Physica D 69 (1993) 327–332
North-Holland

SDI: 0167-2789(93)E0234-3

PHYSICA D

Lattice Boltzmann equation for quantum mechanics

S. Succi[a] and R. Benzi[b]

[a]*IBM ECSEC, European Center for Scientific and Engineering Computing, Viale Oceano Pacifico 171–173, 00144 Rome, Italy*
[b]*Physics Department, Universitá Roma II, Tor Vergata, Rome, Italy*

Received 20 November 1992
Accepted 24 June 1993
Communicated by U. Frisch

It is shown that the lattice Boltzmann equation for hydrodynamics can be extended in such a way as to describe non-relativistic quantum mechanics.

Interesting analogies between quantum mechanics (QM) and fluid-mechanics (FM) have been pointed out since the early days of the formulation of quantum theory [1]. Although it is nowadays (almost) universally accepted that these analogies are purely formal in nature, they retain nonetheless a valuable role for modeling purposes. In fact they often provide a physically sound and intuitive basis for the development of numerical methods aimed at the solution of evolutionary quantum equations [2].

In this paper, we present a new analogy between QM and FM that is mostly inspired by recent developments of the theory of the lattice Boltzmann equation (LBE), a fully discrete kinetic equation stemming from lattice gas cellular automata [3,4] (for a review see ref. [5]). It is shown that the non-relativistic Schrödinger equation results from the hydrodynamical limit of the relativistic Dirac equation pretty much the same way as the Navier–Stokes equations of fluid-dynamics are obtained as the large-scale limit of a discrete kinetic equation such as LBE. This means that the basic merits of LBE as a Navier–Stokes solver, i.e. case of implementation of complex boundary conditions and ideal amenability to massively parallel computing, can in principle be exported to the field of numerical quantum mechanics.

The hydrodynamic lattice Boltzmann equation is a fully discrete kinetic equation of the form

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i, t+1) - f_i(\boldsymbol{x}, t) = \sum_{j=1}^{b} \Omega_{ij}(f_j - f_j^{\mathrm{eq},2}) \qquad (1)$$

where f_i are the mean particle populations propagating along direction $\boldsymbol{c}_i$ and Ω_{ij} is scattering matrix mediating collisions between the ith and jth populations. Here $f_i^{\mathrm{eq},2}$ represents the equilibrium distribution function expanded up to second order terms in the flow field in order to retain convective effects. Formally, one has

$$f_i^{\mathrm{eq},2} = \frac{\rho}{b}(1 + c_{il}u_l + P_{ilm}u_l u_m) \qquad (2)$$

where $\rho = \Sigma_{i=1}^{b} f_i$ is the local flow density, $u_l = \rho^{-1}\Sigma_{i=1}^{b} c_{il}f_i$ is the local flow speed and the tensor P_{ilm} is projector along direction $\boldsymbol{c}_i$, $P_{ilm} = c_{il}c_{im} - (c^2/D)\delta_{lm}$. In order for eq. (1) to reproduce the Navier–Stokes equations in the continuum limit, the following sum-rules have to be fulfilled by the collision matrix

$$\sum_{i=1}^{b} \Omega_{ij} = 0_j , \qquad \sum_{i=1}^{b} c_{il}\Omega_{ij} = 0_{jl} , \tag{3}$$

which correspond to mass and momentum conservation respectively. In addition, fourth order tensors of the form $\Sigma_{i=1}^{b} c_{il}c_{im}P_{ino}$ must be isotropic to ensure rotational invariance at the macroscopic level. These conditions are fulfilled only by a restricted class of lattices, the most popular being the hexagonal lattice proposed by Frisch, Hasslacher and Pomeau in two dimensions and the face-centred-hypercube in four dimensions [6].

By projecting eq. (1) upon the eigenvectors of the collision matrix, a set of finite-difference equations for the hydrodynamical fields ρ, J_l, S_{lm} (density, current and stress tensor) are obtained. In the limit where these finite differences can be replaced by the corresponding partial derivatives, and with the additional assumption that the stress tensor is adiabatically slaved to its equilibrium value.

