

# Comparison of Dynamic Diffusion with an Explicit Difference Scheme for the Schrödinger Equation

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We represent the method of dynamic diffusion for the approximate solution of Schrödinger's equation with decoherence and describe a swarm simulation as a proof of concept. Decoherence occurs as the divergence of the exact solution for the dynamics of the diffusion swarm, which arises when the total number of real particles grows. The method of dynamic diffusion cannot be reduced to the solution of differential equations, in contrast to Bohm's quantum hydrodynamics; hence, direct computer simulation is the mandatory next step. We compare the dynamic diffusion with the explicit finite differences scheme for the Schrödinger equation for some standard one-dimension cases.

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## 1. Introduction

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Experiments on quantum computers [1] show the necessity for developing quantum theory with many particles to investigate the decoherence problem. It is closely connected with the general theory of complex systems and processes, in which quantum effects play the key role. For a system with  $n$  real particles, we can write the Hamiltonian in the form of a general formula, not in the form of a matrix, because such a matrix would have  $\exp(n)$  dimensions; for example, if a value of  $n$  is accessible, the corresponding value of  $\exp(n)$  may be inaccessible due to its huge size. The possibility of writing the explicit formulas for Hamiltonian  $H$  factually also gives us the way to investigate fast quantum algorithms without launching them in reality. When solving the search problem, for example, the problem of finding the solution  $x_{\text{tar}}$  of equation  $f(x) = 1$  for a Boolean function  $f$  of  $n$  variables, we know neither  $f$  nor  $x_{\text{tar}}$ ; however, we can be convinced that

$(\pi/4)\sqrt{N/l}$  iterations of Grover's operator  $G$  gives us the state  $|x_{\text{tar}}\rangle$ , provided we start from the state with equal amplitudes [2]. Here is the force of Cartesian mathematics.

However, if we try to apply this result in practice, for example, to the solution of a certain equation  $f(x) = 1$ , we immediately meet the principal difficulty: the practical realization of the operator  $G$ , which acts in the space of  $N = 2^n$  dimensions. Therefore, to find the root  $x_{\text{tar}}$  of the equation, we must deal physically with a Hilbert space of exponential dimensions. At the same time, only some formulas reflecting general properties of  $G$ , such as its unitarity and its concrete expression as  $G = I_0 I_{x_{\text{tar}}}$ , are sufficient to establish convergence of the algorithm.

Attempts to make quantum computers scalable encounter a serious obstacle, which is usually treated as decoherence. Decoherence should be treated as the divergence of the real evolution of a quantum system from the exact solution of its Schrödinger equation. On the other hand, in the standard apparatus of quantum theory there are no intermediate forms of evolution between unitary dynamics and measurements, and the latter need an external subject, who has rights to measure (or to observe) a state of the small system at hand. We thus treat the observer not only as something (somebody) more complex than our system, but as the subject, whom we cannot include in the investigated system, in principal.

The standard formalism of quantum theory thus establishes the border between “simple” objects, to which we can apply quantum mechanics, and “complex objects,” to which quantum theory is not applicable. This conclusion is new because it follows from our inability to build a scalable quantum computer, at least at this moment. The fundamental role of decoherence forces us to look anew to the attempts of de Broglie and Bohm to build the explicit urn scheme for quantum probability. More exactly, we can call it the building of the “constructive version” of quantum theory, which can be applied to “complex objects” [3].

The method of collective behavior comes from the idea of Bohm about representing a quantum particle as an ensemble, which we call a swarm, of classical pointwise particles, which we call its samples. Each sample has not only its coordinates, but its own velocity. The genesis of this idea is attributed to de Broglie, who proposed the fundamental sense of the wave corresponding to the real particle, which has the dynamical characteristic of velocity. The impulse of the swarm in a given point then becomes connected with the phase  $S/\hbar$  of the wavefunction by the relation  $\nabla S = p$ . Based on this correspondence, Schrödinger derived his famous equation. However, the swarm representation of the quantum particle meets the following fundamental difficulty. In the Schrödinger equation there is the wavefunction  $\Psi$ , connected with the density of samples by the equality  $\rho = |\Psi|^2$ , and we thus have no direct connection between the dynamics and  $\rho$ . To

make sense for this application of the swarm, we have to require that its density is proportional to the density of the probability of the occurrence of the particle in a given point. Then samples must be presented in the time evolution; for example, each sample must have its own history. The dynamics of the swarm, consisting of behaviors of all samples, must approximate the exact solution of the Schrödinger equation for a sufficiently large time frame.

## 2. Bohm Approach

The problem of conservation of the individuality of the samples has been solved by Bohm, who proposed the swarm of classical particles, which are driven by the external potential  $V = V(\vec{r})$  and the so-called quantum potential

$$Q = -\frac{\hbar^2}{2m} \frac{\Delta R}{R},$$

where  $\Psi = R \exp(iS/\hbar)$ . The Schrödinger equation and the external potential  $V$  satisfy two real equations of the form:

$$\frac{\partial S}{\partial t} + \frac{p^2}{2m} + V + Q = 0, \quad (1)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left( \frac{1}{m} \rho p \right) = 0, \quad (2)$$

where equation (1) is the Hamilton–Jacobi equation for the characteristic function  $S$  of a sample, which is defined by the equations  $\nabla S = p$ ,  $\partial S / \partial t = E$ , where  $p = p(\vec{r})$  is its impulse,  $\rho(\vec{r}) = R^2(\vec{r})$ —the density of the swarm—and equation (2) shows the property of continuity of a swarm. This approach is called quantum hydrodynamics, because a quantum particle is represented here by a swarm of its classical samples, which obeys the law of classical dynamics, but its potential  $U = V + Q$  has the quantum summand  $Q$ , which depends on the density of the swarm in this point in time and space.

The algorithm modeling quantum dynamics by the hydrodynamical approach does the following at each step.

- Fulfills the free flight of all samples.
- Changes the speed of each sample according to the rule  $p(t + \Delta t) = p(t) - \nabla U$ .
- Changes the speed of each sample according to the rule  $p(t + \Delta t) = p(t) - \nabla U$ .

We see that the computation of the density of the swarm at each step is very important, because it is required for the computation of  $U$ , due to the addition of the quantum pseudopotential  $Q$ . We can consider that samples merely determine the nodes of division of configuration space, which is the base of the finite differences method for the solution of equations (1) and (2); the value of quantum hydrodynamics is thus limited by the possible acceleration of the solution of the Schrödinger equation. How valuable is this advantage of quantum hydrodynamics? We consider the case of many real particles, for example, a few tens of them. The density of the swarm will then be the density of the swarm in  $R^{3n}$  space, where  $n$  is the total number of particles. To conserve the initial accuracy of the approximation to

$$\rho(t) \approx |\Psi(t)|^2 \quad (3)$$

for the solution  $\Psi$  of the Schrödinger equation, we need to keep a constant linear spatial step, which results in the exponential growth of the total number of cells in the configuration space. To be able to compute derivatives from the density (we need three sequential), we must guarantee that each cell is full of samples that create the same difficulty as the direct solution of the Schrödinger equation for  $n$  particles. The single profit from the quantum hydrodynamics consists of the possibility of optimizing the grid for the finite differences scheme; this advantage is interesting, but it does not resolve our main problem.

