

Formal Analogy between the Dirac Equation in Its Majorana Form and the Discrete-Velocity Version of the Boltzmann Kinetic Equation

F. Fillion-Gourdeau,^{1,*} H. J. Herrmann,² M. Mendoza,² S. Palpacelli,^{3,†} and S. Succi^{4,‡}

¹Centre de Recherches Mathématiques, Université de Montréal, Montréal, Canada H3T 1J4

²ETH Zurich, Computational Physics for Engineering Materials, Institute for Building Materials, Schafmattstrasse 6, HIF, CH-8093 Zurich, Switzerland

³Numidia srl, via G. Peroni, 130, 00131, Roma, Italy

⁴Istituto Applicazioni Calcolo, CNR, via dei Taurini 19, 00185, Roma, Italy

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We point out a formal analogy between the Dirac equation in Majorana form and the discrete-velocity version of the Boltzmann kinetic equation. By a systematic analysis based on the theory of operator splitting, this analogy is shown to turn into a concrete and efficient computational method, providing a unified treatment of relativistic and nonrelativistic quantum mechanics. This might have potentially far-reaching implications for both classical and quantum computing, because it shows that, by splitting time along the three spatial directions, quantum information (Dirac-Majorana wave function) propagates in space-time as a classical statistical process (Boltzmann distribution).

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Boltzmann and Dirac.—Analogies between the nonrelativistic Schrödinger equation and fluid dynamics have been noted since the early days of quantum mechanics. In particular, back in 1927, Madelung noticed that, by expressing the wave function in eikonal form, i.e., $\Psi = Re^{iS/\hbar}$, the Schrödinger equation turns into the hydrodynamic equation of a compressible, inviscid fluid, with number density $\rho = R^2$ and velocity $\vec{u} = -\nabla S/m$. The quantum fluid is subject to the classical potential $V_c(\vec{x})$ plus the quantum potential $V_q(\vec{x}) = -(\hbar^2/2m)(\Delta R)/R$. Although the hydrodynamic analogy is commonly regarded as purely formal in nature, lately, its connections with Bohm's theory of hidden variables and de Broglie's pilot wave picture have received a surge of interest, mostly in connection with experimental investigations on the nonlocal nature of quantum physics [1].

The quantum relativistic fluid analogy seems to have received comparatively less attention. Back in 1993, it was noted that the Dirac equation can be regarded as a special form of a *discrete* Boltzmann kinetic equation, in which the particle velocities are confined to a handful of discrete values [2,3]. The discrete components of the Boltzmann distribution, $f_i(\vec{x}; t) \equiv f(\vec{x}, \vec{v} = \vec{v}_i; t)$, where the index i labels the discrete velocities, are then identified with the spinor components ψ_i of the Dirac equation. This opens up an interesting connection between classical kinetic theory and relativistic quantum mechanics.

Mathematically, the connection is not so surprising, since both Boltzmann and Dirac equations are hyperbolic supersets of the Navier-Stokes and Schrödinger equations, respectively.

The interesting point, however, is that the connection becomes much more direct and compelling by considering the discrete-velocity version of the Boltzmann equation, in

relation to the Majorana form of the Dirac equation, in which all matrices are *real* [4].

Majorana particles have attracted significant interest in recent years, mostly in connection with the fact that they coincide with their own antiparticles, as beautifully discussed in a recent essay by Wilczek [5].

Here, we wish to put forward a different angle of interest of the Majorana representation, namely, the fact that it not only makes Boltzmann-Dirac analogy conceptually more poignant, but it also turns it into a concrete *unified* computational scheme for the simulation of both relativistic and nonrelativistic quantum wave equations, on both classical and quantum computers. The corresponding method is known as the quantum lattice Boltzmann (QLB) method [2]. The QLB method is based on the identification of the discrete Boltzmann distribution with the spinorial wave function $f_i(\vec{x}; t) \leftrightarrow \psi_i(\vec{x}; t)$. Even though both objects are real, they still face a mismatch of degrees of freedom in more than one spatial dimension, since a spinor of order s consists of $2s + 1$ components, regardless of the number of dimensions, while the discrete distribution requires (at least) $2d$ discrete components in d spatial dimensions. Moreover, the Dirac-Majorana matrices cannot be simultaneously diagonalized, reflecting the basic fact that spinors are not ordinary vectors. As a result, in more than one spatial dimensions, it is in principle not possible to keep the particle velocity aligned with its spin.

