the Pauli matrices in the product (15) of three such factors,

$$T_a = \tfrac{1}{8}\sum_{\mathbf{h}}[1 + \epsilon(h_x)\sigma_x] \\ \times [1 + \epsilon(h_y)\sigma_y][1 + \epsilon(h_z)\sigma_z]\exp(\mathbf{h}\cdot\nabla), \qquad (17)$$

and by identifying the evolution operator T_a with the generic evolution operator U_Δ introduced before. The exact evolution operator in the continuum limit is recovered from the Lie-Trotter product formula (cf., for example, Ref. [39]), when $N = t/\Delta t$ tends to infinity,

$$\lim_{N\to\infty}[\exp(a\sigma_x\partial_x)\exp(a\sigma_y\partial_y)\exp(a\sigma_z\partial_z)]^N \\ = \exp(c\,\boldsymbol{\sigma}\cdot\nabla\,\Delta t). \quad (18)$$

I would like to point out that the approximation (15) associated with the Lie-Trotter formula leads automatically to the body-centered lattice (CsCl lattice structure, 8 nearest neighbors). The unitarity conditions represent such severe constraints on the W's that I am inclined to believe that they can be satisfied only for the body-centered lattice owing to the relationship with the Lie-Trotter formula. In particular, I prove in the Appendix that the unitarity conditions (6) and (7) cannot be satisfied for the standard form of a lattice used in gauge field theories — the simple cubic lattice (NaCl lattice structure, 6 nearest neighbors).

In order to find the continuum limit of the evolution equation, I shall use the exponential representation of the evolution operator (5) and then expand both sides of the equation

$$\phi(\mathbf{r}, t + \Delta t) = \sum_{\mathbf{h}} W(\mathbf{h})\exp(\mathbf{h}\cdot\nabla)\phi(\mathbf{r}, t) \qquad (19)$$

in powers of Δt and a ($\mathbf{h}$ is of the order of a). The linear terms in this expansion give the Weyl equation,

$$\partial_t\phi(\mathbf{r}, t) = c\,\boldsymbol{\sigma}\cdot\nabla\phi(\mathbf{r}, t). \qquad (20)$$

Incidentally, to obtain a discretized Weyl equation in two spatial dimensions one may choose as the four matrices W_{++}, W_{+-}, W_{-+}, and W_{--} the real matrices $P_i/2$.

III. UNIQUENESS OF THE WEYL EQUATION

I shall prove now that *for every set* of 2×2 matrices satisfying the unitarity conditions, and not just for the choice (12), one obtains the Weyl equation in the continuum limit. To this end, let me introduce, as in solid state physics, the lattice structure factor $\tilde{W}(\mathbf{k})$,

$$\tilde{W}(\mathbf{k}) = \sum_{\mathbf{h}} W(\mathbf{h})\exp(i\mathbf{k}\cdot\mathbf{h}). \qquad (21)$$

Owing to the unitarity conditions for the W's, this matrix is unitary for all values of $\mathbf{k}$. For the special choice (12) of the W's, the structure factor takes on the form

$$\tilde{W}(\mathbf{k}) = m_0 + m_x\sigma_x + m_y\sigma_y + m_z\sigma_z, \qquad (22)$$

where

$$m_0 = c_x c_y c_z + s_x s_y s_z, \qquad (23a)$$
$$m_x = s_x c_y c_z - c_x s_y s_z, \qquad (23b)$$
$$m_y = c_x s_y c_z + s_x c_y s_z, \qquad (23c)$$
$$m_z = c_x c_y s_z - s_x s_y c_z, \qquad (23d)$$

and

$$c_i = \cos(k_i a), \quad s_i = \sin(k_i a). \qquad (24)$$

The eigenvalues $\lambda_\pm$ of $\tilde{W}(\mathbf{k})$ are

$$\lambda_\pm = \exp(\pm i\varphi) = m_0 \pm i\sqrt{1 - m_0^2}. \qquad (25)$$

For small values of $\mathbf{k}$, the matrix $\tilde{W}(\mathbf{k})$ can be approximated by

$$\sum_{\mathbf{h}} W(\mathbf{h})\exp(i\mathbf{h}\cdot\mathbf{k}) = 1 + ia\,\mathbf{S}\cdot\mathbf{k} + \cdots, \qquad (26)$$

where I have made use of the assumption A that a homogeneous wave function should not change in time,

