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# Lattice Boltzmann schemes for quantum applications

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**Abstract**

We review the basic ideas behind the quantum lattice Boltzmann equation (LBE), and present a few thoughts on the possible use of such an equation for simulating quantum many-body problems on both (parallel) electronic and quantum computers. © 2002 Published by Elsevier Science B.V.

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## 1. Quantum mechanics and fluids

Intriguing analogies between quantum mechanics and fluid mechanics have been pointed out since the earliest days of quantum theory [1]. The orthodox tenet is that these analogies are purely formal in character and do not bear upon the basic physics of quantum phenomena. A less-orthodox, albeit not minor, stream of thought insists instead that quantum mechanics, and notably Heisenberg's uncertainty principle, are nothing but a mirror of our ignorance of the underlying (hidden) microscopic physical level. This leads to the puzzling theory of 'hidden variables' which traces back to Einstein and subsequently to Bohm and others [2]. It is not our intent here to enter this fascinating and still open subject [3]. We turn to a practical question instead: what can the analogy do for us in terms of numerical modeling of evolutionary quantum mechanical phenomena? The question is legitimate because, regardless of its philosophical implications, the fluid analogy certainly provides an intuitive and physical sound basis to develop numerical methods for time-dependent quantum mechanics. In particular, it is reasonable to ask whether the advantages brought about by lattice kinetic methods in fluid dynamics can—by means of the fluid analogy—be exported to the context of quantum mechanics. Before we put forward our discrete kinetic theory version of the analogy, it is useful to provide a cursory survey of the main ideas behind the analogy itself. To this end, a short recap of basic notions of quantum mechanics is in order.

## 2. The fluid formulation of the Schrödinger equation

Let us begin with the Schrödinger equation for a non-relativistic quantum particle of mass $m$ in an external potential $V(\vec{x})$:

$$\mathrm{i}\hbar\partial_t\Psi = \left[-\frac{\hbar^2}{2m}\Delta + V(\vec{x})\right]\Psi, \tag{1}$$

where $\Psi(\vec{x},t)$ is the wavefunction of the material particle. Upon multiplying (1) by the complex conjugate

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$\Psi^*$, and the complex conjugate of (1) by $\Psi$ and then subtracting, we obtain the following set of fluid equations:

$$\partial_t \rho + \partial_a J_a = 0, \tag{2}$$

$$\partial_t J_a + \partial_a P = 0, \tag{3}$$

where, by using the eikonal representation $\Psi = \rho^{1/2} e^{i\theta}$:

$$\rho = |\Psi|^2, \tag{4}$$

$$J_a = \frac{\hbar}{m}\partial_a \theta \equiv \rho u_a, \tag{5}$$

$$P = \rho\left(\frac{u^2}{2} + \frac{V}{m} + \frac{V^Q}{m}\right), \tag{6}$$

and

$$V^Q \equiv -\frac{\hbar^2}{2m}\frac{\Delta\rho^{1/2}}{\rho^{1/2}} \tag{7}$$

is the famous quantum potential advocated by Bohm and coworkers to support the picture of quantum mechanics as an intrinsically non-local description of the microscopic world [4]. This configures quantum matter as an *ideal* (*inviscid, dissipationless*), *irrotational compressible* fluid. The inviscid character of the quantum fluid stems from the reversible nature of the Schrödinger equation, a diffusion equation in *imaginary* time. So much for the analogy in the continuum. What about the discrete lattice world? Interestingly enough, this analogy becomes even *more* compelling once transposed into the language of the lattice world. In fact, the lattice formulation naturally calls for an an "upgrade" from the non-relativistic Schrödinger equation to its relativistic associate, the Dirac equation. Symbolically, the analogy goes as follows (*DE*: Dirac equation, *SE*: Schrödinger equation, *LBE*: Lattice Boltzmann equation, *NSE*: Navier–Stokes equation):

$$DE \to SE, \tag{8}$$

$$LBE \to NSE. \tag{9}$$

### 2.1. Fluid formulation of relativistic quantum mechanics

To unfold this analogy, it proves expedient to cast the Dirac equation into a form where all streaming matrices, known as Weil matrices, become real. This is the so-called *Maiorana form*: In a compact four-dimensional notation, this reads

$$\left[W^\mu_{jk}\partial_\mu\right]\psi_k = iM_{jk}\psi_k, \quad \mu = 0, 3 \tag{10}$$

with

$$W^0_{jk} = \delta_{jk},$$
$$W^1_{jk} = \alpha^x_{jk}, \quad W^2_{jk} = \beta_{jk}, \quad W^3_{jk} = -\alpha^z_{jk},$$
$$M_{jk} = -im\alpha^y_{jk} + qV\delta_{jk} + A^a_{jk}J_a,$$

where all matrices have the standard meaning. Here $J^\mu A_\mu \equiv qV + J_a A^a$ is the interaction of the elementary charge $q$ with an external electromagnetic field described by the 4-vector potential $(V, A^a)$.