$$\partial_t S_{lm} < \lambda(S_{lm} - S_{lm}^{\text{equil}}) , \tag{4}$$

λ being the leading eigenvalue of the collision matrix, these finite-difference equations are shown to converge to the Navier–Stokes equations of a continuum fluid with a viscosity $\nu \sim \lambda^{-1}$. Physically, λ is the particle mean free path in lattice units. As this quantity approaches zero, an increasing number of degrees of freedom take active part to the non-linear evolution of the system. This corresponds to the onset of strong self-interaction of the velocity field (fully developed turbulence). Hence λ^{-1} is the coupling parameter of the theory. Note that the inequality (4) is crucial in breaking the hyperbolic structure of LBE and turn it into a mixed parabolic-hyperbolic equation, as it is appropriate for a dissipative system such as the Navier–Stokes equations. In this respect LBE can be regarded as a hyperbolic approximation of the Navier–Stokes equations. Note in fact that LBE contains some redundancy with respect to Navier–Stokes because the number of populations f_i is higher than the number of hydrodynamic fields. The corresponding extra degrees of freedom, although unactive on a macroscopic scale, are crucial to maintain the correct symmetries of the microscopic dynamics. It is precisely this redundancy that, combined with the adiabatic assumption eq. (4), allows it to account for diffusive effects without introducing any second derivative. The beneficial effect is twofold: first, it relaxes the need of treating diffusion implicitly, as is usually required to bypass the severe constraints on the time-step imposed by stability arguments.

Second, and here lies the key advantage of the method, most of the computational work is placed upon the collision phase. Since this phase is completely local, no communication is required between neighbors, whence its outstanding amenability to parallel computing.

The central idea of this paper is that the nonrelativistic Schrödinger equation ensues from the relativistic Dirac equation under the same conditions which govern the passage from LBE to the Navier–Stokes equation. This analogy is most conveniently developed by starting from the representation of the Dirac equation in which all the spin matrices are real. For a free particle of mass m, this reads (in atomic units $\hbar = 1$, $c = 1$) [2]

$$[\partial_t + \alpha_{ij}^x\partial_x + \beta_{ij}\partial_y - \alpha_{ij}^z\partial_z]\psi_j = -im\alpha_{ij}^y\psi_j , \quad i,j = 1,4 , \tag{5}$$

where α and β are the standard 4×4 Dirac matrices. The analogy proceeds by attempting a formal parallel between the discrete speeds of LBE and the discrete spin states of the Dirac quadrispinor ψ.

More precisely, we formulate the following position:

$$f_i \rightarrow \psi_i ,$$
$$\boldsymbol{c}_i \rightarrow \boldsymbol{L}_{ij} \equiv (\alpha_{ij}^x, \beta_{ij}, -\alpha_{ij}^z) ,$$
$$\Omega_{ij} \rightarrow Q_{ij} \equiv -im\alpha_{ij}^y . \tag{6}$$

Let us examine these positions in light of the distinct physical nature of LBE and the Dirac equation. The basic difference can be summarized as follows:

(1) f_i is a real one-dimensional array of dimension b while ψ_i is a complex quadrispinor.

(2) c_{il} is a set of three one-dimensional arrays of size b, while L_{ij} is a set of three two-dimensional arrays of size 4×4.

(3) The matrix Ω_{ij} is real and symmetric while Q_{ij} is skew-symmetric.

According to point (1), the quantity $\rho_i = f_i^* f_i$ (instead of f_i) represents the probability density of finding a particle along the ith link. In this respect, point (3) is nothing but the necessary condition in order for the probability density $\Sigma_{i=1}^{b} \rho_i$ to be locally conserved.

As an immediate consequence of point (1) it is clear that the LBE formalism has to be extended to a complex-valued distribution functions. Point (2) is entirely related to the quantum nature of the spin variable. This quantum nature manifests itself in two ways: first, unlike usual three-dimensional vectors, only one component of the spin is measurable (conventionally we chose the z-axis). Second, once this component is fixed, its values are quantized to the binary set ± 1. While this latter property is automatically embodied in the LBE formalism (it is actually the starting point of our analogy!) the former requires a careful discussion.

To achieve a full correspondence between LBE and Dirac equations one should be able to:

(1) simultaneously diagonalize the three matrices L_{ij};

(2) fix b to the value of 4.

Point (1) is clearly forbidden for it would be equivalent to state the spin is a common three-dimensional vector. Point (2) seems also unachievable because of its incompatibility with the interpretation of f_i as a (complex) particle population propagating along the links of a three-dimensional lattice. In fact, by symmetry, one requires at least 2D propagation directions, i.e. 2 opposite pairs along each coordinate axis. Thus only the case $D = 2$ would seem consistent with point (2).