$$\tilde{W}(0) = \sum_{\mathbf{h}} W(\mathbf{h}) = 1, \qquad (27)$$

and I have defined the matrices S_i,

$$S_x = W_{+++} + W_{++-} + W_{+-+} + W_{+--} \\ - W_{-++} - W_{-+-} - W_{--+} - W_{---}, \qquad (28a)$$
$$S_y = W_{+++} + W_{++-} - W_{+-+} - W_{+--} \\ + W_{-++} + W_{-+-} - W_{--+} - W_{---}, \qquad (28b)$$
$$S_z = W_{+++} - W_{++-} + W_{+-+} - W_{+--} \\ + W_{-++} - W_{-+-} + W_{--+} - W_{---}. \qquad (28c)$$

The unitarity of the matrix (26) requires that the three matrices S_i must be Hermitian and, therefore, the formulas (28) must also hold with all the matrices W replaced by their Hermitian conjugates. This enables me to use the unitarity conditions (7) and (10) to evaluate the products of the matrices S_i. The unitarity conditions imply that the products of any matrix W by its Hermitian conjugate all commute,

$$[Q(\mathbf{h}), Q(\mathbf{h}')] = 0, \qquad (29)$$

where

$$Q(\mathbf{h}) = W^\dagger(\mathbf{h})W(\mathbf{h}), \qquad (30)$$

and hence all six Q's can be simultaneously diagonalized.

From the equivalence of all six lattice directions (assumption B), I conclude that the eigenvalues of all matrices Q must be the same, and then from equations (6) and (9) I find that these eigenvalues are $1/4$ and 0. It is now a matter of tedious but straightforward algebraic manipulations to show that the matrices S_i satisfy the familiar anticommutation relations,

$$S_i S_j + S_j S_i = 2\delta_{ij}. \tag{31}$$

There exist only two inequivalent two-dimensional representations of these relations: $\mathbf{S} = \boldsymbol{\sigma}$ or $\mathbf{S} = -\boldsymbol{\sigma}$. They describe the propagation of two helicities. Thus, up to a choice of helicity, the universality of the Weyl equation under the listed assumptions is established.

The matrix $\tilde{W}(\mathbf{k})$ determines the discretized time evolution for each Fourier component of the wave function. This matrix is related to the momentum space Hamiltonian through the formula

$$\tilde{W}(\mathbf{k}) = e^{-iH(\mathbf{k})\Delta t}, \tag{32}$$

and from the formulas (22) and (23) we deduce that

$$H(\mathbf{k}) = -\arctan(\sqrt{1/m_0^2 - 1})\frac{\mathbf{m}\cdot\boldsymbol{\sigma}}{|\mathbf{m}|}. \tag{33}$$

Note that for a local time evolution operator U_Δ, the Hamiltonian becomes nonlocal; as a logarithm of a local evolution operator it contains interactions not only among nearest neighbors but with *all the lattice sites*. For small values of $\mathbf{k}$, the spectrum of $\tilde{W}(\mathbf{k})$ determines the energy spectrum uniquely through the formula (26). However, for the values of $\mathbf{k}$ comparable to $1/a$, the spectrum of the Hamiltonian is not unique for one can always add multiples of $2\pi/\Delta t$ to its eigenvalues. This point has been forcefully made by 't Hooft [36,37]. That is why for a discretized time evolution one can escape the conclusion that there are pathological states with large momenta and small energy that lead to the fermion doubling problem. This fact was known to Nielsen and Ninomiya who state explicitly in Ref. [32] that one possibility to avoid their no-go theorem is to introduce discretized time evolution. One can see clearly how the Nielsen-Ninomiya no-go theorem is avoided by going over a simple proof of this theorem given by Pelissetto [33]. In that proof the assumption of locality is used to obtain the continuity of the Lagrangian (or the Hamiltonian) in momentum space which, in turn, leads to the appearance of additional, unwanted poles in the propagator. The possibility of avoiding the conclusions of the Nielsen-Ninomiya theorem for discontinuous energy spectra (in particular for a discrete spectrum of any system occupying a finite volume) has also been stressed by Quinn and Weinstein [30,31].

