Quantum non-equilibrium and relaxation to equilibrium for a class of de Broglie–Bohm-type theories

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2010 New J. Phys. 12 043008
(http://iopscience.iop.org/1367-2630/12/4/043008)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 132.234.251.212
The article was downloaded on 13/06/2010 at 05:34

Please note that terms and conditions apply.
Quantum non-equilibrium and relaxation to equilibrium for a class of de Broglie–Bohm-type theories

Samuel Colin\(^1,4\) and Ward Struyve\(^2,3,4\)

\(^1\) Centre for Quantum Dynamics, Griffith University, Brisbane, QLD 4111, Australia
\(^2\) Institute of Theoretical Physics, KU Leuven, Celestijnenlaan 200D, B-3001 Leuven, Belgium
\(^3\) Institute of Philosophy, KU Leuven, Kardinaal Mercierplein 2, B-3000 Leuven, Belgium
E-mail: s.colin@griffith.edu.au and Ward.Struyve@fys.kuleuven.be

Received 21 December 2009
Published 1 April 2010
Online at http://www.njp.org/
doi:10.1088/1367-2630/12/4/043008

\textbf{Abstract.} The de Broglie–Bohm theory is about non-relativistic point-particles that move deterministically along trajectories. The theory reproduces the predictions of standard quantum theory, given that the distribution of particles over an ensemble of systems, all described by the same wavefunction \(\psi\), equals the quantum equilibrium distribution \(|\psi|^2\). Numerical simulations done by Valentini and Westman (2005 \textit{Proc. R. Soc. A} 461 253) have illustrated that non-equilibrium particle distributions may relax to quantum equilibrium after some time. Here we consider non-equilibrium distributions and their relaxation properties for a particular class of trajectory theories (first studied in detail by Deotto and Ghirardi (1998 \textit{Found. Phys.} 28 1)) that are empirically equivalent to the de Broglie–Bohm theory in quantum equilibrium. In the examples we studied of such theories, we found a speed-up of the relaxation, compared to the ordinary de Broglie–Bohm theory. Hence non-equilibrium predictions that depend strongly on relaxation properties, such as those studied recently by Valentini, may vary across different trajectory theories. As such, these theories might be experimentally distinguishable.

\(^4\) Authors to whom any correspondence should be addressed.
1. Introduction

In the de Broglie–Bohm theory [1–3], an individual closed system is described by its wavefunction that satisfies the Schrödinger equation and by particle positions that move deterministically along trajectories with a velocity that depends on the wavefunction. The theory reproduces the predictions of standard quantum theory, given that the distribution of particle positions over an ensemble of systems, all described by the same wavefunction \( \psi(x, t) \), is given by \( |\psi(x, t)|^2 \). The dynamics is such that if the distribution of particle positions equals \( |\psi(x, t_0)|^2 \) at a certain time \( t_0 \), then it equals \( |\psi(x, t)|^2 \) at other times \( t \), a property called \textit{equivariance} [4]. The distribution \( |\psi|^2 \) plays the role of an equilibrium distribution (see, for example, [4–6]), similar to that of thermal equilibrium in classical statistical mechanics, and is called the \textit{quantum equilibrium distribution}.

Present-day experiments yield a very good confirmation of standard quantum theory and hence of quantum equilibrium. This could be accounted for by a Boltzmann-type argument: as shown by Dürr \textit{et al} [4], most initial configurations of the universe (relative to the natural measure \( |\Psi(X)|^2dX \), with \( \Psi \) being the wavefunction of the universe) yield the quantum equilibrium distribution \( |\psi(x)|^2 \) for actual ensembles described by the effective wavefunction \( \psi(x) \). In addition, it has to be expected that non-equilibrium distributions will tend to evolve to equilibrium and stay close to it for a reasonable amount of time in ‘most’ cases.\(^5\) This was illustrated by Valentini and Westman [7], who presented a numerical simulation of such a

\(^5\) As explained in detail in section 3.2, some distributions do not evolve to quantum equilibrium. For some wavefunctions there is never relaxation to equilibrium. So ‘most’ should in the first place refer to some natural measure \( \nu(d\psi) \) on Hilbert space. For example, considering product states \( \psi(x_1) \ldots \psi(x_N) \) (with \( N \) large), it probably holds that most non-equilibrium distributions (understood as empirical distributions) will tend to evolve to equilibrium, where ‘most’ refers to the measure \( |\psi(x_1) \ldots \psi(x_N)|^2dx_1 \ldots dx_N\nu(d\psi) \). In the following, we will not attempt to make these statements more precise.
relaxation to equilibrium for a free particle in a two-dimensional box. For a particular initial non-equilibrium distribution they found a rapid relaxation to quantum equilibrium (with the relaxation timescale roughly given by $\hbar^2/\varepsilon m^{1/2}(\Delta E)^{3/2}$, where $\varepsilon$ is the coarse-graining length that is used when comparing the coarse-grained non-equilibrium and equilibrium distributions, $m$ the mass of the particle and $\Delta E$ the energy spread of the wavefunction).