### 3. Swarm with Dynamic Diffusion

The task of making explicit the mechanism for the acceleration of samples requires the satisfaction of conservation laws. If we are going to refuse to use the knowledge of density in the vicinity of the point at hand, we must ensure these laws for separate samples, which means the refusal to use such things as the quantum pseudo potential. First of all, we define this mechanism and write the equation on the string of samples through the border, which is induced by this mechanism; then we show that the Schrödinger equation can be reduced to this equation if we fix the grain of the spatial resolution. It turns out that our mechanism of dynamic diffusion critically depends on the choice of this grain, which causes some peculiarities of our approach. However, these peculiarities are an unavoidable price for the advantages we obtain with dynamic diffusion for many particles.

#### 3.1 Mechanism of Bond Creation and Annihilation

We will define the evolution of a swarm, which we call the dynamic diffusion, and which will consist of steps, each of duration  $\Delta t$ . But here the simple scheme from Section 2 is not sufficient, because the

swarm will be substantially transformed; hence, we define the step of evolution anew.

At each step we will have not samples, but simplexes. A simplex  $S$  of an order  $j$  ( $j \in N$ ) is a pointwise particle, which has its own coordinates  $\bar{r}(S)$ , speed  $v(S)$ , and internal shift  $sb(S)$ . Simultaneously, we will define at each step the new objects called bonds. Speaking informally, a simplex is some set of samples connected with each other by bonds, which roll with very high speed, so that their kinetic energy is large, whereas the speed of the simplex as the whole is low. Factually, the swarm will be divided into two fractions: separate samples, traveling with the largest possible speed  $c$ , and simplexes of orders  $j > 1$ , whose speed is much lower. This is the reason for the introduction of the waiting time: this is the time during which the simplex  $S$  flies, but which is not enough that  $S$  can overcome the distance to the neighboring cell. Furthermore, we will see in this section that the fixation of the division of space to cells is necessary for the simulation of quantum dynamics; this is why we cannot consider the continuous movement of simplexes.

For this we first of all define the procedure of association of a sample  $s$  with a simplex  $S$  of the order  $j$ . Let  $S$  be located in the cell  $\bar{r}$  and  $s$  be a sample that has just flown to this cell. We suppose that during the considered step the distance between  $s$  and  $S_j$  reaches its minimal value. We now suppose that the time flies continuously; it will not change the duration of the step, because of the fraction  $c/v(S)$ . At the instant when the minimal distance is reached, we establish the absolutely rigid connection between  $s$  and  $S$ , so these objects start to roll classically around their common center of masses; the resulting object we call a simplex of the order  $j + 1$ . Its speed  $v_1 = (v(s)m + v(S)M)/(m + M)$ , where  $m$ ,  $M$  are masses of  $s$  and  $S$ , respectively, results from the classical consideration of the system  $s + S$ ; the single nonclassical object here is the bond we introduced between  $s$  and  $S$ . We call this bond the main bond of the resulting simplex  $S_1$  and designate it as  $b(S_1)$ . We note that due to the absolute rigidity of the bond, it does not produce any work; the energy, impulse, and momentum of impulse are thus conserved in the course of association.

The process of bond elimination is exactly the reverse of the association; it results in a separate sample, which flies away from the simplex that becomes less than one in its order. The iteration of  $q$  times of the association, starting with  $S$ , gives us the simplex  $S'$ , whose order is  $j + q$ . Factually, a simplex of order  $j$  represents sequentially nested simplexes, each of which is the result of the association between some sample and the preceding simplex. The sequential dissociation goes in the reverse order.

Now we are ready to define the step of the main evolution. The step looks like the following sequence.

- For each simplex  $S$  we change  $sb(S)$  to  $sb(S) + v(S)\delta t$  and check the inequality  $sb(S) < d$ , where  $d$  is the distance to the closest neighboring cell along the direction of  $vS$ . If it is satisfied, we go to the next action; if it is violated, we shift  $S$  to the closest neighboring cell and put its internal shift to zero:  $sb(S) = 0$ .
- Each simplex obtains additional speed as  $b\delta t\nabla V/m$ , where  $V$  is some external potential,  $\delta t$  is the duration of the step,  $m$  is the mass of a sample, and  $b$  is some constant.
- From each simplex  $S$  we take  $[aj]$  last samples from  $S$  and sequentially eliminate the bonds connecting them with the simplex. We consider them as belonging to a thin layer and let them fly to the closest neighboring cells with the speeds they have, where  $j$  is the order of this simplex and  $a$  is some constant  $a \ll 1$ .
- After the arrival of each sample belonging to a thin layer from the closest neighboring cell, we associate it with the corresponding simplex and recalculate its speed by the law of association.

We call the effect of bond annihilation *peak explosion*, because it seems like the explosion of the simplex, where the hidden energy of rolling samples transforms to the visible kinetic energy of released samples, which fly out of the cell at hand. The third item says that these samples are immediately absorbed by the neighboring simplexes; their energy and impulse are thus captured by these simplexes. Peak explosion bears a resemblance to gas fraction; we can call the movement of simplexes following from the first point the liquid stream. The first and second items establish the rules for phase transition: from the liquid phase to the gas and vice versa. The velocity of gas fraction is much higher than that of the liquid phase; this is the representation of the nonrelativistic character of dynamics we are considering:

$$v_{\text{symp}} \ll c. \quad (4)$$

The principal difficulty is caused when  $\rho$  becomes too small, because here the corresponding simplex will obtain a speed comparable with  $c$ . In this case our definition of simplexes loses its validity, because this definition presumes that flying samples are presented to a cell when a simplex stays; this simplex cannot leave the cell until the sample associates with it. We note that this difficulty is the same as in the Bohm hydrodynamical approach; it is hardly possible to overcome it with swarms. On the other hand, the area where  $\rho = 0$  plays the principal role in the simulation of quantum dynamics; its influence shows immediately because of the great speed of gas fraction. In a quantum

swarm, no matter how it is treated (hydrodynamics or dynamic diffusion), it is impossible to make considerations local, as in ordinary hydrodynamics when we separate a “small cube” and consider a stream through its border. The reason is the existence of gas fraction. In addition we will have the more quantitative characteristic of this form of quantum nonlocality.

We choose the initial state of the swarm in such a form, where each cell is occupied by exactly one simplex; the density  $\rho(\bar{r})$  will then be proportional to the order of the simplex occupying the cell  $\bar{r}$ .

The evolution we have defined depends on the constant  $a$ , which is the intensity of the annihilation of the bond; we can treat it as  $1/\Delta T$ , where  $\Delta T$  is the average time of the life of the bond. The process of bond annihilation will thus be the result of a Poisson random process with the given intensity.

We now consider two neighboring cells  $x$  and  $x_1$  with a common border, as well as the density of the stream through this border  $p_{x, x_1}$ , and find its derivative  $dp(x, x_1)/dt$ . The density of the stream is the stream divided by the square  $\delta x^2$  of the border (i.e., the stream through the border of a unit-sized cube—we take it to pass from the quantity of the samples to the density); we call it simply the stream. Why do we focus on the stream variation, not the stream itself? Because the stream depends on the initial state of the swarm, which must be given in advance; we cannot derive it from the mechanism of the speedup of the samples. The mechanism of dynamic diffusion we defined influences the stream only through its variation, which is the dynamical magnitude, as a force. We will see that in the initial moment the stream is created by the movement of simplexes, whereas separate samples belonging to a thin layer create the variation of the stream.

Let  $j$  and  $j_1$  be the orders of the simplexes in the cells  $x$  and  $x_1$ , respectively. We must estimate the deposits to the steam variation from gas and liquid fractions separately.