In order to decide this issue in the present case, we must first define the Hamiltonian as a function of $\mathbf{k}$. The arctan function appearing in Eq. (33) is multivalued, but one can choose uniquely its branches by making a natural assumption that the (positive energy) spectrum of the Hamiltonian $H(s\mathbf{k})$ is a nondecreasing function of the scaling parameter s with only minimal jumps at all discontinuities. This choice is illustrated in Fig. 1 for three
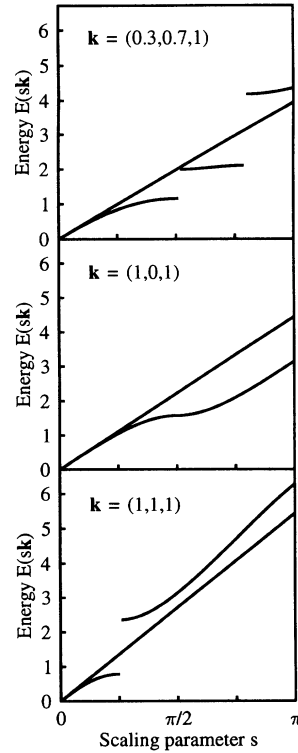

FIG. 1. These graphs show the energy in the form of an increasing function of the length of the momentum vector for three arbitrarily chosen directions of the momentum vector. In each graph the length of the momentum vector varies with the scaling parameter s. Straight lines in each graph represent the energy spectrum of the standard continuum theory. In each case the two spectra clearly coincide for small momenta.

selected values of the momentum vector. For an increasing spectrum there will never be any unphysical states with large momenta and small energies that plague lattice theories with local Hamiltonians. The graphs shown in Fig. 1 exhibit only the positive branch of the energy spectrum. The negative-energy branch is obtained in each case by a mirror reflection.

IV. SUM OVER HISTORIES

I shall now write down the sum over histories for the Weyl particle arising from the time-evolution algorithm (2), and I shall show that the solution of the initial value problem, given as a sum over trajectories, yields in the continuum limit the correct expression for the retarded propagator.

The N-fold iteration of a single-step time evolution leads to the formula

$$\phi(\mathbf{r}, t + N\Delta t) = \sum_{\mathbf{h}_1,\ldots,\mathbf{h}_N} W(\mathbf{h}_1)\cdots W(\mathbf{h}_N)$$
$$\times \phi(\mathbf{r} + \mathbf{h}_1 + \cdots + \mathbf{h}_N, t). \tag{34}$$

When the summation in this formula is restricted to only those terms that produce a given total displacement, we obtain the following discretized form of the propagator

$$K(\mathbf{r} - \mathbf{r}', t) = \sum_{\mathbf{h}_1,\ldots,\mathbf{h}_N} W(\mathbf{h}_1)\cdots W(\mathbf{h}_N)\delta_{\mathbf{r},\mathbf{r}'+\mathbf{h}_1+\cdots+\mathbf{h}_N}, \quad (35)$$

where $t = N\Delta t$. Each term in this sum corresponds to a lattice trajectory that in N steps connects the initial and the final lattice sites. A single step described by a vector $\mathbf{h}$ is represented as a multiplication by the matrix $W(\mathbf{h})$. Contributions from all trajectories are coherently added.

The constraint on the sum in (35) can be handled (cf., for example, [40]) with the help of the Fourier representation of the Kronecker delta, leading to an integral form of the propagator involving our structure factor $\tilde{W}(\mathbf{k})$

$$K(\mathbf{r} - \mathbf{r}', t) = \left(\frac{a}{2\pi}\right)^3 \int d^3k \, [\tilde{W}(\mathbf{k})]^N \exp[i\mathbf{k}\cdot(\mathbf{r} - \mathbf{r}')], \quad (36)$$

where the integration extends over the Brillouin zone: $-\pi/a < k_i < \pi/a$. In the limit, when $a \to 0$ and $N \to \infty$ with t fixed, the Nth power of $\tilde{W}$ can be written, on account of (26), in the form

$$\lim_{N\to\infty} [\tilde{W}(\mathbf{k})]^N = \exp(i\boldsymbol{\sigma}\cdot\mathbf{k}\,t). \quad (37)$$

This result was to be expected since it is just the momentum-space representation of the Lie-Trotter formula (18). The exponential of the Weyl Hamiltonian is, of course, the Fourier representation of the propagator for the Weyl equation. Thus, the sum over histories (34) reproduces correctly in the continuum limit the retarded propagator.