Remarkably, both problems can be circumvented by resorting to operator splitting. Essentially, this amounts to splitting the spinor propagation along the three spatial dimensions into a series of three one-dimensional propagations, each using the diagonalized form of the corresponding Dirac-Majorana streaming matrix. As a result, at each propagation step the particle spin is kept aligned with

its velocity, so that the identification $f_i \leftrightarrow \psi_i$ continues to hold.

In this Letter we show that this “heuristic stratagem” is backed up by a rigorous mathematical treatment, which leads to a unified computational approach to quantum wave mechanics. The resulting computational scheme offers outstanding amenability to parallel computing on electronic computers [6] and is also suitable to prospective quantum computing simulations [7–9].

To show its versatility also towards the inclusion of nonlinear interactions, as an application, we shall solve a specific form of the nonlinear Dirac equation including a dynamical-symmetry breaking term, as first proposed by Nambu and Jona-Lasinio (NJL).

Discrete Boltzmann and Dirac.—To set up the framework, let us write down the two equations in full display. The discrete Boltzmann equation reads as follows:

$$\partial_t f_i + v_i^a \nabla_a f_i = \Omega_{ij} (f_j - f_i^e), \quad (1)$$

where $f_i = f(\vec{x}, \vec{v} = \vec{v}_i; t)$ is the probability density of finding a particle around position \vec{x} at time t with discrete velocity \vec{v}_i . The latin index $a = x, y, z$ runs over spatial dimensions and the Einstein summation rule is assumed. The left-hand side represents the particle free streaming (in the absence of external forces, for simplicity), while the right-hand side is the collisional step steering the distribution function towards a local Maxwell equilibrium f_i^e . The (symmetric) scattering matrix Ω_{ij} encodes the mass-momentum-energy conservation laws underpinning fluid dynamic behavior.

The Dirac equation, in Majorana form, reads as follows:

$$\partial_t \psi_i + S_{ij}^a \nabla_a \psi_j = M_{ij} \psi_j, \quad (2)$$

where S_{ij}^a are the three Majorana streaming matrices and M_{ij} is the (antisymmetric) mass matrix, acting upon the real spinor ψ_i , $i = 1, 2s + 1$. This clearly shows a formal analogy with the Boltzmann equation: the left-hand side describes the free streaming of the spinors, while the right-hand side can be regarded as a simple form of local collision between the various spinorial components. Note that the mass matrix has dimensions of an inverse time scale, typically given by the Compton frequency $\omega_c = mc^2/\hbar$. In 1D, this analogy is “exact”: by choosing a representation where the Dirac matrix is diagonal (Majorana representation), we recover Eq. (1). In multiple dimensions, however, the story is different: the connection can be realized only by resorting to operator splitting, whereby each step can be written in the form of Eq. (1). This will be discussed in the following.

Quantum lattice Boltzmann.—Let us consider the case of spin $s = 1/2$ particles and start from a relativistic wave equation with matrices β, α_a in the Dirac representation. The goal here is to find the discrete time evolution of the wave function by using the formal analogy with the Boltzmann equation. In the QLB setting, this time

evolution proceeds by a sequence of streaming and collisional steps, given by (we use natural units where $c = \hbar = 1$)

$$\partial_t \psi^{(x)}(t) = -\alpha_x \partial_x \psi^{(x)}(t), \quad \psi^{(x)}(t_n) = \psi(t_n), \quad (3)$$

$$\partial_t \psi^{(y)}(t) = -\alpha_y \partial_y \psi^{(y)}(t), \quad \psi^{(y)}(t_n) = \psi^{(x)}(t_{n+1}), \quad (4)$$

$$\partial_t \psi^{(z)}(t) = -\alpha_z \partial_z \psi^{(z)}(t), \quad \psi^{(z)}(t_n) = \psi^{(y)}(t_{n+1}), \quad (5)$$

$$\partial_t \psi^{(c)}(t) = -i\beta m \psi^{(c)}(t), \quad \psi^{(c)}(t_n) = \psi^{(z)}(t_{n+1}), \quad (6)$$

$$\psi(t_{n+1}) = \psi^{(c)}(t_{n+1}), \quad (7)$$

where the superscript labels the step of the splitting and $t_n = n\Delta t$ is the time after n iterations. In these equations, the calculated solution at a given step provides an initial condition for the next step in the sequence. Eqs. (3)–(5) correspond to streaming while the last step in Eq. (6) is collisional.