Non-equilibrium distributions have been studied in detail by Valentini, who suggested possible domains where such non-equilibrium distributions might occur and how they might be detected, see, for example, [6], [8–10]. In particular, Valentini suggested that one should look for non-equilibrium in astrophysical and cosmological scenarios. Assuming that the universe started in a special state of non-equilibrium (just as our universe seems to have started from a very special state of non-equilibrium on the classical statistical level), he considered the circumstances under which this non-equilibrium might be preserved and even be transferred to macroscopic scales. A priori, any non-equilibrium seems possible. Nevertheless, in the case of a scalar field on expanding space, Valentini was able to come up with a quantitative prediction [11, 12]. He showed that relaxation to equilibrium is expected to be suppressed for a specific range of modes. One of the possible consequences is a correction to the predictions for the temperature fluctuations of the cosmic microwave background in the context of inflation theory.

In this paper, we consider a certain class of trajectory theories that, just as the de Broglie–Bohm theory, leave $|\psi|^2$ equivariant. In this class of theories, which was studied in detail by Deotto and Ghirardi [13], the velocity field of the particles is changed by an additive term compared to that of the de Broglie–Bohm theory. From the point of view of these theories, standard quantum theory emerges as an effective theory describing the state of equilibrium. As such they may only be distinguished in quantum non-equilibrium. The goal of this paper is to examine quantum non-equilibrium and possible relaxation to equilibrium for these theories, by means of numerical simulations.

In the examples we studied of such theories, the relaxation proceeds more rapidly than in the ordinary de Broglie–Bohm theory. This was as expected, since the additional term in the velocity field, in general, just adds to the irregularity of the motion and hence to its mixing-like behaviour. In particular, in the case of the ordinary de Broglie–Bohm theory, it was reported earlier that nodes, in general, induce chaotic behaviour for trajectories that come in their neighbourhood (see, for example, [7], [14–19]). In the alternative theories under consideration, the additional term in the velocity fields tends to lead to an overall increase of its amplitude, causing the particles to travel larger distances, compared to the ordinary de Broglie–Bohm theory, in a given time interval. As such, particles tend to reach nodes sooner and undergo the chaotic motion sooner.

Non-equilibrium predictions that depend strongly on relaxation properties, such as those studied recently by Valentini, may hence vary for different trajectory theories. As such these theories might be experimentally distinguishable.

The outline of the paper is as follows. In section 2, we start with reviewing this class of de Broglie–Bohm-type theories. In section 3, we consider non-equilibrium distributions and some issues that are relevant to possible relaxation. In section 4, we present numerical simulations of relaxation for a number of de Broglie–Bohm-type theories, for a particle in a two-dimensional box (just as in the simulations of Valentini and Westman), showing a correlation between relaxation time and the choice of dynamics.

6 See, for example, [19] or [20] for a collection of references on chaos in the de Broglie–Bohm theory.
2. de Broglie–Bohm theory

2.1. Standard velocity field

In the de Broglie–Bohm theory, an individual closed system is described by its wavefunction $\psi(x, t)$, with $x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N}$, which satisfies the non-relativistic Schrödinger equation

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\sum_{k=1}^{N} \frac{\hbar^2}{2m_k} \nabla_k^2 \psi(x, t) + V(x) \psi(x, t),$$

(1)

and by particle positions $X_1(t), \ldots, X_N(t)$, whose configuration $X(t) = (X_1(t), \ldots, X_N(t))$ satisfies the guidance equation

$$\frac{dX(t)}{dt} = v_s(X(t), t),$$

(2)

where the velocity field $v_s$ is given by

$$v_s(x, t) = \frac{j_s(x, t)}{|\psi(x, t)|^2},$$

(3)

with $j_s = (j_{s,1}, \ldots, j_{s,N})$ the standard quantum probability current, given by

$$j_{s,k} = \frac{\hbar}{m_k} \text{Im} (\psi^* \nabla_k \psi) = \frac{1}{m_k} \nabla_k S |\psi|^2, \quad \psi = |\psi| \exp(iS/\hbar),$$

(4)

and which satisfies the continuity equation

$$\frac{\partial |\psi|^2}{\partial t} + \nabla \cdot j_s = 0$$

(5)

as a consequence of the Schrödinger equation.

An arbitrary distribution $\rho(x, t)$ transported along the de Broglie–Bohm trajectories satisfies the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (v_s \rho) = 0.$$  

(6)

Also $|\psi|^2$ satisfies this continuity equation, because of (5). This implies equivariance: if the distribution $\rho$ equals $|\psi|^2$ at a certain time, then they are equal at all times (and $|\psi|^2$ is actually the only equivariant distribution that is also a suitably local functional of $\psi$ [21]). It is the generalization of the property of stationarity in classical statistical mechanics.