### 3.1.1 Liquid Fraction: Inertia

We estimate the deposit of the first item. The function of density  $\rho$  typically has the strongly discontinuous form, where “peaks” are interspersed with “holes.” Of course, it is the influence of the fixation of  $\delta x$ ; we also recognize that it is unavoidable. To cope with this discontinuity, we can reform the first item and let samples fly by the annihilation of bonds, as in the second item. Here part of the  $a_l j$  samples will fly in the direction  $\bar{l}$ , where  $a_l = a_0 \bar{l} \cdot v(r)$ , where  $a_0$  is a small constant  $a_0 \ll a$ . This way of making  $\rho$  more continuous, however, violates the invariance with respect to the change of inertial read-

out system. Our mechanism must not depend on this choice. We make this agreement temporarily, in order to estimate the deposit of such part of the swarm, which belongs to the liquid phase, to the change of stream. Thus, this deposit will be  $v_{\text{norm}}(r) \nabla \rho(r)$ , where  $v_{\text{norm}}$  is the component of the speed of the swarm, orthogonal to the border, because it comes from the variation of the order of simplexes, which comes through this border.

### 3.1.2 Liquid Fraction: External Potential

This deposit equals  $b \rho \nabla V$ .

### 3.1.3 Gas Fraction

In view of the second item of our definition of a step, this stream equals the difference between the number of samples that flew from the cell  $x$  to  $x_1$  and the number of samples that flew in the opposite direction, that is, the difference between  $j$  and  $j_1$ . The deposit of gas fraction is thus  $a \nabla \rho$ .

We can make the following conclusion. If constants  $a$  and  $b$  are substantially larger than  $a_0$ , the change of the stream in the unit of time follows

$$\frac{dp_{x,x_1}}{dt} = a \nabla \rho + b \rho \nabla V. \quad (5)$$

This equation characterizes dynamic diffusion. To show that this mechanism can serve as the approximation of quantum unitary dynamics, we now have to derive it from the Schrödinger equation.

## ■ 3.2 Reducing of Schrödinger Equation to Swarm

We now consider the swarm, for which equation (3) is true where  $\Psi$  is an exact solution of the Schrödinger equation, and try to derive the evaluation of the stream variation from the Schrödinger equation directly, accepting some features of sample moving that agree with the mechanism of dynamic diffusion. Our aim is to show that this variation satisfies equation (5).

To ensure the main requirement of equation (3) we must define swarm density as

$$\rho(r) = \frac{N_d}{dx^3 N_{\text{total}}}, \quad (6)$$

where  $N_d$  is the number of samples occurring in a cube with center  $r$  and side  $dx$ ;  $N_{\text{total}}$  is the total number of samples in the swarm. To compare with the solution of the Schrödinger equation, we would

have to take limits in this definition  $\delta x \rightarrow 0$ , which would mean that we consider not one swarm but the sequence of swarms with densities  $\rho_n$  with increasing  $n$ . We will not do it in order to avoid useless complication; instead each time when it is necessary, we agree that it is possible to continue our division of the space into cubes so that  $\delta x$  will decrease in the admissible limits. We write  $\rho(x) = |\Psi(x)|^2$ , which means that

$$\rho_n(x) \rightarrow |\Psi(x)|^2 \quad (n \rightarrow \infty), \quad (7)$$

without special mention. Such a sequence of swarms realizing the approximation to the density of the wavefunction—the solution of the Schrödinger equation—we call the *admissible approximation of quantum evolution*. Now having this agreement, we fix the grain  $\delta x$  of spatial resolution. This fixation is necessary for computing of the stream variation. We call the stream with the fixed  $\delta x$  the *detailed stream*, to emphasize its substantial dependence on  $\delta x$ .

At first we show that there exists a quantum swarm with the local shifts of samples; for example, that equation (3) can be guaranteed by only shifting samples on the closest distances (i.e., between neighboring cells).

We would easily guarantee the satisfaction of equation (3) if we did not impose any limitations on the speeds of samples and on their changes. This means that samples can move any distance in the course of one step, and equation (3) will be true at each step with the required accuracy; it will be conserved in some time frame  $\delta t$ . However, this mechanism is useless because it depends on knowledge of the wavefunction, whereas our aim is to manage without the wavefunction at all.

We take up the quantum swarm, and start from the Schrödinger equation

$$i\hbar \frac{\partial \Psi(r, t)}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi(r, t) + V_{\text{pot}}(r, t) \Psi(r, t), \quad (8)$$

which we can rewrite as

$$\begin{aligned} \Psi_t^r(r) &= -\frac{\hbar}{2m} \Delta \Psi_t^i(r) + \frac{V_{\text{pot}}}{\hbar} \Psi^i(r), \\ \Psi_t^i(r) &= \frac{\hbar}{2m} \Delta \Psi_t^r(r) - \frac{V_{\text{pot}}}{\hbar} \Psi^r(r) \end{aligned} \quad (9)$$

for the real and imaginary parts  $\Psi^r$ ,  $\Psi^i$  of the wavefunction  $\Psi = \Psi^r + i\Psi^i$ . We are interested in the evolution of density only, for ex-

ample, the function

$$\rho(r, t) = (\Psi^r(r, t))^2 + (\Psi^i(r, t))^2.$$

We fix the value  $\delta x$  and apply for the approximation of second derivatives the difference scheme of the form

$$\frac{\partial^2 \Psi(x)}{\partial x^2} \approx \frac{\Psi(x + \delta x) + \Psi(x - \delta x) - 2 \Psi(x)}{(\delta x)^2} \quad (10)$$

for each time instant, provided the wavefunction satisfies all conditions for such an approximation. Since the addition of any constant to the potential energy  $V_{\text{pot}}$  does not influence the quantum evolution of the density, we can consider instead of  $V_{\text{pot}}$  the other, equivalent, potential  $V_{\text{pot}} + \alpha$ , where  $\alpha = -3 h^2 / m(\delta x)^2$ , which results in the disappearance of the summand  $2 \Psi(x)$  in the difference schemes for second derivatives on  $x, y, z$  (from that the coefficient 3 appears) after its substitution in the Schrödinger equation. This trick is not accurate from the mathematical viewpoint: we use the fact (the possibility of adding a constant to the potential), which is substantiated by analysis, whereas we fix  $\delta x$ , and after that we cannot send it to zero. However, it is not critical. We could preserve the last summand and continue our computations; it gives the same result but complicates computations.

For the simplicity of notation, we introduce the coefficient

$$\gamma = \frac{h}{2m} \frac{1}{(\delta x)^2}.$$

Since we do not yet know the mechanism of moving samples in the quantum swarm, we suppose that we simply remove some samples from one cell or place them onto another cell from some storage. We divide the evolution of the quantum swarm to such small frames of the longitude  $\delta t$  that on each frame, samples travel in the framework of two neighboring cells. If we prove that the diffusion mechanism provides the evolution on each of such frames, it will be true for the whole evolution, because our supposition about the exchange between two closest cells does not limit the generality. We also agree that these cells differ from each other on the shift to  $\delta x$  along the axis  $x$ , which does not limit the generality either. We denote the centers of these cells by  $x$  and  $x_1 = x + \delta x$ .