The streaming steps for a given coordinate a proceed as follows. First, it should be noted that the matrix α_a (for $a = x, y, z$) is not diagonal and, thus, the Dirac equation is not in the form of Eq. (1). However, the latter can be recovered by using the unitary transformation of spinors $S_a = (1/\sqrt{2})(\beta + \alpha_a)$. This equation allows us to transform the Dirac matrices to a Majorana-like representation, where the matrix $\tilde{\alpha}_a = S_a^\dagger \alpha_a S_a = \beta$ is diagonal, with eigenvalues ± 1 . Then, by introducing the transformed spinor as $\tilde{\psi}^{(a)} = S_a^{-1} \psi^{(a)}$, the streaming steps can be turned into

$$\partial_t \tilde{\psi}^{(a)}(t) = -\beta \partial_a \tilde{\psi}^{(a)}(t), \quad (8)$$

which is clearly in the form of Eq. (1) without the collisional term. This has a solution given by

$$\tilde{\psi}_{1,2}^{(a)}(t_{n+1}, \mathbf{x}) = \tilde{\psi}_{1,2}^{(a)}(t_n, x_a - \Delta t), \quad (9)$$

$$\tilde{\psi}_{3,4}^{(a)}(t_{n+1}, \mathbf{x}) = \tilde{\psi}_{3,4}^{(a)}(t_n, x_a + \Delta t), \quad (10)$$

where $x_a + v_i^a = x_a \mp \Delta t$, $i = -1, 1$, is the lattice neighbor pointed by the discrete speed $v_i^a = \mp c$. This corresponds to an *exact* integration of the streaming operator along the characteristics $\Delta x_a = \pm c \Delta t$ (light cones), which is typical of the lattice Boltzmann method.

The collision step can also be integrated exactly by using the solution

$$\psi^{(c)}(t_{n+1}) = e^{-i\beta m \Delta t} \psi^{(c)}(t_n) \equiv C \psi^{(c)}(t_n). \quad (11)$$

It is then possible to write $C = e^{-M \Delta t}$ explicitly as a 4×4 matrix by using properties of Dirac matrices [10].

It is readily shown that the above discrete system is unitary for any value of the time step Δt . Moreover, it looks like a classical motion of two discrete walkers, hopping by one lattice unit along every coordinate at

each time step and colliding according to the scattering matrix $M = i\beta m$. More complex interactions can be treated in a similar way by including the interaction terms into the scattering matrix. As long as the matrix is local, it is not necessary to diagonalize S and M simultaneously, and due to the operator splitting, the simplicity of the lattice Boltzmann formalism is not compromised. For instance, for the coupling to an electromagnetic field, the scattering matrix is given by $M = i\beta m - ie\alpha_a A_a(x, t) + ieV(x, t)$, where (A_a, V) is the electromagnetic potential.

Symbolically, the 3D evolution of the Dirac spinor reads like a sequence of three one-dimensional stream steps and one collisional step:

$$\psi(t_{n+1}, \mathbf{x}) = C(S_z P_z S_z^{-1})(S_y P_y S_y^{-1})(S_x P_x S_x^{-1})\psi(t_n, \mathbf{x}), \quad (12)$$

where $P_a = e^{-\Delta t \beta \partial_a}$ is a translation operator along the direction a . The latter shifts the “1,2” and “3,4” spinor components by $\mp \Delta t$, respectively.

Of course, this procedure is not exact: as shown in the following, it corresponds to an operator splitting method where the streaming and collision matrices do not commute. However, each step of the splitting is exact and, thus, the only source of error comes from the splitting which scales like $O(\Delta t^2)$ (second order accuracy). We refer the reader to [11] for the numerical analysis of the scheme. Other schemes where the error scales like $O(\Delta t^3)$ can also be obtained [6,11]. Most importantly, it does not spoil the unitarity of the scheme for any value of the time step: this is required to conserve the probability density (L^2 norm). Full details of the algorithm can be found in [6] and slightly different versions are in [2,12].