As mentioned in the introduction, $|\psi|^2$ plays the role of an equilibrium distribution, called the quantum equilibrium distribution. Given the quantum equilibrium distribution and the fact that measurement results are generally ultimately recorded in positions of macroscopic pointers, like instrument needles, computer output, etc, it almost follows immediately that the de Broglie–Bohm theory reproduces the standard quantum mechanical predictions (see, for example, [1–3], [22, 23]).
2.2. Alternative velocity fields

The flow defined by (2) and (3) is not the only one for which the distribution $|\psi|^2$ is equivariant. The continuity equation for $|\psi|^2$ still holds if the current $j_s = v_s |\psi|^2$ is replaced by

$$ j = j_s + j_a, $$

where $\nabla \cdot j_a = 0$. As a result, for the velocity field

$$ v = \frac{j}{|\psi|^2} = v_s + \frac{j_a}{|\psi|^2}, $$

the distribution $|\psi|^2$ will also be equivariant. As such, one can consider alternative theories that, just as the ordinary de Broglie–Bohm theory, agree with standard quantum theory in quantum equilibrium.

This ambiguity in the choice of possible guidance equations was first studied in detail by Deotto and Ghirardi [13], who found that the requirement of Galilean covariance is insufficient to determine the guidance equation uniquely. Uniqueness could be obtained by extra requirements [3, 4] or by different ones [24–27]. These uniqueness results merely indicate the possible naturalness of certain guidance equations.

An interesting example of this ambiguity turns up in the context of the Pauli equation, which describes non-relativistic spin-1/2 particles [1]. Considering a single particle, one possible current is given by

$$ j_s = \frac{\hbar}{m} \text{Im} \left( \Psi^\dagger \nabla \Psi \right). $$

When the magnetic field is negligible and $\Psi$ is a spin eigenstate, that is, $\Psi(x, t) = \psi(x, t) \chi$, where $\chi$ is a constant spinor, the Pauli equation will imply the non-relativistic Schrödinger equation for $\psi$ and the current will reduce to the one in (4). Another natural current is obtained by adding the divergence-free term

$$ j_a = \frac{\hbar^2}{m} \nabla \times (|\psi|^2 \chi^\dagger \sigma \chi) $$

(10)

to $j_s$. For a spin eigenstate this term survives, so that the latter current yields the velocity field

$$ v = v_s + \frac{\hbar}{2m|\psi|^2} \nabla \times (|\psi|^2 \chi^\dagger \sigma \chi) $nabla \times (|\psi|^2 \chi^\dagger \sigma \chi) = \frac{1}{m} \nabla S + \frac{\hbar}{2m|\psi|^2} \nabla \times (|\psi|^2 \chi^\dagger \sigma \chi). $$

This velocity field is very natural when one considers the non-relativistic spin-1/2 theory as the limiting case of the relativistic Dirac theory [1]. The natural current and velocity field for the Dirac theory namely yield the spin term in the non-relativistic limit. The trajectories for this velocity field have been studied in, for example, [28–31]. (For other spins a similar ambiguity can be considered [32].)

Note that one can have other trajectory theories in which the velocity field is not of the form (9), but which are still empirically equivalent to the de Broglie–Bohm theory in quantum equilibrium, see, for example, [33, 34]. There even exist such theories where the equilibrium distribution is, in general, different from $|\psi|^2$ [35].

2.3. Some properties of the alternative velocity fields

The velocity fields \( v \) given in (8) are not defined at the nodes of the wavefunction (that is, points where \( \psi = 0 \)). In general they also diverge near nodes. Nevertheless, in the case of the ordinary de Broglie–Bohm velocity field, the set of initial configurations that run into a node has \( |\psi|^2 \)-measure zero [36, 37]. Probably similar results hold for a reasonable class of alternative velocity fields.

In the case of the ordinary de Broglie–Bohm velocity field, the nodes are the only potential source of vorticity, while the alternative velocity fields yield vorticity even away from nodes. This can be seen as follows. Consider a single particle for simplicity. The average vorticity \( \omega_\Sigma \) over a surface \( \Sigma \) with boundary \( \partial \Sigma \) is given by

\[
\omega_\Sigma = \frac{1}{A(\Sigma)} \oint_{\partial \Sigma} v \cdot d\mathbf{l},
\]

(12)

where \( \oint_{\partial \Sigma} v \cdot d\mathbf{l} \) is the circulation of the velocity field and \( A(\Sigma) \) is the area of the surface. If the surface does not contain any node, Stokes’ theorem can be applied to write \( \oint_{\partial \Sigma} v \cdot d\mathbf{l} = \int_{\Sigma} \omega \cdot d\mathbf{S} \), where \( \omega = \nabla \times v \) is the vorticity vector. This vorticity vector is not defined at nodes (although alternatively one could define it in a distributional sense, see, for example, [38] for the case of the ordinary de Broglie–Bohm theory).