A scalar product of Eq. (10) with $\psi^*_j$ yields the desired set of continuity equations:

$$\partial_t \rho_j + \partial_a J^a_j = S_j, \quad j = 1, 4 \tag{11}$$

where $\rho_j = \psi^*_j\psi_j$ is the partial density of the $j$th fluid, $J^a_j = \psi^*_j\alpha^a_{jk}\psi_k$ the corresponding current density, and $S_j = i\psi^*_j M_{jk}\psi_k$ is a "chemical" source term transferring mass across the different components of the relativistic mixture. Note that in the above expressions only the index $k$ is summed upon. Unitarity, read norm conservation, implies $\sum_j S_j = \sum_{jk}\psi^*_j M_{jk}\psi_k = 0$. This is automatically secured by the antihermitian character of the mass matrix: $M_{kj} + M^*_{jk} = 0$. As promised, the fluid analogy comes by *more* naturally than in the non-relativistic case, because the Dirac equation only involves first order derivatives. Another pleasing feature is that the external interaction is easily accommodated into a formal redefinition of the mass matrix, without compromising the local nature of the theory. The fluid interpretation of the Dirac equation is equally transparent: four types of *spinning particles* stream in space and, once on the same space-time location, they interact via the "scattering matrix" $M_{jk}$. A qualitative difference with classical particle motion is apparent, though. In a classical fluid, particles do not "mix" during the streaming phase. A type-1 particle at location $x$ at time $t$ with speed $v$ propagates to $x + v\,dt$ at time $t + dt$ and it is still entirely of type 1.

A relativistic particle however undergoes mixing during free propagation, because its spinning motion implies a rotation around the direction of motion which mixes up the four spinorial components. This is why the streaming matrix is generally non-diagonal, echoing the fact that spin is not an ordinary vector. This suggests that the discrete space-time of a relativistic particle should be represented by a 'hypernet-

ted lattice' in which each link is made up of four distinct but communicating channels, one per spinorial state. This "Hypernetted Lattice Theory" is less of a joke than it seems. It has been recently realized that lattice formulations of field theory based upon spinning particle motion may offer potential advantages over more popular techniques such as path-integration [5]. This is because in quantum lattice models "*instead of seeking discretized versions of the Hamiltonian or the Lagrangian, a discretized version of the evolution operator is introduced*" [5]. In fact, what this author finds is that "*the rotation group, the Lorentz group and spin emerge automatically in the continuum limit from unitary dynamics on a cubic lattice*". The reader fond of more details is directed to the original reference.

### *2.2. Dirac to Schrödinger: the adiabatic approximation*

As noted in [6], the way the Schrödinger equation is obtained as a long wavelength (low energy) limit of the Dirac equation involves a sort of adiabatic approximation which is formally very similar to the low-Knudsen adiabatic expansion taking the (lattice) Boltzmann equation into the Navier–Stokes equations. The formal parallel emerging from this analogy is

$$Kn = l_\mu / l_M \sim \beta = v/c, \tag{12}$$

where $l_\mu$ is the particle mean free path, $l_M$ a typical coherence length of the macroscopic fluid and $\beta$ is the relativistic particle to light speed ratio. Detailed calculations can be found in the original reference [6] and need not be repeated here.

The relativistic motion implies that any particle of momentum $p_a$ is invariably associated with an antiparticle with opposed momentum $-p_a$. The symmetric combination of these two gives rise to a smooth, emergent field, $\phi^+$, whereas the antisymmetric combination defines a low amplitude, high-frequency mode which decouples from the system dynamics in the limit $\beta \to 0$. The scenario is exactly the same as the adiabatic approximation in kinetic theory, with a key difference. Kinetic theory describes dissipative phenomena in which adiabatic elimination wipes out the initial conditions, the transient modes die out, never to return. Quantum mechanics is reversible, and fast modes never die out: they just oscillate so fast that any observation on timescales longer than their period of oscillation simply overlooks them. But they are still there and more resolved (higher energy) measurements could always bring them back again. Note that it is the fast mode, not the antiparticle mode that fades away; the particle–antiparticle twin-link does not dissolve even in the low energy limit.