General operator-splitting framework.—The QLB was derived on heuristic grounds, based on a intuitive analogy between a genuinely *quantum* variable, the particle spin, and a *discrete* one, the particle momentum in the lattice formulation of the Boltzmann equation. Since quantization is a physical concept while discretization is a numerical one, it might be argued that the analogy is somewhat artificial, hence perhaps coincidental and of limited applicability.

In the following, we shall show that this is not the case: QLB can be shown to fall within the *general* theory of operator splitting, as applied to the Dirac equation.

This might have potentially deep implications for both classical and quantum computing, because it implies that, by splitting time along the three spatial directions, and augmenting the stream-collide dynamics with proper global rotations, quantum information (the Dirac wave function) propagates in space-time as a classical statistical process (Boltzmann distribution). It would be of great interest to explore whether such insight could be used to simulate the Dirac equation on trapped-ion analogue computers based on the QLB dynamics [13].

The starting point of the general operator splitting theory is the formal solution of the Dirac equation given by

$$\psi(t_{n+1}) = T \exp\left[-i \int_{t_n}^{t_{n+1}} H(t) dt\right] \psi(t_n) \quad (13)$$

$$\psi(t_{n+1}) = e^{-i\Delta t(H(t_n) + \mathcal{T})} \psi(t_n), \quad (14)$$

where $H(t)$ is the Dirac Hamiltonian, T is the time-ordering operator, and $\mathcal{T} = i\overleftarrow{\partial}_{t_n}$ is the “left” time-shifting operator. The second form of the solution was obtained in [14] and constitutes a great starting point for deriving approximation schemes. Then, the operator-splitting method consists of decomposing the Hamiltonian as $H(t) = \sum_{j=1}^N H_j(t)$ and approximating the evolution operator in Eq. (14) by a sequence of exponentials in the form

$$\psi(t_{n+1}) \approx \prod_{k=1}^{N_{\text{seq}}} \left[e^{-is_0^{(k)} \Delta t \mathcal{T}} \prod_{j=1}^N e^{-is_j^{(k)} \Delta t H_j(t_n)} \right] \psi(t_n), \quad (15)$$

where the coefficients $N_{\text{seq}} \in \mathbb{N}$ and $s_j^{(k)} \in \mathbb{R}$ are chosen to obtain an approximation with a given order of accuracy. It is then straightforward to conclude that the QLB scheme, shown in Eq. (12) and in Eqs. (3)–(6), corresponds to a particular decomposition of the Hamiltonian [15] and to a specific realization of Eq. (15).

The conclusion is far-reaching; the Majorana representation exposes a concrete connection between the (discrete) Boltzmann equation and the Dirac equation in Majorana form. As a result, the information contained in the quantum relativistic four-spinor $\psi(t, \mathbf{x})$ can be processed on entirely classical terms, i.e., free streaming along constant directions and local collisions, complemented with diagonalization steps to keep speed and spin constantly aligned. Remarkably, the scheme is also viable for prospective quantum computer implementations [7–9,16].

The QLB has been applied to a variety of quantum wave problems, mostly in the nonrelativistic context [17–19]. Here we present a new application to an important non-linear relativistic problem, namely, the Dirac equation augmented with Nambu–Jona-Lasinio dynamic symmetry breaking terms.

NJL-Dirac equation.—The NJL model was prompted by a profound analogy between the Bardeen-Cooper-Schrieffer theory of superconductivity and chiral symmetry breaking in relativistic quantum field theories [20,21] and it has served ever since as a model paradigm to study symmetry-breaking phenomena in both fields.

The NJL Lagrangian reads [20]

$$\mathcal{L}_{\text{NJL}} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi + \frac{g}{2}[(\bar{\psi}\psi)^2 - (\bar{\psi}\gamma^5\psi)^2]. \quad (16)$$

This corresponds to the free-particle Dirac Lagrangian, plus an interaction term, driven by the coupling parameter g . This coupling term reflects four-fermion interactions, in direct analogy with the BCS theory of superconductivity.