In the case of the ordinary de Broglie–Bohm theory the velocity field is given by \( v_s = \nabla S / m \), so that the corresponding vorticity vector is zero. Hence if the surface \( \Sigma \) does not contain any node, then the average vorticity over that surface is zero. The average vorticity can only be nonzero when the surface contains nodes. In that case the vorticity is quantized [39, 40]. This is because the circulation is given by \( \oint_{\partial \Sigma} v \cdot d\mathbf{l} = \oint_{\partial \Sigma} \nabla S \cdot d\mathbf{l} / m = nh / m \), with \( n \) being an integer, since \( S \) is multivalued, where different values of \( S \) at a point can only differ by an integer multiple of \( 2\pi \hbar = \hbar \) (since \( \psi \) is single-valued).

Note that in case the particle is moving in an external magnetic field \( B = \nabla \times A \), the standard velocity field becomes \( v_s = \nabla S / m - eA / mc \), so that the vorticity vector obtains a contribution \(-eB / mc\).

In the case of alternative velocity fields, the vorticity vector \( \omega \) is, in general, different from zero, so that there is vorticity even away from nodes.

In the ordinary de Broglie–Bohm theory, the chaotic motion near nodes probably finds its origin in the vorticity, together with the divergent behaviour of the velocity field. In the case of alternative velocity fields, similar features hold even in the neighbourhood of quasi-nodes (where \( |\psi| \) becomes very small). In this context, it would therefore be interesting to study the implications of vorticity, possibly combined with nodal or quasi-nodal structure, for possible chaotic behaviour.

3. Quantum non-equilibrium and relaxation to quantum equilibrium

3.1. Coarse-graining

For an arbitrary distribution \( \rho \) one can introduce the quantity \( f = \rho / |\psi|^2 \). Because \( \rho \) and \( |\psi|^2 \) satisfy the same continuity equation (with velocity field \( v \)), one has that \( \partial f / \partial t + v \cdot \nabla f = 0 \). This means that \( f \) is conserved along trajectories, that is, \( f(X(t), t) = f(X(0), 0) \) for all times \( t \) [5–8]. As such it would seem that \( \rho \) can never really relax to \( |\psi|^2 \) because their ratio is conserved along trajectories. However, relaxation should be understood in the sense that \( \rho \) goes
to $|\psi|^2$ on a coarse-grained level [6–8]. That is, if we consider the coarse-grained densities $\bar{\rho}$ and $|\psi|^2$, whose value is obtained by averaging over non-overlapping cells (so that their value is constant over those cells), then $\bar{\rho}/|\psi|^2$ is not necessarily conserved along the trajectories, so that $\bar{\rho}$ may relax to $|\psi|^2$. The coarse-graining could be understood as corresponding to a finite accuracy of physical measurements.

The deviation of $\rho$ from $|\psi|^2$ can be quantified by means of minus the relative entropy of $\rho$ with respect to $|\psi|^2$ [6–8]:

$$H = \int \mathrm{d}x \rho \ln(\rho/|\psi|^2).$$

(13)

Valentini called this quantity $H$ in analogy with the $H$-function in classical statistical mechanics. It is strictly positive and zero for the quantum equilibrium distribution. However, since this quantity is conserved in time, just like $f$, it is not really suitable to quantify relaxation. Instead the coarse-grained $H$-function

$$\bar{H} = \int \mathrm{d}x \bar{\rho} \ln(\bar{\rho}/|\psi|^2)$$

(14)

should be considered.

3.2. Relaxation

While we typically expect a non-equilibrium distribution to relax to equilibrium (on a coarse-grained level), this will definitely not happen always. That is, while we typically expect the coarse-grained $H$-function, $\bar{H}$, to decrease over time, it may also increase over time or stay constant. This depends on both the initial distribution and the initial wavefunction. Let us expand on this.

Firstly, for a given wavefunction, not every initial distribution $\rho(x)$ will have relaxed to the quantum equilibrium distribution $|\psi(x, T)|^2$ in a given time $T$. Just consider some distribution $\rho(x) \neq |\psi(x, T)|^2$ and evolve that distribution backwards in time along the de Broglie–Bohm trajectories. The resulting distribution $\rho(x, -T)$ will then lead to the non-equilibrium distribution $\rho(x)$ after time $T$. The distribution might of course relax at a later time.

Secondly, for some wavefunctions there will even be no relaxation, regardless of the initial distribution. For example, in the case of the ordinary de Broglie–Bohm theory, there will not be relaxation for a plane wave or a Gaussian wavefunction (see [41] for further examples). For a single-particle plane wave any distribution will just be translated over time. For a Gaussian wavefunction any distribution will either spread or contract over time, depending on whether the Gaussian itself is spreading and contracting. Note that relaxation might still occur for alternative velocity fields.