V. DIRAC EQUATION ON A LATTICE

For massless particles each helicity state propagates independently. Chiral invariance (or CP symmetry) is expressed in my discretized form of time evolution by the fact that the matrices W corresponding to the two helicities are related by the spatial reflection

$$W(\mathbf{h}) \to \sigma_y W^*(\mathbf{h})\sigma_y = W(-\mathbf{h}), \quad (38)$$

as seen from the formulas (28). For massive particles, however, the two helicity states are mixed by the mass term. Therefore, the discretized time evolution for a massive particle must be described, as in the standard Dirac equation, in terms of two two-component wave functions. The discrete time-evolution algorithm for a massive Dirac particle can again be written in the same general form (8) as for the massless case

$$\psi(\mathbf{r}, t + \Delta t) = \sum_{\mathbf{h}} D(\mathbf{h})\psi(\mathbf{r} + \mathbf{h}, t). \quad (39)$$

The 4×4 matrices D that act on four-component wave functions $\psi(\mathbf{r}, t)$ can be expressed in terms of the matrices $W(\mathbf{h})$ and $W(-\mathbf{h})$ by the following block-matrix formulas (from now on, I set $c \equiv a/\Delta t = 1$ and $\hbar = 1$)

$$D(\mathbf{h}) = \begin{pmatrix} \cos(ma) & i\sin(ma) \\ i\sin(ma) & \cos(ma) \end{pmatrix}\begin{pmatrix} W(\mathbf{h}) & 0 \\ 0 & W(-\mathbf{h}) \end{pmatrix}. \quad (40)$$

It is clear that such a modification does not affect the unitarity conditions; the matrices D will also satisfy all of them. The continuum limit of (39) gives the Dirac equation in the Weyl representation of the Dirac matrices

$$\partial_t \psi(\mathbf{r}, t) = (\rho_3\,\boldsymbol{\sigma}\cdot\nabla + i\rho_1 m)\psi(\mathbf{r}, t). \quad (41)$$

Having reproduced in the previous section the propagator of a massless particle as a sum over histories, I can easily include the mass in this sum since that part of the problem has been already solved by Feynman [1,2] in one dimension. More recently Feynman's "checkerboard" picture of a particle zigzagging through spacetime, reversing its helicity at each bend, has also been described by a Poisson process [9,15,20,21,40]. This Poisson process must be combined with the propagation of definite helicity states. Thus, the propagator for a massive Dirac particle will be a sum of terms, each term describing a fixed number of helicity reversals. Between the reversals induced by the mass term the propagation is described by the sum over histories (35), evaluated separately for each helicity.

VI. MAXWELL EQUATIONS ON A LATTICE

An extension of my lattice algorithm to wave equations describing massless particles with higher spins is most easily accomplished with the help of the spinor representation of relativistic wave functions. In the simplest case of spin-1 particles — the photons — the wave function can be represented as the self-dual (or the anti-self-dual) part of the electromagnetic field tensor (cf. Ref. [41]). More explicitly, I construct a second rank symmetric spinor ϕ_{AB} from the components of a complex vector $\mathbf{F} = (\mathbf{E} + i\mathbf{B})/\sqrt{2}$,

$$\phi_{00} = -F_x + iF_y, \quad (42a)$$

$$\phi_{01} = F_z = \phi_{10}, \quad (42b)$$

$$\phi_{11} = F_x + iF_y. \quad (42c)$$

The Maxwell equations can be expressed in the spinor notation in the form (cf., for example, Ref. [41])

$$\sigma^{\mu C'A}\partial_\mu \phi_{AB} = 0, \quad (43)$$

where the four spin matrices $\sigma^{\mu A'B}$ are equal to the unit matrix and to the Pauli matrices,

$$\{\sigma^{\mu A'B}\} = \{\mathbf{1}, \sigma_x, \sigma_y, \sigma_z\}^{A'B}. \quad (44)$$

The equations (43), together with the symmetry condition for ϕ_{AB}, are equivalent to the Maxwell equations. I shall write these equations in the following form that is directly amenable to the treatment applied before to the spin-1/2 case,

$$\partial_t \Phi = -\boldsymbol{\rho}\cdot\nabla\,\Phi. \quad (45)$$

The vector Φ is related to the spinorial components ϕ_{AB} through the formula

$$\Phi_1 = \phi_{00}, \quad \Phi_2 = \phi_{01}, \quad \Phi_3 = \phi_{10}, \quad \Phi_4 = \phi_{11} \quad (46)$$

and the matrices ρ_i have the form

$$\rho_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad (47a)$$

$$\rho_2 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \quad (47b)$$

$$\rho_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (47c)$$

The set of four equations (45) becomes equivalent to the full set of Maxwell equations if one imposes two auxiliary conditions

$$\Phi_2 = \Phi_3 \quad (48)$$

and

$$-(\partial_x + i\partial_y)\Phi_1 + \partial_z\Phi_2 + \partial_z\Phi_3 + (\partial_x - i\partial_y)\Phi_4 = 0. \quad (49)$$