Now we divide the segment  $\Delta t$  into two parts, 1 and 2, and agree about the following. On part 1 we will consider only the change of  $\rho(x)$ , which is caused by  $\rho(x_1)$ , and on part 2 the change of  $\rho(x_1)$ , caused by  $\rho(x)$  (the effect from the small change of  $\rho(x)$  on part 1 has

a higher order and we ignore it). The density is uniquely defined by the wavefunction; hence, we will consider the change of the wavefunction on each part. We show that the required change of the wavefunction can be obtained in this way: on part 1 we consider the change of  $\Psi$  corresponding to

$$\frac{\partial^2 \Psi(x)}{\partial x^2} \approx \frac{\Psi(x + \delta x) - 2\Psi(x) + \Psi(x - \delta x)}{(\delta x)^2} \quad (11)$$

and on part 2, corresponding to

$$\frac{\partial^2 \Psi(x_1)}{\partial x^2} \approx \frac{\Psi(x_1 - \delta x) - 2\Psi(x_1) + \Psi(x_1 + \delta x)}{(\delta x)^2}. \quad (12)$$

Really, if we accept that the wavefunction changes according to these two equations for all nodes, we obtain that the final change resulting from the described process on all possible  $x$  coincides with the change resulting from the difference scheme of equation (10). Taking into account that equation (12) follows from equation (11) after the replacement of  $x$  by  $x_1$  and vice versa, we obtain that the result of the sequential actions can be represented by the system of equations

$$\begin{aligned} \Psi_t^r(x) &= -\gamma \Psi^i(x_1) + V(x) \Psi^i(x), \\ \Psi_t^i(x) &= \gamma \Psi^r(x_1) - V(x) \Psi^r(x), \end{aligned} \quad (13)$$

and the analogous system obtained by the replacement of  $x$  by  $x_1$  and vice versa, where the lower index means differentiation by  $t$ . This means that we consider only the exchange of samples through one fixed border between cells  $x$  and  $x_1$ . If we then sum the other deposit corresponding to the exchange between  $x$  and  $x_0 = x - \delta x$ , we obtain the full change of density within the effect of the separation into two fractions: gas and liquid. This exchange has an analogous form, and all further computations can be fulfilled for it with the corresponding result; we thus take up only the exchange between  $x$  and  $x_1$ .

Equation (13) is true if samples move from  $x$  to  $x_1$ . When samples move from  $x_1$  to  $x$ , we obtain the analogous system obtained by the replacement of  $x$  by  $x_1$  and vice versa. The Schrödinger equation will then express the result of the general evolution process consisting of all cases where we can place  $x$  and  $x_1$  by six ways along three coordinate axes. By the time frame  $\Delta t$ , we now mean just such a short time segment when the exchange goes only between  $x$  and  $x_1$  (and, possibly, the storage; we will shortly see that the storage is not needed).

For such a segment we have

$$\begin{aligned} \dot{p}_{x,x_1} &= \frac{\partial \rho(x)}{\partial t} \Big|_{x,x_1} = 2 \Psi^i(x) (\Psi^r(x_1) - V(x) \Psi^r(x)) + \\ &2 \Psi^r(x) (-\Psi^i(x_1) - V(x) \Psi^i(x)) = \\ &2 (\Psi^i(x) \Psi^r(x_1) - \Psi^r(x) \Psi^i(x_1)) = - \frac{\partial \rho(x_1)}{\partial t} \Big|_{x,x_1}, \end{aligned} \quad (14)$$

where by

$$\frac{\partial \rho(x)}{\partial t} \Big|_{x,x_1}$$

we denote the deposit to the derivative of density by time, which appears from the moving of samples through the border separating cubes that contain points  $x$  and  $x_1$ . The result is that the decrease of samples in one cell equals the increase of them in the other; for example, the evolution of the quantum swarm satisfies the condition of locality, and we can speak about the stream of samples through the element of the surface when we fix the value of  $\delta x$ .

### ■ 3.3 Dependence of Swarm Dynamics on Grain

We approach the most important thing in the description of quantum dynamics: the dependence on the grain  $\delta x$ . We cannot confirm that equation (14) determines the number of samples, which increase the density of the corresponding cell when they pass through the considered surface in the unit of time. The expression for a detailed stream (equation (14)) is not an expression for an ordinary stream of particles through a surface. The reason is that it critically depends on a value  $\delta x$ , and it is impossible to direct this value to zero. We cannot apply to a swarm the fundamental features of mathematical analysis, such as that it is possible to divide intervals without limit  $(x, x_1)$  and to pass to a limit at  $\delta x \rightarrow 0$  so all values of group magnitudes (the density and speed) will keep their values. Equation (14) indirectly specifies that at the swarm there are samples with essentially different speeds, so we cannot speak about the speed of all of the swarm at a given point. Let us recollect that the swarm has two parts: fast (separate samples from the thin layer) and slow (simplexes). The mechanism of moving samples of the fast part is that each of them on each step  $\Delta t$  jumps along the direction of its movement by the number of cells proportional to  $\Delta t$ . The mechanism of moving of a sample of the slow part of the swarm is that it waits a number of the steps, proportional to  $1/\Delta t$ , being at a stop, and only then moves exactly in one step along the direction of its movement. In this case we cannot

write for the detailed vector stream (density)  $\bar{p}$  the expression

$$\frac{\partial \rho(r, t)}{\partial t} = \frac{1}{N(\delta x)^3} \int_{S(r)} \bar{p}(r, t) \bar{n}(\bar{r}_1) ds(r_1) \quad (15)$$

that is true for the ordinary stream  $p$ . Instead we must use the expression

$$\frac{\partial \rho(r, t)}{\partial t} = \frac{1}{N(\delta x)^3} \int_{S(r)} \bar{p}(r, t) |_{(x, x_1)} \bar{n}(\bar{r}_1) ds(r_1) + \Lambda, \quad (16)$$

where the summand  $\Lambda$  has the following nature.

Let  $\delta x$  and  $\Delta t$  be fixed. To write equation (15), it is necessary to guarantee that all samples of the fast part of the swarm, which have passed through the border in a direction  $r$ , remain in the corresponding cell and do not jump out of it because of their great speed. For this, it is necessary to make  $\Delta t$  small enough. But then samples of the slow part of the swarm will not have time to move even a little. For maintenance of the movement of both fast and slow samples there is only one way: to reduce the grain  $\delta x$ . But we cannot do that either, because then at once speeds of the fast part of the swarm will increase, and we have to consider another swarm.

Thus, it is impossible to replace the discrete character of motion of the samples of fast and slow parts of the swarm with continuous movement, as in the case of the classical continuous environment. Summand  $\Lambda$  makes sense of the phase transition between fast and slow parts of the swarm. We arrive at the need to consider two fractions: slow liquid and fast gas. (Otherwise, if we make it possible for simplexes to move at each step, we would have to consider jumps of samples of a thin layer. The jump of a fast sample means that it disappears in one cell then appears in another cell, which can have no common borders with the first.) There is no usual stream in a quantum swarm; we can thus operate with the detailed stream only.

The inapplicability of the usual analytical methods to the quantum swarm does not mean the impossibility of a substantiation of a way of modeling offered to us by means of classical mathematics. (In one case the delta function of Dirac, the classical mathematical substantiation, formally has been found in the form of linear functionals.) I do not exclude the discovery of such a substantiation, but it is only for the case of one real particle. However, it is impossible to find a classical substantiation of the method of collective behavior in its general form for many particles, because here the limitation of the quantity of samples plays the central role that makes impossible the application of the ideology of mathematical analysis. In particular, it means that

it is hopeless to attempt to prove formally that our mechanism of moving of samples of the swarm gives a good approximation in all cases of the exact solution of the Schrödinger equation. Therefore the substantiation of the proposed mechanism in Section 3.4 should be treated as an explanation for the algorithm's correctness, but not as the strict proof of its suitability in all cases. The general ideology of constructivism [3] offers us one method: to rely on direct computer modeling.