Another interesting remark concerns the symmetry breaking induced by a non-zero mass $m$. If $m$ is made zero the up and down walkers do not see each other and go across with no interaction, the result being the wave equation for photons. Manifestly this is a singular limit which cannot be described by the Schrödinger equation (diffusion coefficient goes to infinity). Any non zero mass causes "collisions" which slow down the wavepackets and confer them a subluminal speed $v < c$ as it befits material particles.

### *2.3. The interacting case*

Interactions with an external or self-consistent fields are readily included by a minor extension of the "collision operator". They read as follows:

$$\partial_t u_{1,2} - \partial_z u_{1,2} = m d_{2,1} + \mathrm{i} g d_{2,1}, \tag{13}$$

$$\partial_t d_{1,2} + \partial_z d_{1,2} = -m u_{2,1} + \mathrm{i} g u_{1,2}, \tag{14}$$

where $g = eV/\hbar$ is the coupling frequency of the potential. Self-consistent potentials, such as those arising in connection with the non-linear Schrödinger equation, are easily accommodated by making $g$ a function of the local density $u^2 + d^2$.

## 3. The quantum lattice Boltzmann equation

We are finally in the position to reformulate the basic analogy in quantitative terms. This is based on the following position: *The* 4*-spinor* $\psi_j(\vec{x}, t) \equiv \psi(\vec{x}, \vec{s}_j, t)$ *is identified with a complex discrete particle distribution* $f_i(\vec{x}, t) \equiv f(\vec{x}, \vec{v}_i, t)$. The analogy is tantalizing, but a minute's thought reveals two severe flaws:

(1) While the 4-spinor $\psi_j$ (we consider spin 1/2 throughout) has always four components in any dimensions, the discrete population $f_i$ is a set of $b$ real functions with $b$ a sensitive function of space dimensionality.

(2) While LBE streaming is always diagonal in momentum space, the three Weil matrices can*not* be simultaneously diagonalized.

Both problems are intimately related to the quantum nature of the spin variable. Fortunately, there is a way out. As observed in [6] in the limit of 'small' timesteps, actually much shorter than the inverse Compton frequency $\omega_c^{-1}$, *both flaws can be circumvented by decomposing the three-dimensional particle motion into a sequence of three one-dimensional motions along the coordinate directions* $x, y, z$. The technical key to achieve this task is a well known tool-of-the-trade in computational fluid dynamics: "Operator Splitting". The main use of operator splitting in Computational Fluid Dynamics is to handle 3D problems as a sequence of lower dimensional ones. In quantum field theory, a very similar technique goes under a different name: "Trotter formula": $e^A = (e^{A/n})^n$ with $n$ integer and $A$ any 'reasonable' operator. Consider the formal solution to the Dirac equation for a massless particle (the collisional operator plays no role at this stage):

$$\Psi_j\left(x^\mu + \mathrm{d}x_\mu\right) = \left[e^{\mathrm{d}t\sum_{\mu=0}^{3} W_{jk}^{\mu}\partial_\mu}\right]\Psi_k(x^\mu). \tag{15}$$

Manifestly, the propagator taking the wavefunction from $x^\mu \equiv (x, y, z, t)$ to $x^\mu + \mathrm{d}x^\mu \equiv (x + \mathrm{d}x, y + \mathrm{d}y, z + \mathrm{d}z, t + \mathrm{d}t)$ is the direct product of three one-dimensional partial propagators $P^a \equiv e^{\mathrm{d}t[\partial_t + W_{jk}^a\partial_a]}$, $a = x, y, z$ (no summation upon $a$ implied). This is the natural consequence of the additivity of the streaming operator. This expression is a good starting point for "conventional" numerical treatment of the Dirac equation [7], but is definitely unsuitable to a quantum LBE formulation because spinorial states get mixed during the propagation step, something that would not occur to a classical particle.

Therefore, a naive application of operator splitting is not viable.