Hence, despite the appealing qualitative analogies, a deeper insight seems to reveal a basic quantitative clash between LBE and the Dirac equation.

Yet, we shall see that a way out of both these difficulties can be found.

The basic idea is to realize that, although the *simultaneous* diagonalization of the three matrices L is impossible, nothing prevents a sequential diagonalization of each of them *separately*.

Mathematically this is tantamount to saying that we can find two 4×4 transformation matrices X, Y such that $L^x = X^{-1} L^x X$ and $\tilde{L}^y = Y^{-1} L^y Y$ are diagonal with eigenvalues ± 1. Straightforward algebra yields

$$X = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 \end{pmatrix},$$

$$Y = -\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}. \tag{7}$$

This means that one is given the possibility of working with three distinct formulations of the same equation, each having one diagonal streaming operator along x, y, z respectively. This immediately suggests operator splitting. Within operator splitting techniques, the evolution from t to Δt driven by the operator $L = L^x + L^y + L^z$ is splitted into three separate steps, each driven by L^x, L^y, L^z respectively. More precisely, the scheme proceeds as follows:

Propagation along $z(P_z \equiv P + \Delta z \hat{k})$:

$$f(P_z, t + \Delta t) = (1 + Q\,\Delta t) f(P, t)\,, \tag{8a}$$

Propagation along $y(P_{yz} \equiv P + \Delta y \hat{j} + \Delta z \hat{k})$:

$$f^y \equiv Yf\,, \quad Q^y = Y^{-1} Q Y\,, \tag{8b}$$

$$f^y(P_{yz}, t + \Delta t) = (1 + Q^y\,\Delta t) f^y(P_z, t + \Delta t)\,. \tag{8c}$$

Propagation along $x(P_{xyz} \equiv P + \Delta x\hat{i} + \Delta y\hat{j} + \Delta z\hat{k})$:

$$f^{xy} \equiv Xf^{y}, Q^{xy} = X^{-1}Q^{y}X, \tag{8d}$$

$$f^{xy}(P_{xyz}, t + \Delta t) = (1 + Q^{xy}\Delta t)f^{xy}(P_{xy}, t + \Delta t). \tag{8e}$$

Finally, the updated value at $P_{xyz} \equiv P + \Delta P, t + \Delta t$ can be restored according to

$$f(P + \Delta P; t + \Delta t) = X^{-1}Y^{-1}f^{xy}(P + \Delta P; t + \Delta t). \tag{8f}$$

With respect to a classical fluid, the quantum nature of the problem reflects in the extra-computations associated with the diagonalization procedure. However since the matrices Q^{y} and Q^{xy} can be prepared once forever right at the outset, they do not cause any additional overhead. Simply, instead of a single matrix Q, one has to use a triplet of distinct matrices Q, Q^{y}, Q^{xy} each acting on the three nodes linking P to $P + \Delta P$ via P_z, P_{yz}, i.e., along a path lying on the coordinate axes. Hence, the only additional overhead is the one associated with the transformation from/to f to/from f^{y}, f^{xy}. It should be noted that, due to the non-commutativity of L^{x} and L^{y}, the above procedure introduces an error of the order of $[L^{x}, L^{y}]\Delta t^{2}$. This error is, however, within the same range of accuracy of the general discrete formulation.

The nice point about this scheme is that each of the three steps has the form of a 1D-LBE algorithm; i.e. propagation of two pairs of walkers moving along opposed directions. To better clarify this point, it is useful to rewrite the one-dimensional version of eq. (5) for movers propagating along z. According to the standard notation, we split the 4-spinor ψ into a pair of bispinors $\chi = (\chi_1, \chi_2)$ and $\eta = (\eta_1, \eta_2)$, where index 1, 2 refer to spin-up and -down, respectively. The Dirac equation reads as

$$\begin{aligned} &\partial_t u_{1,2} - \partial_z u_{1,2} = m d_{2,1}, \\ &\partial_t d_{1,2} + \partial_z d_{1,2} = m u_{2,1}, \end{aligned} \tag{9}$$

where $u_1 \equiv \chi_1, u_2 \equiv \eta_2$ are the up-movers along direction $+z$ and $d_1 \equiv \chi_2, d_1 \equiv \eta_1$ are the down movers. The above equations look exactly as a one-dimensional linear LBE for two pairs of movers along the z axis. After the appropriate diagonalizations, the same formal structure is obtained along the x and y axis.