Thirdly, if there is relaxation of a distribution $\rho$ for a particular wavefunction, then by time-reversal invariance there exists a wavefunction for which the time evolution of the distribution becomes time reversed [7]. The de Broglie–Bohm dynamics has the time-reversal symmetry $(X(t), \psi(x, t)) \rightarrow (X(-t), \psi^*(x, -t))$, which reverses the direction in which the trajectories are traversed. As a result, an initial distribution $\rho(x)$ whose time evolution is given by $\rho(x, t)$ under the dynamics determined by $\psi(x, t)$, will evolve according to $\rho(x, -t)$ under the dynamics determined by $\psi^*(x, -t)$.
4.1. A particle in a two-dimensional square box

We consider a particle that moves in two dimensions and that is confined to a two-dimensional square box of side \( \pi \) by an infinite potential well \((\hbar, \text{the mass } m \text{ and the length unit are all set to } 1)\). As such, the wavefunction is given by a superposition of the energy eigenfunctions

\[ \phi_{mn}(x_1, x_2) = \frac{2}{\pi} \sin(mx_1) \sin(nx_2) \]  

with energy eigenvalues \( E_{mn} = (m^2 + n^2)/2 \), where \( m \) and \( n \) are strictly positive integers.

Note that, except in one dimension [43], the trajectories, in general, do not inherit the periodicity of the wavefunction, that is, in general \( x_{t+\tau} \neq x_t \). Note also that the maps \( x_t \), in general, do not form a group.
We first consider a superposition of the four lowest energy eigenstates, with equal weights and different phases $\theta_{mn}$:

$$
\psi_1(x_1, x_2, t) = \sum_{m,n=1}^{2} \frac{1}{2} e^{i\theta_{mn}} \phi_{mn}(x_1, x_2) e^{-iE_{mn}t} 
= \sum_{m,n=1}^{2} \frac{1}{\pi} \sin(mx_1) \sin(nx_2) e^{i(\theta_{mn} - E_{mn}t)}. 
$$

The wavefunction is periodic, with period $4\pi$. The corresponding density $|\psi_1(x_1, x_2, 0)|^2$, at time $t = 0$, is given in figure 1. The wavefunction has only one node (within the box), whose trajectory is given in figures 2 and 3.

We also consider the following wavefunction:

$$
\psi_2(x_1, x_2, t) = \frac{\sqrt{3}}{2} e^{i\theta_{11}} \phi_{11}(x_1, x_2) e^{-iE_{11}t} + \sum_{m,n=2}^{\infty} \frac{1}{2\sqrt{3}} e^{i\theta_{mn}} \phi_{mn}(x_1, x_2) e^{-iE_{mn}t}, 
$$

which also has a period of $4\pi$, but which does not have any nodes. The corresponding density $|\psi_2(x_1, x_2, 0)|^2$ is given in figure 1.

In two dimensions a divergence-free two-vector field $a_i(x_1, x_2)$ can always be written as $a_i = \varepsilon_{ij} \partial_j f(x_1, x_2)$, where $\varepsilon_{ij}$ is anti-symmetric with $\varepsilon_{12} = 1$ (as a consequence of Poincaré’s lemma), so that the velocity field of the particle can be put into the form

$$
v_i(x_1, x_2, t) = v_{ij}(x_1, x_2, t) + \mu \frac{\varepsilon_{ij} \partial_j f(x_1, x_2, t)}{|\psi(x_1, x_2, t)|^2}, 
$$

For the record, the phases are given by $\theta_{11} = 1.1525988926093297$, $\theta_{12} = 4.2775762116024665$, $\theta_{21} = 2.166032988555025$ and $\theta_{22} = 2.8960554218806349$. They are obtained from [7], where they were randomly generated.

---

Figure 1. The equilibrium densities at time $t = 0$, for the wavefunctions $\psi_1$ and $\psi_2$, given in equations (17) and (18), respectively.
Figure 2. Panel (a) displays the trajectory of the node of the wavefunction $\psi_1$. The other panels display particle trajectories for different values of $\mu$ and $f$ for the wavefunction $\psi_1$. In each case, the initial position is the centre of the box. The final position is denoted by an arrow. All trajectories are for the time interval $[0, 4\pi]$. Note that the trajectory in panel (e) does not display periodicity over this time interval.

with $\mu$ being a constant. We will consider a number of different values for $\mu$ and the following choices for the function $f$: 9

$$f_1 = |\psi|^2, \quad f_2 = \epsilon_{ij} \partial_i f_{s,j}, \quad f_3 = \partial_i f_{s,i}.$$  \hspace{1cm} (21)