### ■ 3.4 Reduction of Schrödinger Equation to Dynamic Diffusion

We introduce the following parameters depending on  $\delta x$ :

$$I = \frac{h^2}{2m^2(\delta x)^3}, \quad \kappa = \frac{h}{m\delta x} \quad (17)$$

where  $h$  is the Planck constant. The parameter  $I$  is called the *intensity of action of the density gradient*, and  $\kappa$  is called the *intensity of potential*.

Now to construct the mechanism for changing the speed of samples, we will find the change of the detailed stream  $(\partial/\partial t)p|_{(x,x_1)}\bar{n}dS$  of the quantum swarm through a surface of a small cube, the normal to which is parallel to the axis  $OX$ . For this purpose it is necessary to differentiate equation (14) by the time variable:

$$\begin{aligned} \bar{p}'_t &= 2\gamma[(\gamma\Psi^r(x_1) - V(x)\Psi^r(x))\Psi^r(x_1) + \\ &\quad \Psi^i(x)(-\gamma\Psi^i(x) + V(x_1)\Psi^i(x_1)) - \\ &\quad (-\gamma\Psi^i(x_1) + V(x)\Psi^i(x))\Psi^i(x_1) - \\ &\quad \Psi^r(x)(\gamma\Psi^r(x) - V(x_1)\Psi^r(x_1))] = \\ &2\gamma^2(\Psi^r(x_1))^2 - 2\gamma V(x)\Psi^r(x)\Psi^r(x_1) - \\ &2\gamma^2(\Psi^i(x))^2 + 2\gamma V(x_1)\Psi^i(x)\Psi^i(x_1) + \\ &2\gamma^2(\Psi^i(x_1))^2 - 2\gamma V(x)\Psi^i(x)\Psi^i(x_1) - \\ &2\gamma^2(\Psi^r(x))^2 + 2\gamma V(x_1)\Psi^r(x)\Psi^r(x_1) = \\ &2\gamma^2((\Psi^r(x_1))^2 + (\Psi^i(x_1))^2 - ((\Psi^r(x))^2 + (\Psi^i(x))^2)) + \\ &2\gamma[(V(x_1) - V(x))((\Psi^r(x))^2 + (\Psi^i(x))^2) + o(\delta x)], \end{aligned} \quad (18)$$

where

$$\begin{aligned} o(\delta x) &= (\Psi^r(x)\Psi^r(x_1) + \Psi^i(x)\Psi^i(x_1) - ((\Psi^r(x))^2 + (\Psi^i(x))^2)) \\ &\quad (V(x_1) - V(x)). \end{aligned}$$

We thus can write for the detailed stream the formula

$$\Delta p |_{(x,x_1)} = (-I \nabla \rho - \kappa \rho \nabla V) \Delta t. \tag{19}$$

We see that the Schrödinger equation gives the same change of stream as the dynamic diffusion (see equation (5)), if we put  $a = -I$ ,  $b = -\kappa$ .

**3.5 Restoration of Wavefunction from Dynamical Diffusion Swarm**

In order to compare the standard description of a quantum state through its wavefunction  $\Psi$  and its swarm representation, we will assume that the latter is described by a pair of functions

$$\rho(t, \bar{r}), \bar{p}(t, \bar{r}), \tag{20}$$

where the scalar function  $\rho$  is the density of samples, and the vector of impulse of the swarm  $\bar{p}(r)$  is the sum of the speeds of the samples that occurred in the small cell with side  $\delta x$  and center in the point  $r$ . The swarm impulse does not include the weight of the real particle  $p(r)$ ; there is the swarm characteristic in which “the weight” role is played by the total number of samples.

Such a pair does not use the concept of complex numbers and does not give the beautiful differential equations of the Schrödinger type for  $\rho$  and  $\bar{p}$ . Moreover, the mechanism of dynamic diffusion introduced by us for imitation of quantum evolution differs considerably from classical processes (e.g., a heat transfer or fluctuations), in that its intensity depends on the chosen grain of the spatial resolution. We have tried it for the sake of the main thing: economy of computing resources, which are not only necessary for modeling of quantum dynamics of complex systems, but are absolutely necessary for its research in general.

Given a state of swarm, we will show how the usual complex wavefunction  $\Psi$  can be restored from the pair in equation (20). We accept that the carrier of the wavefunction is connected; that is, any two points in it can be connected by a curve that is not crossing any area of zero density  $\rho = 0$ . This restriction is related to that which is used in the diffusion Monte Carlo method. For this purpose we consider equation (14) and substitute in it the expression for the wavefunction through density:  $\Psi(r) = \sqrt{\rho(r)} \exp(i\phi(r))$ . The problem consists of the calculation of the phase  $\phi(r)$  of wavefunction. We will notice that as only the relative phase between various points has a physical sense, we can fix some point  $r$  and consider a phase of another point  $r_1$  relatively to  $r$ . If  $r_1$  is close to  $r$ , equation (14) gives us

$$\phi(r) - \phi(r_1) = \arcsin k(\delta x)^2 \frac{\bar{p}(\bar{r} - \bar{r}_1)}{\sqrt{\rho(r) \rho(r_1)}},$$

which leads to the following formula for the relative phase:

$$\phi(r_1) = \int_{\gamma} k(\delta x)^2 \bar{v} d\bar{\gamma}, \quad (21)$$

where the path  $\gamma$  goes from  $r$  to  $r_1$ . This equation explicitly depends on the choice of the path  $\gamma$ ; hence, we have to prove its correctness, for example, independent of the choice of  $\gamma$ .

We mention that this derivation will be correct only in the case when  $\rho > e > 0$  for some constant  $e > 0$ ; for example, the density must be separated from zero in all areas of consideration. Since the phase is determined only to within an integer multiple of  $2\pi$ , different choices of the path can lead to at most the change of the phase to such a number that takes place, for example, for excited states of an electron in a hydrogen atom with nonzero magnetic number. We show that the integration of the speed  $\bar{v}$  of the swarm along a closed path preserves its value in time more exactly when the spatial resolution  $\delta x$  is smaller. The result is that if in the initial time instant equation (21) is correct, it preserves the correctness for the following instants as well.

We thus consider the derivative of the integral of the speed of the swarm along the closed path  $\gamma_c$ . Applying equation (19) and taking into account that  $\partial \bar{p} / \partial t$  is proportional to  $\rho \partial \bar{v} / \partial t$ , we obtain

$$\frac{\partial}{\partial t} \int_{\gamma_c} \bar{v} d\gamma = - \int_{\gamma_c} A I(\delta x)^2 \frac{\nabla \rho}{\rho} + B \kappa(\delta x)^2 \nabla V \quad (22)$$

for some  $A, B$ . The first summand gives zero after the integration along the closed path, because it is  $\nabla \ln \rho$ ; the second summand gives zero by the analogous reason.

It is now sufficient to check that equation (21) is correct in the initial instant, and that can be done straightforwardly for each possibility. In the case where the wavefunction of the initial state can be obtained from the ground state of the electron in the hydrogen atom, where  $\bar{v} = 0$ , the correctness follows from what has been shown, because there is no phase shift to  $2\pi k$ . The phase of each ground state does not depend on the point. If to obtain the initial state in the considered problem we have to start from some excited state, we must first check the correctness for this state.

Based on these computations, we can write formulas connecting swarm parameters with the wavefunction:

$$\begin{aligned}
 |\Psi(r)| &= \sqrt{\rho(r)}, \\
 \phi(r) &= \int_{\gamma:r_0 \rightarrow r} k \bar{v} \cdot d\gamma, \\
 \bar{v} &= b \nabla \phi(r),
 \end{aligned}
 \tag{23}$$

for some  $a, b$ . These formulas permit us to pass from the wavefunction to the swarm and vice versa. This description has two features. First, beyond the Schrödinger dynamics on the level of the grain,  $\delta x$  corresponds with the swarm dynamics of the lower level with grains  $\Delta x, \Delta t$ , so that there is the substantial dependence of swarm parameters (intensity) from the chosen grain of spatial resolution  $\delta x$ . Second, quantum dynamics presupposed the presence of the thin layer and the specific behavior of samples toward it.