The first condition reduces the number of components from four to three, and the second one expresses the vanishing of the divergence of the field vectors. If these conditions are imposed initially, they will be valid for all times as a result of the evolution equations (45). Note that the divergence condition can be obtained by demanding that the time derivative of Φ also obeys the first condition. In other words, one may just impose initially at each point in space two orthogonality conditions of the form

$$(A|\Phi) = 0, \quad (A|\boldsymbol{\rho} \cdot \nabla \Phi) = 0, \quad (50)$$

where the vector A is equal to $(0, 1, -1, 0)$.

The matrices ρ_i can be expressed as tensor products $\sigma_i \times I$, where I is the 2×2 unit matrix. Therefore, the equation (45) is ready for discretization along the lines adopted in this paper. One can just take the basic formula (1) for the discrete time evolution, replace the two-dimensional vector ϕ by the four-dimensional vector Φ and enlarge all 2×2 matrices $W(\mathbf{h})$ to the size 4×4 by substituting for all matrix elements in the formulas (14) the appropriate multiples of the unit 2×2 matrix. For example,

$$W_{---} = q_- \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix} \rightarrow q_- \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (51)$$

Such a substitution leads to the formula for the structure factor analogous to (22) but with all the matrices σ_i replaced by the matrices ρ_i. The only new ingredient needed for the spin-1 case is the discretized form of the second auxiliary conditions that must be imposed on the vector Φ to bring about the equivalence with the Maxwell

theory. While the first auxiliary condition is again the same equality (48) of the second and the third component of Φ, the divergence condition (49) must be replaced by its discretized version. The proper form of this condition is obtained from the continuous case by adapting it to the present situation. In that way, instead of Eq. (50) one obtains

$$(A|U_\Delta \Phi) = 0, \quad (52)$$

where U_Δ is the discretized evolution operator for the Maxwell field. One may check that these conditions are preserved during the discretized time evolution.

As in the case of the Weyl equation, the propagation of particles of opposite helicity is described by a complex conjugate wave function whose components form a second rank symmetric primed spinor $\phi^{A'B'}$ built from the components of the complex conjugate vector $\mathbf{F}^*$,

$$\phi^{0'0'} = -F_x^* - iF_y^*, \quad (53a)$$

$$\phi^{0'1'} = -F_z^* = \phi^{1'0'}, \quad (53b)$$

$$\phi^{1'1'} = F_x^* - iF_y^*. \quad (53c)$$

The unitarity condition for the photon wave function Φ (or its complex conjugate) leads to the exact energy conservation in each evolution step for the associated electromagnetic field.

An extension of my discretization algorithm to massless particles of arbitrary spin can be based again on the spinor form of the wave equations describing all such particles (cf. Ref. [41]). The only case that is not covered by my algorithm is that of a spinless particle.

VII. CONCLUSIONS

A discretized version of the evolution equations for relativistic wave functions, described in this paper, has been originally intended as a new numerical algorithm for solving these equations. However, being accurate only up to the lowest order in lattice spacing, my algorithm cannot successfully compete with nonunitary though more efficient and flexible numerical methods of solving the Dirac equation (such as those described, for example, in Refs. [42] and [43]). The results presented here do indicate, however, what challenges are to be met in a construction of a fundamental theory with discretized space and time in order to satisfy the requirements of locality and unitarity. These requirements impose severe restrictions on the theory; in particular, they allow only for some lattice structures. It came as a surprise to me to find that the simplest lattice form with 6 nearest neighbors, that has become a standard choice in all lattice gauge theories, is ruled out by the unitarity conditions.