9 Note that the velocity field (11), for the case of a spin-eigenstate $\chi = (1 \ 0)^T$ and for a factorizable wavefunction $\psi(x_1, x_2, x_3, t) = \psi(x_1, x_2, t) \eta(x_3, t)$, reduces to

$$v_1 = \frac{1}{m} \partial_1 S_\psi + \frac{\hbar}{2m|\psi|^2} \partial_2 |\psi|^2, \quad v_2 = \frac{1}{m} \partial_2 S_\psi - \frac{\hbar}{2m|\psi|^2} \partial_1 |\psi|^2, \quad v_3 = \frac{1}{m} \partial_3 S_\eta,$$  \hspace{1cm} (20)

where $S_\psi$ and $S_\eta$ are the phases of $\psi$ and $\eta$, respectively. Hence, in this case the motion in the $(x_1, x_2)$-plane decouples from that in the $x_3$ direction and the velocity field in the $(x_1, x_2)$-plane is of the form (19), with $\mu = \hbar/2m$ and $f = f_1 = |\psi|^2$. 

Figure 3. Space–time trajectories of the node (bold lines) and particle trajectories (thin lines), for the wavefunction $\psi_1$, over the time interval $[0, 4\pi]$. In each case, the initial position is the centre of the box.

The value $\mu = 0$ corresponds to the ordinary de Broglie–Bohm theory. The choices are such that there is no outgoing or incoming quantum probability flux at the boundary of the box (which means that the components of the currents normal to the boundary vanish). This means that there is no flow of $|\psi|^2$ in or out of the box. In figures 2 and 3, some trajectories are given for the wavefunction $\psi_1$ given in (17).

We consider different non-equilibrium distributions at time $t = 0$. The first one, denoted by $\rho_0$, is chosen to be the square of the modulus of the ground state, that is,

$$\rho_0(x_1, x_2, 0) = |\phi_{11}(x_1, x_2)|^2 = \left(\frac{2}{\pi}\right)^2 \sin^2 x_1 \sin^2 x_2. \tag{22}$$
The other non-equilibrium distributions, denoted by \( \rho_i, i = 1, \ldots, 4 \), are obtained from \( \rho_0 \) by translation and contraction, that is,

\[
\begin{align*}
\rho_1(x_1, x_2, 0) &= 4\rho_0(2x_1, 2x_2, 0), \quad (x_1, x_2) \in [0, \pi/2] \times [0, \pi/2], \\
\rho_2(x_1, x_2, 0) &= 4\rho_0(2(x_1 - \pi/2), 2x_2, 0), \quad (x_1, x_2) \in [\pi/2, \pi] \times [0, \pi/2], \\
\rho_3(x_1, x_2, 0) &= 4\rho_0(2x_1, 2(x_2 - \pi/2), 0), \quad (x_1, x_2) \in [0, \pi/2] \times [\pi/2, \pi], \\
\rho_4(x_1, x_2, 0) &= 4\rho_0(2(x_1 - \pi/2), 2(x_2 - \pi/2), 0), \quad (x_1, x_2) \in [\pi/2, \pi] \times [\pi/2, \pi],
\end{align*}
\]

and are zero outside the domains specified. So these distributions have their support in the four different quadrants of the square box.

4.2. Some details of the algorithm

The algorithm to calculate the evolution of the non-equilibrium densities is similar to that of Valentini and Westman [7]. Just as in their work, the calculation of the trajectories is based on the Runge–Kutta–Fehlberg algorithm with Cash–Karp parameters [44] (but with a starting value of \( \Delta \) equal to \( 10^{-3} \) and the maximal number of time steps equal to \( 10^5 \)).

In order to calculate the time-evolved non-equilibrium density \( \rho(x_1, x_2, t) \) from the initial density \( \rho(x_1, x_2, 0) \), a uniform lattice is placed over the box, whose lattice points have the coordinates \((k\pi/1024 - \pi/2048, l\pi/1024 - \pi/2048)\), where \( k, l = 1, 2, \ldots, 1024 \) (with hence a total of \( 1024 \times 1024 \) lattice points). Each lattice point is then evolved backwards in time from time \( t \) to time \( t = 0 \) using the de Broglie–Bohm dynamics. Then, using the constancy of \( f = \rho/|\psi|^2 \) along a trajectory (see section 3.1), one has that the time evolved density at a lattice point with coordinates \((x_1, x_2)\) is given by

\[
\rho(x_1, x_2, t) = |\psi(x_1, x_2, t)|^2 f(x_1(0), x_2(0), 0),
\]

where \((x_1(0), x_2(0))\) are the coordinates of the backtracked position. This method of using the backtracked positions is advantageous compared to one where positions are evolved forward in time [7]. If the calculation of the backtracked position involves more than the \( 10^5 \) time steps, it is halted and the lattice point is ignored when calculating the coarse-grained and smoothed density.