By imposing the chiral symmetry, the NJL Lagrangian should not present any explicit bare mass term, so we set $m = 0$. However, the NJL dynamics leads to the formation of a chiral condensate, corresponding to an effective mass term and a spontaneous symmetry breaking of the chiral symmetry. Much of the current interest in the NJL model is motivated by the fact that it serves as a phenomenological model of quantum chromodynamics (for a full account, see [22]).

The associated equation of motion reads (see the Appendix)

$$(\partial_t + \alpha_a \partial_a + im\beta)\psi = ig\beta[(\psi^\dagger \beta \psi) - (\psi^\dagger \beta \gamma^5 \psi)\gamma^5]\psi. \quad (17)$$

A solution of this equation is required for the quantum study of this model, in the mean-field approximation.

The space-time discretization of the NJL-Dirac equation can be cast in the standard QLB format by adding the nonlinear term into the collision step as in the case of the electromagnetic field, by replacing $C \rightarrow C_{\text{NJL}}$. The collision step becomes

$$\begin{aligned} \psi^{(c)}(t_{n+1}) &= C_{\text{NJL}} \psi^{(c)}(t_n) \\ &= T \exp\left[\int_{t_n}^{t_{n+1}} dt M_{\text{NJL}}(t)\right] \psi^{(c)}(t_n), \end{aligned} \quad (18)$$

$$M_{\text{NJL}}(t) \equiv -i\beta[m - g\rho_S(t)] - g\rho_A(t)\Sigma, \quad (19)$$

where $\rho_S \equiv \psi^\dagger \beta \psi$ and $\rho_A \equiv i\psi^\dagger \beta \gamma^5 \psi$ depend on time, hence the time-ordering operator, and $\Sigma \equiv \beta \gamma^5$. The time ordering can be approximated by using Eqs. (14) and (15): the ensuing ordinary exponential can be converted exactly to a 4×4 unitary matrix C_{NJL} . A similar treatment of the nonlinear term, albeit using spectral methods, can be found in [23].

Numerical application.—As an application of the QLB scheme, we simulate the emergence of a dynamic fermion mass as a result of the spontaneous breaking of the chiral symmetry of the NJL equation.

For this purpose, let us consider an initial condition given by the following Gaussian minimum-uncertainty wave packet,

$$\psi(t=0, z) = S_y \begin{bmatrix} -C_u e^{ikz} + C_d e^{-ikz} \\ C_u e^{ikz} - C_d e^{-ikz} \\ C_u e^{ikz} + C_d e^{-ikz} \\ C_u e^{ikz} + C_d e^{-ikz} \end{bmatrix} \frac{e^{-z^2/4\sigma^2}}{(2\pi\sigma^2)^{1/4}}, \quad (20)$$

centered about $z = 0$, with initial width σ . Let $\omega = k$ be the initial energy of the wave packet. The coefficients C_u and C_d obey the condition $2C_u^2 + 2C_d^2 = 1$, so that $\psi^\dagger \psi = |G_0|^2$. Moreover, an asymmetry can be set by tuning the ratio $C_u/C_d \equiv \alpha \neq 1$.

We analyze our numerical results for the case of $m = 0$, which ensures that the axial current is conserved by the

free part of the equation, as a function of the coupling coefficient g . For this test, the following parameter setting is used: $k = 0.006$, $\sigma = 48$, $C_u = 1.177$, and $C_d = 0.784$. Numerical results for $\rho(z) = |\psi|^2$ at times $t = 10, 50, 100$, and 200, for the case $g = 0, 1$, and 2, are shown in Fig. 1.

This calculation requires 200 time steps (for a mesh size of 1024 lattice sites) and about 0.01 CPU seconds on a standard PC. This amounts to a processing speed of about 20 MLUPS (million lattice updates per second), which is in line with the performance of lattice Boltzmann schemes for classical fluids. Since the latter is known to be very competitive, the same conclusion is likely to hold for the quantum case. A final statement in this direction must be left to detailed head-on comparison between QLB and state-of-the-art numerical methods for the Dirac and Schrödinger equations.