We are now in position to prove the initial assertion according to which the Schrödinger equation ensues from the Dirac dynamics under the same large-scale and adiabaticity assumptions which govern the passage from the LBE to the Navier–Stokes equation. To this purpose we note that under the unitary transformation

$$\phi^{\pm} = 2^{-1/2}(u \pm \mathrm{i}d)\exp \mathrm{i}mt, \tag{10}$$

the eqs. (9) are readily checked to turn into

$$\partial_t \phi^{+} - \partial_z \phi^{-} = 0, \qquad \partial_t \phi^{-} - \partial_z \phi^{+} = 2\,\mathrm{i}m\phi^{-}. \tag{11}$$

From these, one sees that, after adiabatic elimination of the "fast" antisymmetric mode

$$|\partial_t \phi^{-}| \ll 2m|\phi^{-}|, \tag{12}$$

the "slow" symmetric mode ϕ^{+} obeys the Schrödinger equation for a free particle of pass m. Again, the analogy between eq. (4) and (12) needs some clarification. In the case of eq. (1), the damping factor λ is real which means that fast transient modes die out in a time lapse of the order of λ^{-1}. This is also the time taken by the stress tensor to be slaved to its equilibrium value. In the quantum case, the damping factor is purely imaginary, so that fast modes never die out but just oscillate with a frequency of the order of c^{2}/ν^{2} times higher than slow hydrodynamic modes. Note that in physical units the inequality (12) can be written as $\omega^{-} \ll \omega^{+}\beta^{-2}, \omega^{+}$ being the De Broglic frequency associated with a particle of momentum p ($\omega^{+} = 2\pi\nu p/h$). These modes, in close analogy with the redundant populations of LBE, although needed to guarantee relativistic covariance, are not observable on a macroscopic time scale longer than

$1/\omega^-$. This is precisely the scale marking the transition from the covariant, hyperbolic Dirac dynamics to the non-covariant parabolic dynamics of the Schrödinger equation (diffusion in imaginary time). Note that, unlike the classical case in which this transition carries along irreversibility, both quantum dynamics remain reversible because the damping factor is purely imaginary. This basic physical difference has some important implications on the numerical scheme, as will be detailed in the following. Equation (1) can be regarded as an explicit first-order Lagrangian scheme proceeding along the characteristic directions c_i of the lattice. Standard stability analysis reveals that this scheme is linearly stable and free of numerical dispersion under the sole constraint that the spectrum of the collision matrix be confined to the interval $(-2, 0)$. Such an explicit scheme cannot, however, be straightforwardly applied to the quantum case without incurring in unconditionally unstable modes growing like $\exp \gamma\, \Delta t \sim 1 + m^2\, \Delta t^2$. The unstable modes can be stabilized, and unitarity restored, by adopting a linearly implicit scheme. This consists of evaluating the collision operator as a weighted average between time t and $t + \Delta t$. Choosing 0.5 as a weighting factor (Cranc–Nicolson scheme) we obtain

$$\hat{u} - u = -m\Delta t(d + \hat{d})/2\,,$$
$$\hat{d} - d = m\,\Delta t(u + \hat{u})/2\,, \qquad (13)$$

where $\hat{u} \equiv u(z + \Delta z, t + \Delta t)$ and $\hat{d} \equiv d(z - \Delta z, t + \Delta t)$. This is equivalent to an explicit LBE with a modified collision matrix $(1 - Q\,\Delta t/2)^{-1}(1 + Q\,\Delta t/2)$:

$$\hat{u} - u = 2\mu(1 + \mu^2)^{-1}u - 2\mu^2(1 + \mu^2)^{-1}d\,,$$
$$\hat{d} - d = 2\mu^2(1 + \mu^2)^{-1}u - 2\mu(1 + \mu^2)^{-1}d\,, \qquad (14)$$

where $\mu = m\,\Delta t/2$. It is easy to show that this system leads to the following dispersion relation $(\omega \equiv \omega_R + i\omega_L)$

$$\omega_R - kc = \frac{1}{\Delta t}\tan^{-1}[2\mu(1 - \mu^2)^{-1}]\,, \qquad \omega_L = 0\,, \qquad (15)$$

which is stable and coincides with the continuum dispersion relation $(\omega_r - kc = 0)$ up to corrections of order μ^3.