The coarse-graining of a density \( \rho \) is done by averaging over square non-overlapping cells of side \( \pi/32 \) (with a total of \( 32 \times 32 \) cells). Each such coarse-graining cell \( C \) contains 1024 lattice points, of which a certain number \( N_C \) can be backtracked. So the coarse-grained density \( \bar{\rho} \) in a certain cell \( C \) is given by

\[
\sum_C \rho(x_1, x_2, t)/N_C,
\]

where the sum ranges over coordinates \((x_1, x_2)\) of lattice points that are contained in the cell \( C \) and that could be backtracked.

Lattice points near nodes are generally harder to backtrack because the velocity field generally diverges there. This is in particular the case for the lattice points near the boundary of the box. Therefore in order to speed-up the calculation of the time-evolved non-equilibrium densities, we have ignored those lattice points that lie within two coarse-graining cells near the boundary. As such there is an error in calculating the coarse-grained \( H \)-function, since the ignored regions near the boundary yield no contribution to the integral. Therefore, our calculated coarse-grained \( H \)-function only measures the difference between the calculated coarse-graining cells.

In the figures, smoothed densities \( \tilde{\rho} \) are displayed, instead of the coarse-grained densities \( \bar{\rho} \). The reason for the smoothing is to average out fine-grained fluctuations. It is done by averaging
Figure 4. Smoothed densities $|\psi_1|^2$ and $\tilde{\rho}_0$ at times $t = 0, 4\pi$ and $8\pi$, for guidance equations with different values of $\mu$ and $f = f_1$, for the wavefunction $\psi_1$. Note that the relaxation to equilibrium is better for higher value of $\mu$.

over square cells of side $\pi/16$, ignoring again the cells near the boundary. The cells may be overlapping and can be mapped to one another by translations over an integer multiple of $\pi/108$ along the $x_1$- and $x_2$-directions. More explicitly, we consider the points with coordinates $(k\pi/128 + 3\pi/32, l\pi/128 + 3\pi/32)$, with $k, l = 0, 1, 2, \ldots, 104$, and calculate $\tilde{\rho}$ at those points by averaging the density $\rho$ over cells of size $\pi/16$, ignoring again the lattice points that could not be backtracked (so that each average is done over at most 4096 lattice points). In generating the plots with Matlab an interpolation of those densities values is then introduced.

4.3. Results of the numerical simulations

Figures 4–7 display the time evolution of the distributions $|\psi_1|^2$ and of the different non-equilibrium distributions $\rho_i, i = 0, \ldots, 4$ for $\psi_1$ (given by (17)), and this for different guidance
Figure 5. Smoothed densities $\tilde{\rho}_1$ and $\tilde{\rho}_2$ at times $t = 0, 4\pi$ and $8\pi$, for guidance equations with different values of $\mu$ and $f = f_1$, for the wavefunction $\psi_1$. 

The calculated values of the coarse-grained $H$-function are given in tables 3 and 4. Note that some values of $\bar{H}$ are negative, which is theoretically impossible. In general, there will be some deviations from the actual values because of several reasons. Firstly, these densities are
calculated using only a lattice sampling; secondly, there are numerical errors that arise when calculating the time evolution of the distributions; and thirdly, by ignoring the contributions of regions near the boundary in the integral that defines $\bar{H}$, we have effectively put $\bar{\rho}$ zero in those regions. Valentini and Westman [7] estimated the error in $\bar{H}$ to be about 2%. Assuming a similar error in our case, we have presented the values of $\bar{H}$ rounded to the nearest integer.

From the pictures, as well as from the values of the coarse-grained $H$-function, it is clear that the non-equilibrium distributions evolve closer to equilibrium over time. Furthermore, the relaxation time decreases when the value of $\mu$ increases. As mentioned before, this might be

Figure 6. Smoothed densities $\tilde{\rho}_3$ and $\tilde{\rho}_4$ at times $t = 0, 4\pi$ and $8\pi$, for guidance equations with different values of $\mu$ and $f = f_1$, for the wavefunction $\psi_1$. (In the case of $\tilde{\rho}_4$, $\mu = 0$ and $t = 8\pi$, one peak in the distribution is not fully plotted.)
Figure 7. Smoothed densities $|\psi_1|^2$ and $\tilde{\rho}_0$ at times $t = 0$, $2\pi$ and $4\pi$, for guidance equations with different values of $\mu$ and $f$, for the wavefunction $\psi_1$. (In the case of $\tilde{\rho}_0$, $\mu = 0$ and $t = 2\pi$, one peak in the distribution is not fully plotted.)

explained by the fact that the extra term in the velocity adds to the overall irregularity of the motion and to the vorticity in particular.