However, we can argue that we *do not* need to work with the same representation of the Dirac equation during the three separate streaming steps. As long as we are able to develop a recipe securing uniqueness of the representation in $x_\mu$ and $x_\mu + \mathrm{d}x_\mu$, we are free of choosing the representation that better fits our needs. The idea is to perform each 1D partial streaming in the representation where the corresponding Weil matrix is diagonal. In practice, one propagates along one direction, say $x$, then 'rotates' the system so as to diagonalize the Weil matrix along, say, $y$, so that propagation along $y$ can be performed like for a classical particle, and finally 'rotates back' the propagated solution at $(x + \mathrm{d}x, y + \mathrm{d}y, t + \mathrm{d}t)$. New errors are introduced in the numerical treatment, but we shall argue that they are $O(\mathrm{d}t^2)$, namely within the general accuracy of the LBE method.

The quantum LBE bears many similarities with other quantum lattice schemes discussed in the recent [5,8,9] and not so recent [10] literature. What sets it apart from all these schemes is the fact of insisting on a diagonal representation of the Weil matrices, so as *to retain the notion of classical trajectories as much as we can*. In fact, the "turn" operator $R$ can formally be interpreted as an "internal scattering" between particle–antiparticle states [9], thus leaving the concept of quantum trajectory still well defined, although in a generalized sense. In a pictorial sense [10], we might say that while classical particles just "Stream and Collide", quantum particles, like swimmers, need a somersault before they can turn in space: they "Stream, Turn and Collide"! The 'Turn' step is a necessity induced by the internal structure of the relativistic particle.

Leaving the details to the original work, here we simply report the final result for a pair of 'up' and 'down' walkers in one-dimension. Upon using a Cranck–Nicholson time-marching procedure (securing unitarity of the numerical scheme), the quantum LBE takes the following form:

$$u(z + \mathrm{d}z, t + \mathrm{d}t) = Au(z, t) + Bd(z, t), \tag{16}$$

$$d(z - \mathrm{d}z, t + \mathrm{d}t) = Ad(z, t) - Bu(z, t), \tag{17}$$

where

$$A = \frac{1 - \Omega/4}{1 - \Omega/4 - \mathrm{i}g}, \tag{18}$$

$$B = \frac{m}{1 - \Omega/4 - \mathrm{i}g}, \tag{19}$$

$$\Omega = m^2 - g^2. \tag{20}$$

A few comments are in order.

First, with $g = 0$ (no-interaction), implicit time marching translates into a mere redefinition of the particle mass $m \to m' = m/(1 - m^2/4)$. By reinstating the time-step $\Delta t$, it is easily recognized that

$m' \to m$ in the limit $\Delta t \to 0$, which means that quantum LBE fulfills the requirement of numerical *consistency*. Large timesteps $m\Delta t > 1$ lead to unphysical results, as it is to be expected since the natural Compton frequency $m$ (in atomic lattice units $\hbar = c = \Delta t = \Delta x = 1$), is no longer resolved. Simple algebra also shows that quantum LBE is *unconditionally stable and* norm-preserving (the all-important unitarity condition). This is fairly remarkable for an explicit numerical scheme [11], and ultimately traces back to the (implicit) lightcone discretization hidden behind the quantum LBE, Eq. (16). Finally, note that at no point in our treatment did we need to care about stringent symmetry requirements: apparently a simple cubic lattice is good enough to our purpose. This probably relates to the diagonal nature of the quantum-mechanical pressure tensor and to the fact that, unlike fluid dynamics, the theory is *not* self-interacting. Finally, we observe that quantum LBE is as computationally lean and amenable to parallel processing as an explicit scheme can be.

All in all, a good set of credentials for a numerical scheme.

## 4. Numerical tests

The quantum LBE scheme has been validated on a series of one-dimensional textbook calculations, including

(i) free particle propagation,
(ii) harmonic oscillator,
(iii) scattering from a rectangular barrier [12].

In addition, the scheme has also been demonstrated for simple cases of non-linear Schrödinger equations of direct relevance to Bose–Einstein condensation [13] (as an example, see Fig. 1). These tests provide evidence of the viability of the quantum LBE in one-dimension. The scheme performs efficiently and, what's more, provides *stability* and *unitarity* at a time, a very valuable property for an explicit scheme. As we said, this is related to the peculiar light-cone space-time marching technique inherent to quantum LBE. Higher-dimensional versions akin to the quantum LBE discussed here have been developed systematically by Boghosian and coworkers [8].