In the formulas of equation (23) the mean speed  $\bar{v}$  of the swarm approximately equals the mean speed of such a part of the swarm, which does not contain a thin layer in each point where the density does not converge to zero. There the thin layer does not give a substantial contribution to the impulse of the swarm because in each small cube there is only one sample from the thin layer. If we apply to the quantum particle the external potential  $V_{\text{pot}}$ , it brings a contribution to the impulse of the swarm because it influences the main part of the swarm that does not belong to the thin layer.

#### 4. Case of Many Particles

Now we show that the method of dynamic diffusion can be generalized to the case of many quantum particles. Take as given the set of  $n$  quantum particles, which we enumerate by natural numbers:  $1, 2, \dots, n$ . To find the efficient scheme of modeling we should apply sequentially the method of collective behavior, where the algorithmic reduction of quantum states is the inbuilt property. The most correct decoherence model, which we named absolute, says that decoherence is the reduction of the quantum state

$$|\Psi\rangle = \sum_j \lambda_j |j\rangle,
 \tag{24}$$

while the memory of the modeling computer cannot contain a full record of this state. In Section 3 we have shown such a model gives Born's rule for calculation of probabilities by an outcome of the measurement of a quantum state of the system, and it proves the correctness of the given model. But such a form of an absolute model of deco-

herence cannot yet serve as a heuristic for a modeling algorithm, as we do not have any way of modeling unitary quantum dynamics for many particles, except calculations within the limits of matrix algebra, and this way, as we saw, is too expensive.

We will consider swarm representations of our  $n$  particles  $1, 2, \dots, n$ , where  $S_1, S_2, \dots, S_n$  are their swarms, corresponding to their states

$$|\Psi_1\rangle, |\Psi_2\rangle, \dots, |\Psi_n\rangle.$$

If we consider the ensemble consisting of all these samples, it will represent a simple state of a kind

$$|\Psi_1\rangle \otimes |\Psi_2\rangle \otimes \dots \otimes |\Psi_n\rangle.$$

But for representation of the entangled state of a kind

$$\Phi = \sum_{j_1, j_2, \dots, j_n} \lambda_{j_1, j_2, \dots, j_n} |j_1, j_2, \dots, j_n\rangle, \quad (25)$$

we need to introduce a new essential element into the method of collective behavior. These are bonds between samples of different swarms, which we call own bonds, to distinguish them from non-own bonds, which we introduced in Section 3.1 to join samples in simplexes. The basic state  $j_i$  can be considered as coordinates of the particle  $i$  in the corresponding configuration space. Representation of the wavefunction in the form of equation (25) means that there are bonds, which connect points  $j_1, j_2, \dots, j_n$  in one cortege.

In the method of collective behavior [4], we will accept that bonds connect not spatial points, but samples of various real particles. These bonds can be written down as corteges

$$\bar{s} = (s_1, s_2, \dots, s_n), \quad (26)$$

where for any  $j = 1, 2, \dots, n$   $s_j \in S_j$ . Wavefunction  $|\Phi\rangle$  then is represented as a set  $\bar{S}$  of corteges  $\bar{s}$ , so that for any  $j = 1, 2, \dots, n$  and  $s_j \in S_j$  there is exactly one cortege of the form in equation (26). Each cortege plays a role in the so-called world of the many-world interpretation of quantum theory. We consider a cortege of equation (26) as a sample of a system of  $n$  particles. In the case of one particle, we saw that the action on a thin layer of the force proportional to the gradient of density of the swarm can simulate quantum dynamics. We will see that this process directly generalizes also to the case of  $n$  particles. We name  $\bar{S}$  the swarm representation of the system of  $n$  particles.

The swarm density  $\bar{S}$  is defined as

$$\rho_{\bar{S}}(r_1, r_2, \dots, r_n) = \lim_{dx \rightarrow \infty} \frac{N_{r_1, r_2, \dots, r_n, dx}}{N(dx)^3 n}, \quad (27)$$

where  $N_{r_1, r_2, \dots, r_n, dx}$  is the total number of the corteges that have appeared in the  $3n$ -dimensional cube with side  $dx$  and center  $r_1, r_2, \dots, r_n$ , and  $N$  is the total number of corteges.

If the wavefunction  $|\Phi\rangle$  is the tensor product of partial wavefunctions:

$$|\Phi\rangle = \bigotimes_{i=1}^n |\phi_i\rangle,$$

the corresponding bonds then can be obtained by the random choice of samples from the uniform distribution  $s_j \in S_j$  for each  $j = 1, 2, \dots, n$ , which will thus form each cortege  $s_1, s_2, \dots, s_n$ . With such choice of corteges, the result is that the density of a corresponding swarm satisfies Born's condition, which for swarms can be written down as

$$\sum_{\bar{r} \in D} |\langle \bar{r} | \Phi \rangle|^2 = \frac{N_{\bar{r}, \bar{S}}}{N}, \tag{28}$$

where  $D \subset R^{3n}$ ,  $N_{\bar{r}, \bar{S}}$  is the total number of corteges that have appeared in area  $D$ . But for the entangled state  $|\Phi\rangle$ , such choice of corteges for a set of swarms  $\bar{S}$  will not give us a condition as in equation (28). We should thus take equation (28) for the definition of a choice of corteges in  $\bar{S}$ . But for the definition of a swarm, we should define also the speeds of all the samples, namely, to generalize equation (23) to the case of  $n$  real quantum particles.

Let  $\Psi(r_1, r_2, \dots, r_n)$  be a wavefunction of a system of  $n$  particles and

$$\Psi = |\Psi| \exp(i\phi(r_1, r_2, \dots, r_n))$$

be its Euler decomposition. We will designate through  $\nabla_j \phi(r_1, r_2, \dots, r_n)$  the gradient  $\Psi$ , taken on coordinates of the particle  $j$  where  $j \in \{1, 2, \dots, n\}$  is a fixed number. Generalization of equation (23) to  $n$  particles looks like

$$\begin{aligned} |\Psi(\bar{r})| &= \sqrt{\rho(\bar{r})}, \\ \phi(r) &= \int_{\bar{\gamma}: \bar{r}_0 \rightarrow \bar{r}} k \bar{v} \cdot d\gamma, \\ \bar{v} &= a \bar{\nabla} \phi(\bar{r}), \end{aligned} \tag{29}$$

where  $\bar{r}$  designates  $r_1, r_2, \dots, r_n$ ,  $\bar{\nabla}$  designates  $(\nabla_1, \nabla_2, \dots, \nabla_n)$ , and  $\bar{\gamma}$  is a path in  $3n$ -dimensional space. Equation (29) is enough of a rule

for the definition of the swarm for a given wavefunction if we agree to unite samples in corteges irrespective of their speeds. At transition from the case of one particle to the case of many particles, it is necessary to insert a sample of the swarm for all systems of many particles instead of a sample of the swarm for one particle everywhere.

The external description of the change in speeds is the direct generalization of the case of one particle. The gradient  $\bar{\nabla}\rho$  of the density of this swarm will cause a change of speed for each sample of a separate particle in those corteges, which belong to the thin layer. Return of an impulse from the thin layer to all of the swarm occurs in each cell of configuration space in the same way, as in the case of one particle. Dynamic smoothing of formed peaks also goes by the general rule.