From Fig. 1, a symmetry breaking between the left- and right-moving wave packets is clearly seen at increasing values of g . The generation of a dynamic mass is expected to reflect into a slowing-down of the group velocity of the wave packets, according to $(v_{\text{group}}/c) = (k/\sqrt{k^2 + m'^2}) < 1$, where $m' = -g\rho_S$ is the dynamic mass of zero-rest mass particles. Indeed, since the initial condition is symmetric with respect to $1 \leftrightarrow 2$ exchange, the quantity ρ_A is initially zero, and remains such all along the simulation.

The results can be checked against the analytic solution to Eq. (17) in 1D and for the case of small g [24], which gives $v_{\text{mean}}/c \simeq 1 - 0.04g + \mathcal{O}(g^2)$ at early times. It can be checked (not shown for space limitations) that this is consistent with the numerical results in Fig. 1.

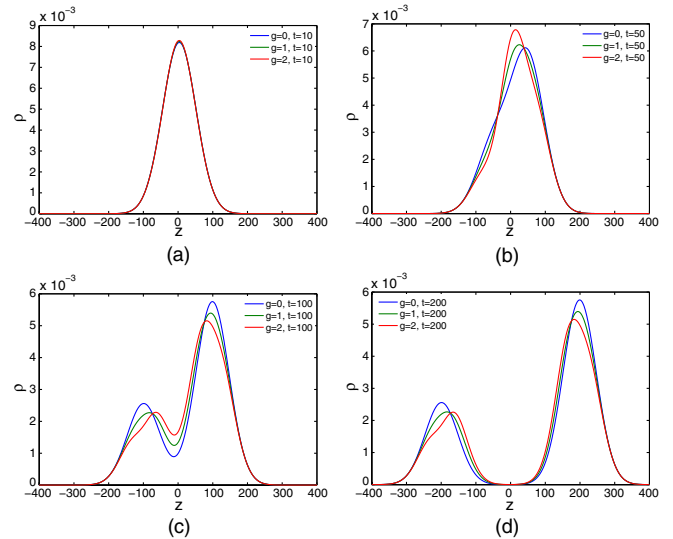


FIG. 1 (color online). $\rho = |\psi|^2$ at times (a) $t = 10$, (b) $t = 50$, (c) $t = 100$, and (d) $t = 200$ for $g = 0, 1$, and 2. The figure shows the separation of the left- and right-moving wave packets in the course of the evolution. The noninteracting case shows no deformation of the Gaussian profile, as expected, while the interacting case leads to a slowdown and deformation of both wave packets.

The same phenomenon can be simulated in two dimensions, and the details shall be presented in a future, lengthier publication.

Extending the above work to the case of quantum many-body systems and nonlinear multidimensional quantum field theory [25] represents an outstanding challenge for future research in the field.

Appendix: NJL-Dirac equation using Pauli representation.—From the NJL Lagrangian of Eq. (16), the associated equation of motion Eq. (17) is derived as follows. Variation of Eq. (16) against $\bar{\psi}$ delivers

$$(i\gamma^\mu \partial_\mu - m)\psi + g[(\bar{\psi}\psi)\psi + (\bar{\psi}\gamma^5\psi)\gamma^5\psi] = 0, \quad (\text{A1})$$

where $\gamma^5 \equiv i\gamma^0\gamma^1\gamma^2\gamma^3$ and $\bar{\psi} = \psi^\dagger\gamma^0$.

The actual definition of the gamma matrices depends on the specific chosen representation. By using Pauli-Dirac representation, γ^i matrices are defined as follows [26]:

$$\gamma^0 = \beta, \quad \gamma^i = \beta\alpha^i, \quad \text{with } i = 1, \dots, 3, \quad (\text{A2})$$

where β and α^i are the standard Dirac matrices.

Inserting these definitions into Eq. (A1), yields

$$(\beta\partial_t + \beta\alpha_a\partial_a + im)\psi = ig[(\psi^\dagger\beta\psi) - (\psi^\dagger\beta\gamma^5\psi)\gamma^5]\psi. \quad (\text{A3})$$

*filliong@CRM.UMontreal.ca

†silviapalpacelli@gmail.com

‡Also at Physics Department, Harvard University, Cambridge MA, 02138, USA.
succi@iac.cnr.it

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