## 5. The quantum $N$-body problem

In this section we shall explore the question of whether/what the lattice techniques discussed so far can bring any new insight into the problem of solving the Schrödinger equation for a collection of, say, $N$ particles (quantum $N$-body problem):

$$i\hbar\partial_t \Phi = \sum_{n=1}^{N} \big[-\Delta_n + V(X_n)\big]\Phi, \tag{21}$$

where $X_n = (x_n, y_n, z_n)$ is the spatial coordinate of the $n$th particle, $\Phi(X_1 \ldots X_N)$ the $N$-body wavefunction and $V$ the interparticle potential, typically in a two-body format $V(X_n) = \sum_{m>n} V(|X_n - X_m|)$. It has been recently pointed out [9] that quantum lattice algorithms constitute excellent candidates as numerical schemes for quantum computers. In the $N$-body quantum LBE, each quantum particle is represented by $bG$ walkers, $b$ being the coordination number of the lattice, namely the number of discrete momentum states attached to each lattice site. These walkers move around according to a fictitious microdynamics whose macroscopic limit is precisely the $N$-body Schrödinger equation.

What would this $N$-body quantum LBE algorithm look like?

"Simply" evolve $N$ replicas of the single-particle quantum LBE scheme and tie them up together via a two-body potential collecting the sum of all contributions $V_g^n = \sum_{g'} \sum_m V(X_g^n - X_{g'}^m)$ at each given site $X_g^n$. If one does not insist on the idea of a particle generalized-trajectory, and turns instead to a 'information-network' picture, a generic quantum lattice algorithm would take the form of a first-order, explicit, non-local, map for the complex array $\Phi_j$:

$$\Psi_j(X,t) = \sum_k T_{jk}\Psi_k(X - V_k\Delta t, t - \Delta t), \tag{22}$$

where $V_k$ scans the $3N$-dimensional neighborhood of $X_n = (x_n, y_n, z_n)$, $n = 1, N$ and $T_{jk}$ is the complex transfer matrix fulfilling the unitarity condition $\sum_l T_{jl}T_{lk} = \delta_{jk}$. The kinetic energy operator is sweet since any walker in a given single-particle state can be moved independently of the others, resulting in a linear $O(bGN)$ complexity. Unfortunately, the two-body long-range potential generates a daunting quadratic complexity, $(bGN)^2$, to say nothing of the $(bG)^N$ requirement in computer storage.... The scheme meets

with a "exponential complexity wall" which rules out any possible use of conventional electronic computers for more than a few hundreds particles [17]. Although this statement can probably be challenged by modern multiscale techniques (Achi Brandt, private communication), we shall assume that such exponential complexity is indeed beyond electronic computation capabilities. This brings us back to quantum computers. Since the matter of solving the $N$-body Schrödinger equation in full on a quantum computer has been described in the existing literature, here we shall take a different path, and discuss how efficient real-space single-particle quantum solvers may contribute to advancing the $N$-body frontier *without solving the full $N$-body Schrödinger equation*. Incidentally we note that this is of actual interest not only for current electronic parallel computers, but hopefully also for actual *software emulators of quantum computers* [14,15].

### 5.1. Quantum LBE and Density Functional Theory

As previously discussed, numerical algorithms for the quantum many-body wavefunction are very hard (to say the least) on electronic computers. Many ways out have been developed to cope with this problem, including,

(i) Quantum Monte Carlo techniques [18],
(ii) Multiscale methods [19],
(iii) Effective one-body theories.

In this paper, we shall be concerned with option (iii).

Effective one-body theories developed in the last fourteen years permit to learn a great deal about the properties of quantum many-body systems without ever invoking the use of many-body wavefunctions. Particularly successful in this respect is the famous Density Functional Theory developed in the 60's by Hohenberg–Kohn and Kohn–Sham [16,17]. The core idea of Density Functional Theory is that the ground state of a many-electron wavefunction (nuclei are regarded as classical particles on account of their higher mass) is uniquely determined by the electronic density $n(\vec{x}) = \sum_j |\phi_j|^2(\vec{x})$, where $\phi_j$ are one-particle orbitals. The ground-state energy can then be obtained by summing up the single-particle orbital energies obtained by solving the Kohn–Sham equations:

$$H_{\mathrm{KS}}\phi_j = E_j\phi_j, \tag{23}$$

where the Kohn–Sham Hamiltonian consists of four contributions

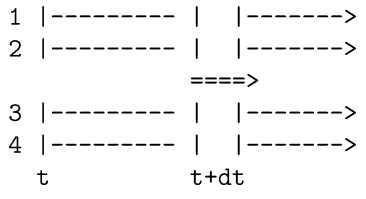
$$H_{\mathrm{KS}} = -\frac{\hbar^2}{2m}\Delta_j + V_{\mathrm{ext}}(\vec{x}) + \mathrm{e}^2\int \frac{n(\vec{y})}{|\vec{y}-\vec{x}|}\,\mathrm{d}\vec{y} + V_{\mathrm{ex}}[n]. \tag{24}$$