Let us consider now the swarm of samples of a quantum system with  $n$  particles. Each of them represents an Everett quantum world and looks like  $\bar{s} = (s_1, s_2, \dots, s_n)$ . How does such a cortege receive an increment of speeds  $\Delta\bar{p}_{\bar{s}} = (\Delta p_1, \Delta p_2, \dots, \Delta p_n)$ ? For this purpose it should be in the thin layer. Let it already be there. Then we will consider all other corteges lying close to  $\bar{s}$  in the sense of the metrics of  $n$ -particle configuration space, and we will find the gradient of their density which looks like:

$$\bar{\nabla}\bar{\rho} = (\nabla_1, \nabla_2, \dots, \nabla_n). \quad (30)$$

Now each sample  $s_j$  receives an increment of its own impulse on  $-I\nabla_j$ . The cortege elements in equation (30) are not defined by the density of separate particles. They are defined by the density of the swarm for all systems with  $n$  particles. That is, influence on  $\nabla_j$  renders not only the swarm density of the  $j^{\text{th}}$  particle taken separately, but samples of all other particles that are connected in one cortege with an environment of the  $j^{\text{th}}$  particle, provided that these corteges lie close to  $\bar{s}$ . We could consider only the density of separate particles only in the case when the state is not entangled (only for non-entangled states is the classical consideration of ensembles legal). Thus if we wish to study the general case of the entangled system in the swarm representation, we should enter into consideration bonds between samples in individual swarms, in particular, for corteges belonging to a thin layer. As in the case of one particle, we redefine the thin layer at each step.

Here again in the case of a non-entangled state, the role that will be played is only an affinity of samples of separate particles. Bonds between the different samples entering into one cortege will be involved only if we have an entangled state. Thus, the thin layer in a case of the entangled state of  $n$  particles also cannot be received as a simple

combination of something like “thin layers” for separate particles. It is defined through bonds in corteges, and has essentially a multi-partial character.

Let  $m$  be the number of samples of each separate particle. Then, owing to our condition of uniqueness of the cortege containing the given sample of any particle, we have exactly  $m$  various corteges, which are not overlapping pairwise. If we send the number of real particles  $n$  to infinity, having left  $m$  to be constant, we will get an increasing deviation of our model from the exact solution of the corresponding Schrödinger equation with the growth of the number of real particles  $n$ . Thus, fixing  $m$  means the presence of an internal factor of decoherence, which is independent from any “environment.” On the other hand, the complexity of the model will linearly increase with growth  $n$ , instead of exponentially, as in the standard formalism. That is, the method of collective behavior realizes an absolute model of decoherence, which rests on the limitation of the memory of the modeling computer.

Acceleration of a thin layer as a result of the action of a density gradient of a swarm in the case of a limited number of samples can be written in a specific form. A division of the configuration space with  $n$  real particles on  $s$  cubes will appear as  $s^n$  cubes. Therefore we can speak about any “calculation of a gradient of density” in Bohm’s sense only in that case when  $m \gg s^n$ , that is, when there are not a lot of real particles. If this inequality is not true, division of the force operating on a separate cortege from the swarm on an “analytically described component” and “processing of peaks” lose meaning. The “peaks” will actually be everywhere, and it is necessary to describe the process of their dynamic smoothing correctly.

Now we take up the mechanism of changing speeds for samples of  $n$  particle systems. It is formulated as in the case of one particle, but the close samples will be replaced by close corteges. Namely, for a cortege we treat it as a simplex of the first order. If two corteges  $\bar{s}_1$  and  $\bar{s}_2$  are close in the sense of  $n$ -particle configuration space, for example, they belong to the same cell in this space. Then in the instant when the distance between them is minimal, the own bonds between the corresponding samples are established, and we obtain the  $n$ -particle simplex of the second order. We call the sequence of these one-particle bonds an  $n$ -particle bond, where one-particle bonds are its components. A simplex for the  $n^{\text{th}}$  order arises from a simplex of the  $n - 1^{\text{th}}$  order and a sample by the same procedure. The decay of all one-particle components of a bond happens simultaneously; that is, we can speak about the decay of  $n$ -particle bonds in a given time instant. The decay results in the flying away of a sample, and so on. A thin layer consists of samples, which move from cell to cell in a short

time frame. With this mechanism, we again obtain the action of the gradient of an  $n$ -particle swarm of corteges, which acts on the thin layer.

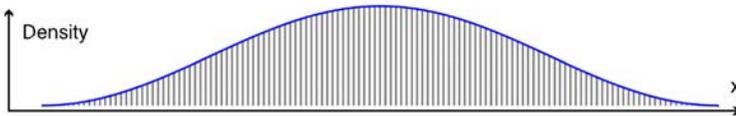
## 5. Computer Simulation of Dynamic Diffusion

This computer model should be considered as a proof-of-concept of the dynamic diffusion swarm.

Thus, we decided to model a few basic experiments inside a one-dimensional rectangular potential hole: dispersion of a Gaussian wave packet, ground state of the wavefunction (in comparison with the linear modulus function), collision of two Gaussian wave packets (as an illustration of quantum interference effects).

The algorithm's convergence is very close to implicit Runge–Kutta after a few time scheme collapses, but consistently shows quantum effects.

Figure 1 shows the swarm representation of the ground state of the particle in the deep potential hole, whose density equals  $\sin^2(x)$ . We obtained its stability by a numerical experiment with the swarm model.



**Figure 1.** Swarm representation of ground state.

### 5.1 Algorithm Overview

The workflow of the algorithm is an evolution iterating the array of simplexes and its interaction with the potential array of barriers (the potential hole is represented as two very high potential barriers). The scheme of simplex creation will be provided in this way:

```
SimplexName (speed, samples, position)
```

There are three phases: explosion, flight, and rearrangement.

- *Explosion.* Coefficient  $a$  indicates the number of samples ( $[0; 1]$ ) detached from a simplex (see Section 3.1). In place of the simplex, three others are created: one will then fly to the left, another one to the right, and the third remains in place. Here is pseudocode for the explosion phase (let the original simplex be “original” (original.samples, original.speed, original.position)):

```

for each original simplex in the array create a new
  simplex with speed : (original.speed - max_speed)
samples : (a * original.samples)
position : (original.position)
create new simplex with
  speed : (original.speed + max_speed) samples :
  (a * original.samples)
position : (original.position)
create new simplex with speed : (original.speed)
samples : ((1-2*a) * original.samples)
position :
  (original.position) remove original simplex from array

```

- *Flight.* Here is pseudocode for the flight phase.

```

for each simplex and for each barrier if simplex
  flights through barrier, then handle barrier
simplex.position = simplex.position + simplex.speed

```

- *Rearrangement.* As the flight of the simplexes continues and they do not interact with each other, a rearrangement phase is needed to perform interaction of nearby simplexes and perform some kind of measurement, arranging simplexes back to the grain-dependent grid. Here is pseudocode for the rearrangement phase:

```

for each point on the grid find all
  simplexes close to each other that can interact

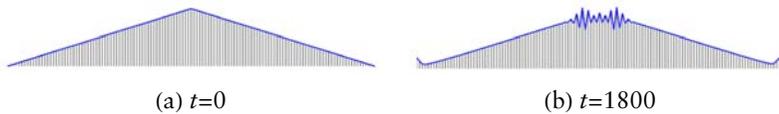
```

## 5.2 Results

Figures 2 and 3 compare the ground state with an artificial linear modulus function. These systems evolve for the same time. It is obvious that the ground state appears to be more stable.