Eqs. (14) can be regarded as the LBE form of the Schrödinger equation in the sense that on a timescale longer than $1/m$ and provided that $m\,\Delta t \ll 1$ to avoid spurious numerical corrections, their continuum limit yields the Schrödinger equations for a free particle of mass m. The present formalism is straightforwardly extended to the case of a matter field interacting with a vector potential A_μ, $\mu = 1.4$. As is well known, the interacting Dirac equation is obtained from the non-interacting one by the replacement $p_\mu \equiv i\partial_\mu \rightarrow (p_\mu - eA_\mu)$. From the point of view of the LBE formalism the presence of the vector potential translates into an effective mass matrix $m\beta_{ij} \rightarrow m\beta_{ij} + \beta^{-1}_{ik} A_\mu L^\mu_{kj}$ $(L^0_{kj} = \delta_{kj})$ which contains the interaction between the fields A_μ and ψ via a quadratic coupling. This can be interpreted as the counterpart of the LBE equilibrium term f^{equil} which contains a "hidden" quadratic dependence on the field f (self-interaction) via the local flow field u. In other words, while in FM the local field is dragged to a local equilibrium depending on the field itself, in QM the local field oscillates around a local equilibrium which is fixed by the vector potential A_μ. Due to presence of the vector potential, the Dirac equation can be written in a conservative form as

$$\partial_t \rho + \partial_l J^l = ig\, A_l J^l \qquad (16)$$

where $J^l = \Sigma^4_{i,j=1}\, \psi^*_i \alpha^l_{ij} \psi_j$ and $g = e^2/hc$ is the fine-structure constant (i.e. the analogue of λ^{-1} in lattice units).

This highlights an important difference with respect to fluid mechanics. In FM the self-interaction enters at the second-order level in the moments hierarchy, through the equilibrium stress tensor which results from projection of $f^{eq.2}$ upon the second order tensor P_{ilm}. Since the equilibrium population depends on P_{ilm}, fourth-order tensors of the form $P_{ilm}P_{ino}$ are

needed to describe the non-linear self-interaction of the velocity field. On the contrary, in QM, the interaction is already present at the zero-th level of the moment hierarchy in the form of a mass production/annihilation term.

Hence, while hydrodynamics imposes stringent isotropy requirements on fourth-order tensors, only second-order tensors are involved by QM. This has a definite impact on the computational complexity of the algorithm.

In conclusion, this work presents a two-fold result. From the theoretical viewpoint, it shows that QM and FM can be described within the unique framework of a (suitably extended) discrete kinetic theory. From the practical point of view, it suggests that a judicious combination of operator splitting and implicit time marching may lead to an efficient numerical scheme for solving the time-dependent Schrödinger equation. In other words, the lesson learned in FM, i.e. that for certain flows it may be more convenient to solve a hyperbolic superset of the Navier–Stokes equations (the lattice Boltzmann) rather than the Navier–Stokes equations themselves, can be exported to QM. The emergence of massively parallel computing implies that it may sometimes be convenient to tackle non-relativistic problems using a relativistic (hyperbolic) formalism[#1]. Given the fact that one of the basic merits of LBE is the ability to deal with grossly irregular boundary conditions, we may speculate that the present scheme should be particularly useful to study wavefunctions in random potentials on massively parallel computers.

[1] Similar advantages have been recently pointed out in the contest of numerical relativity in ref. [8].

Acknowledgements

G. Betello and G. Parisi are kindly acknowledged for useful discussions and advises.

References

[1] E. Madelung, Z. Phys. 40 (1926) 332.
[2] K.C. Kulander, ed., Time Dependent Methods for Quantum Dynamics, thematic issue, Comput. Phys. Commun. 63 (1991).
[3] U. Frisch, B. Hasslacher and Y. Pomeau, Phys. Rev. Lett. 56 (1986) 15.
[4] G. McNamara and G. Zanetti, Phys. Rev. Lett. 61 (1988) 20;
F. Higuera and J. Jimenez, Europhys. Lett. 9 (1989) 663.
[5] R. Benzi, S. Succi and M. Vergassola, Phys. Rep. 222 (3) 1992.
[6] D. d'Humieres, P. Lallemand and U. Frisch, Europhys. Lett. 2 (1986) 291.
[7] L. Landau and E. Lifshitz, Relativistic Quantum Theory (Pergamon, Oxford, 1960).
[8] C. Bona and J. Masso, Phys. Rev. Lett. 8 (1992) 1097.