The first two contributions are the usual kinetic energy and external potential operators, the third one relates to the self-consistent Hartree–Fock potential. Finally, the fourth one is an effective 'exchange' energy functional which collects the effects of $N$-body interactions. The idea is that an effective functional of the electron density exists such that the ground state energy of a fictitious system of *independent* electrons moving in such a potential is *exactly the same* ground-state energy of the interacting system! Describing how such a magic comes about is certainly beyond the scope of this work. Here, we shall simply remark that Density Functional Theory heavily leans on the intuitive picture of a quantum many-body system as a backbone of ions tied up together by a very mobile *electronic fluid*. In this respect, it certainly puts a premium on efficient real-space solvers for the one-particle (non-linear) Schrödinger equation, both in the time-independent (ground-state) and time-dependent (excited states) form. A practical scheme which could be implemented today on either electronic or quantum computer emulators is briefly outlined in the following.

Consider the task of solving a set of $N$ effective time-dependent, one-particle, Kohn–Sham equations coupled via an effective potential $V_{\mathrm{KS}}[\rho]$:

$$\mathrm{i}\hbar\partial_t\phi_j = H_{\mathrm{KS}}\phi_j. \tag{25}$$

Since the LBE grid is uniform, the non-local Hartree–Fock potential is best turned into the corresponding Poisson problem $\Delta V_{\mathrm{HF}} = n$, which is efficiently solved by standard methods such as rapid elliptic solvers or Fast-Fourier techniques. The exchange functional is local and can therefore be handled by the same procedure already discussed and tested for Bose–Einstein condensation.




Sketch 1. Parallel solution of the set of $N$ Kohn–Sham equation ($N = 4$). The double line === indicates the serial phase in which each slave processor forwards its partial density to the master and subsequently receives the effective potential to initiate the next step.

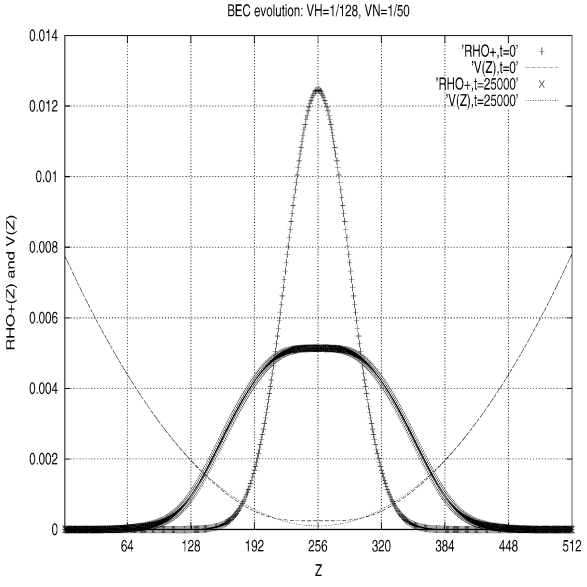



Fig. 1. Probability density $\rho^{+}(z)$ at $t = 0$ and $t = 25{,}000$ for the case of a self-consistent potential of the form: $V(z) = \frac{4V_H}{L^2}(z - z_0)^2 + V_N\rho$. The flattening of the wavefunction due to self-consistent interactions is well visible. The superscript $+$ indicates the slow, hydrodynamic mode.

The system of Eqs. (25) is also particularly well-suited to parallel computing. In fact, each of these equations can be advanced concurrently in time. Upon completing a single time-step calculation, each processor forwards its partial density $\rho_j(t + \mathrm{d}t) = |\phi_j^2|(t + \mathrm{d}t)$ to a master processor whose task is to collect all contributions, form the effective potential $V_{\mathrm{KS}}$ and send it back to each processor to initiate the next time step. This process can be performed fairly efficiently on a electronic parallel since it entails a very lean communication-to-computation ratio. For instance, a parallel computing consisting of $P = N$ processors would solve the $N$-body problem in (slightly more than) the same time it takes a serial one to solve the single-body quantum equation. Since the same statement applies to a *single-processor* quantum computer, one might dream of quantum-computers applications of paramount scientific problems, such as electronic structure calculations of large molecules of biological interest.

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