**Figure 2.** Ground state.

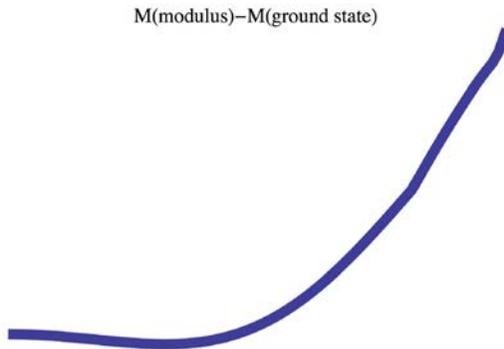


**Figure 3.** Modulus function.

Numeric comparison of convergence was analyzed with a metric:

$$M(\text{wavefunction}, T) = \sum_{i=1}^N |\text{wavefunction.samples}_{x=i}^{t=0} - \text{wavefunction.samples}_{x=i}^{t=T}|.$$

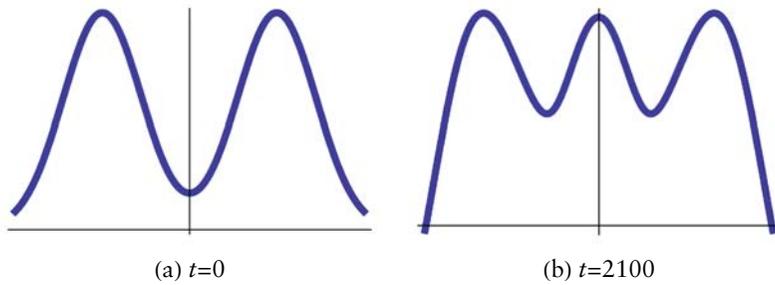
The result is presented in Figure 4.



**Figure 4.**  $M(\text{modulus}, t) - M(\text{ground state}, t)$ .

Figure 5 shows the interference of two wave packets. Results were compared to the Schrödinger equation's numeric solution, performed in Wolfram *Mathematica*. Firstly, this experiment was modeled in Wolfram *Mathematica* with implicit R-K, explicit R-K, and “Automatic” computation methods. The implicit method is absolutely inconsistent. The explicit method does not show the interference effect and deconverges. Automatic results are represented in Figure 5.

Figure 6 shows the results received in dynamical diffusion swarm (DDS) modeling.



**Figure 5.** Two Gauss wave packets, Wolfram *Mathematica*.



**Figure 6.** Two Gauss wave packets, DDS.

### 5.3 Modeling Conclusion

These results can be interpreted as a proof of the constructive approach to wavefunction dynamic modeling. As described, this model can be expanded to the multiparticle case, which is impossible with the classic Schrödinger equation. Certainly there is a lot of work to be done before it can be successfully used in real computations of many-particle systems.

The program was built on the .Net WPF platform. The program has an architecture that separates model and view so it can be integrated into other software (e.g., Experiment Work).

## 6. Conclusion

We show how quantum unitary dynamics can be simulated in terms of a swarm of classical pointwise samples, that is, the embodiment of prequantum dynamics in the sense of [5]. The mechanism of the speedup of samples rests on the new object—bonds, which are absolutely rigid connections joining samples into simplexes. A simplex is a set of close samples, which roll with high speed, whereas a simplex as a whole moves with low speed. The quantum dynamics come from the creation and annihilation of bonds that formed in a kind of Poisson process. In the course of the time evolution, samples fly out from

their parent simplexes and rapidly jump to the other close simplexes, giving them their impulses. This process results in the rapid transmission of impulses. The derivative of a stream of samples through the small border between cells becomes proportional to the density gradient, where the coefficient depends on the grain of spatial resolution as  $\delta x^{-3}$ .

This dependence makes it impossible to send the grain to zero, and hence, to use the exact analytic apparatus on the swarm dynamics. The reason for this lies in the nature of the diffusion swarm—it consists of two fractions: slow (simplexes) and fast (separate samples, flying with the speed of light). The advantage of dynamic diffusion is that this approach to simulation of quantum dynamics can be easily generalized to the many-particle case, because the mechanism of the speedup of the samples depends only on the density at the current point, but not on the closest vicinity of it. In this generalization a sample of the whole  $n$ -particle system is the cortege, consisting of samples of the separate particles. This is the idea of collective behavior for swarm quantum dynamics. These corteges do not intersect, and their total number equals the total number of samples of one particle. The limitation of this number plays the role of decoherence when the number of real particles converges to infinity. In this case the approximation via collective behavior becomes further and further from unitary quantum dynamics.

Rotation of samples inside simplexes bears a resemblance to the spin of particles [6]. We cannot claim that there is the conventional quantum mechanical spin. This spin we can call “hydrodynamic spin.” The establishing of the relation of this “spin” with the usual spin represents an interesting problem.

The check of the validity of dynamic diffusion is done by computer simulation. The main problem arises with the area where  $\rho \approx 0$ . For example, for the particle in the rectangular potential hole, its ground state has the form  $\sin^2 ax$ . The influence of a wall is represented by the elastic reflection of samples and simplexes from the walls. The density then will have peaks along the whole area, and they move faster when the density is smaller. Just the existence of these peaks preserves the form of  $\sin^2$  for a sufficiently long time in comparison to the other functions. The other example is oscillation of a particle between two potential holes separated by high potential barrier. The huge velocity of samples in a thin layer makes it possible to overcome this barrier, if the general speed created by slow simplexes has the same direction. If the direction of this slow part of a swarm is in the reverse direction, the thin layer cannot overcome the barrier. This effect gives the known oscillation, as follows from the Schrödinger equation.

It is interesting to compare our variant of quantum hydrodynamics with cellular automata (as described in [7]). The result of a cellular automaton, defined by very simple rules, is unpredictable, as this computation model is universal. Quantum evolution, in theory, can be represented as a quantum gate array, in other words a quantum computer, whose computational capabilities exceed the classic computational model. This is why there is no sense in raising the question about prediction of quantum computing. This computational model is even more universal than a cellular automaton.

But the fundamental role of decoherence, which affects all aspects of quantum computers, suggests the possible existence of a non-Feynman's quantum computing paradigm. And in this new paradigm, based on algorithms, it is possible to achieve, in some cases, predictable results. As we have shown, quantum evolution is completely different from a cellular automaton. Decrease of the grain size, which increases the accuracy of the cellular automaton (e.g., diffusion), does not increase the accuracy of the quantum system at all.

The uncertainty principle, which leads to the unpredictability of the impulse of any fixed part of the swarm, defines a fundamental limitation for fixed-grain models. For quantum hydrodynamics, this results in a quantum pseudo-potential with singularity at the origin, which is not applicable for real calculations. In dynamic diffusion, described in this paper, this results in characteristics of density equation coefficients when the grain tends to zero.

These characteristics could be calculated for simple systems on a desktop computer, but with an increasing amount of particles the chances of "modeling" in the old paradigm, with fixed, possibly smallest grain fade. Our computation results show that there is a fundamental chaos behind the marvelous quantum computing apparatus. And this gives an absolutely new chance for complex systems computer modeling methods, which can be implemented if we use algorithms instead of classic "modeling" methods, nowadays being used in physics and quantum chemistry calculations. And software like Wolfram *Mathematica* will play a key role in this approach.

The further development of collective behavior lies in the effect of decoherence in complex systems [8, 9]. Here the approximate representation of quantum dynamics in the form of dynamic diffusion will have the advantage over the Bohm approach, because it does not require the density to have a smooth shape.

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