I have confined the discussion to free propagation, but the inclusion of interaction with external fields does not present any new problems. For nongauge couplings one may simply introduce at each evolution step in the Lie-Trotter formula an additional local and unitary factor describing the interaction. The simplest choice for this factor will be, of course, the exponential function of the

interaction Hamiltonian. This is quite analogous to the treatment of the mass term in Sec. V. In the case of a coupling to a gauge field, the problem is a bit more complicated since the interaction term cannot be fully separated from the free evolution lest we violate gauge invariance. A possible way to proceed can be inferred from

the formula (15) in which in the presence of a gauge field one may replace all ordinary derivatives by appropriate covariant derivatives. As a result of this replacement, the updated values of the wave functions will be modified, as compared to the field-free formula (2), by the presence of the standard unitary gauge factors U,

$$\phi(\mathbf{r}, t + \Delta t) = \sum_{\mathbf{h}} U(\mathbf{r}, \mathbf{r}+\mathbf{h_x})U(\mathbf{r}+\mathbf{h_x}, \mathbf{r}+\mathbf{h_x}+\mathbf{h_y})U(\mathbf{r}+\mathbf{h_x}+\mathbf{h_y}, \mathbf{r}+\mathbf{h_x}+\mathbf{h_y}+\mathbf{h_z})W(\mathbf{h})\phi(\mathbf{r} + \mathbf{h}, t). \tag{54}$$

The factor $U(\mathbf{r_1}, \mathbf{r_2})$ represents the element of the Abelian or non-Abelian gauge group associated with the link connecting the points $\mathbf{r_1}$ and $\mathbf{r_2}$. The three vectors $\mathbf{h_x}$, $\mathbf{h_y}$, and $\mathbf{h_z}$ are the components of the vector $\mathbf{h}$ pointing in the direction of one of the links,

$$\mathbf{h} = \mathbf{h_x} + \mathbf{h_y} + \mathbf{h_z}. \tag{55}$$

Note that there are three factors $U(\mathbf{r_1}, \mathbf{r_2})$ in each term in the formula (54). Thus, one must use three links to connect each pair of neighboring lattice sites instead of just one link needed in the standard formulation on a cubic lattice. This proliferation of links is due to the use of the Lie-Trotter formula, and that is the price to be paid for preserving strictly the unitarity at each step of the discretized time evolution.

In the present paper I have restricted myself entirely to the study of a discretized *time evolution* of relativistic wave functions. In this study the preservation of unitarity at each evolution step was important. I have made no attempt to extend this approach to quantized fields. I do not know to what extent the unitary discretization algorithm described here may be useful for applications in quantum field theory, in particular, for the evaluation of the partition function. However, the connection between the time-evolution operator and the transfer matrix of statistical physics, often used in lattice field theories [44–46], may perhaps provide a link between these two problems.

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APPENDIX

In the case of a simple cubic lattice there are 6 matrices W_i, and I shall denote them by W_i where the subscript i takes on the values $\pm x$, $\pm y$, and $\pm z$. The unitarity

conditions in this case lead to 2×19 equations for the matrices W,

$$\sum_i W_i^\dagger W_i = 1, \tag{A1}$$

$$W_i^\dagger W_{-i} = 0, \tag{A2}$$

$$W_i^\dagger W_j + W_{-j}^\dagger W_{-i} = 0, \quad (i \neq j), \tag{A3}$$

and

$$\sum_i W_i W_i^\dagger = 1, \tag{A4}$$

$$W_i W_{-i}^\dagger = 0, \tag{A5}$$

$$W_i W_j^\dagger + W_{-j} W_{-i}^\dagger = 0, \quad (i \neq j). \tag{A6}$$

In order to prove that representations of these relations in the form of 2×2 matrices do not exist, I first observe that, as in the case of a body-centered lattice [cf. Eq. (30)], all products $Q(\mathbf{h})$ can be simultaneously diagonalized, and each has one eigenvalue equal to 0. Thus, three matrices Q, say Q_1, Q_2, and Q_3, have the form

$$\begin{pmatrix} \alpha_i & 0 \\ 0 & 0 \end{pmatrix}, \tag{A7}$$

and the remaining three have the form

$$\begin{pmatrix} 0 & 0 \\ 0 & \beta_i \end{pmatrix}. \tag{A8}$$

In the representation in which the formulas (A7) and (A8) hold, each matrix W can be parametrized by two complex numbers,

$$W_i = \begin{pmatrix} a_i & 0 \\ b_i & 0 \end{pmatrix}, \quad i = 1, 2, 3, \tag{A9}$$

$$W_k = \begin{pmatrix} 0 & c_k \\ 0 & d_k \end{pmatrix}, \quad k = 4, 5, 6. \tag{A10}$$

The unitarity conditions (A3) imply that all three vectors (a_i, b_i) [and also the three vectors (c_k, d_k)] must be mutually orthogonal. This completes the proof, for there exist at most two mutually orthogonal vectors in two dimensions.

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