Note that in the case of the ordinary de Broglie–Bohm velocity field, the relaxation is not as good as in the simulation of Valentini and Westman [7], where a superposition of the first 16 modes was considered instead of the first 4. This is probably related to the fact that more chaotic behaviour is expected when the number of nodes increases [14]. The wavefunction of Valentini and Westman has much more than one node.

In the case of the guidance equation with $f = f_2$, there is not a very good relaxation neither for $\mu = 0.5$ nor for $\mu = 1$, compared to the other alternative guidance equations (although
Table 1. Percentage of backtracked lattice points, for the wavefunction $\psi_1$, and for the guidance equations with different values of $\mu$ and $f$ (up to two decimal places).

<table>
<thead>
<tr>
<th></th>
<th>$t = 4\pi$</th>
<th>$t = 8\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu = 0$</td>
<td>99.89</td>
<td>99.62</td>
</tr>
<tr>
<td>$\mu = 1$, $f_1$</td>
<td>99.98</td>
<td>99.52</td>
</tr>
<tr>
<td>$\mu = 2$, $f_1$</td>
<td>99.52</td>
<td>94.44</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>$t = 2\pi$</th>
<th>$t = 4\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu = 0$</td>
<td>99.95</td>
<td>99.89</td>
</tr>
<tr>
<td>$\mu = \frac{1}{2}$, $f_2$</td>
<td>100</td>
<td>99.62</td>
</tr>
<tr>
<td>$\mu = 1$, $f_2$</td>
<td>99.99</td>
<td>91.71</td>
</tr>
<tr>
<td>$\mu = 1$, $f_3$</td>
<td>100</td>
<td>99.82</td>
</tr>
<tr>
<td>$\mu = 2$, $f_3$</td>
<td>99.99</td>
<td>97.16</td>
</tr>
</tbody>
</table>

Figure 8. Smoothed densities $\tilde{|\psi_2|^2}$ and $\tilde{\rho}_0$ at times $t = 0$, $6\pi$ and $12\pi$, for the ordinary de Broglie–Bohm guidance equation and for the one with $\mu = 2$ and $f = f_1$, for the wavefunction $\psi_2$.

It is still better than for the ordinary de Broglie–Bohm theory. We have tried to perform the simulations also for $\mu = 1.5$, but found that only 76.78% of the lattice points could be backtracked. Since this percentage is rather low, we did not include these results in the
Table 2. Percentage of backtracked lattice points, for the nodeless wavefunction \( \psi_2 \), for the ordinary de Broglie–Bohm guidance equation and for the one with \( \mu = 2 \) and \( f = f_1 \) (up to two decimal places).

<table>
<thead>
<tr>
<th>( t = 6\pi )</th>
<th>( t = 12\pi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mu = 0 )</td>
<td>100</td>
</tr>
<tr>
<td>( \mu = 2, f_1 )</td>
<td>99.45</td>
</tr>
</tbody>
</table>

Table 3. Values of \( \bar{H} \) (rounded to the nearest integer) for the densities plotted in figures 4–7. Note the decrease of \( \bar{H} \) with an increase in \( \mu \).

<table>
<thead>
<tr>
<th>( t = 0 )</th>
<th>( t = 4\pi )</th>
<th>( t = 8\pi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \bar{\rho}_0, \mu = 0 )</td>
<td>54</td>
<td>31</td>
</tr>
<tr>
<td>( \bar{\rho}_0, \mu = 1, f_1 )</td>
<td>54</td>
<td>10</td>
</tr>
<tr>
<td>( \bar{\rho}_0, \mu = 2, f_1 )</td>
<td>54</td>
<td>1</td>
</tr>
<tr>
<td>( \bar{\rho}_1, \mu = 0 )</td>
<td>168</td>
<td>126</td>
</tr>
<tr>
<td>( \bar{\rho}_1, \mu = 1, f_1 )</td>
<td>168</td>
<td>16</td>
</tr>
<tr>
<td>( \bar{\rho}_1, \mu = 2, f_1 )</td>
<td>168</td>
<td>14</td>
</tr>
<tr>
<td>( \bar{\rho}_2, \mu = 0 )</td>
<td>169</td>
<td>129</td>
</tr>
<tr>
<td>( \bar{\rho}_2, \mu = 1, f_1 )</td>
<td>169</td>
<td>26</td>
</tr>
<tr>
<td>( \bar{\rho}_2, \mu = 2, f_1 )</td>
<td>169</td>
<td>17</td>
</tr>
<tr>
<td>( \bar{\rho}_3, \mu = 0 )</td>
<td>130</td>
<td>94</td>
</tr>
<tr>
<td>( \bar{\rho}_3, \mu = 1, f_1 )</td>
<td>130</td>
<td>12</td>
</tr>
<tr>
<td>( \bar{\rho}_3, \mu = 2, f_1 )</td>
<td>130</td>
<td>5</td>
</tr>
<tr>
<td>( \bar{\rho}_4, \mu = 0 )</td>
<td>300</td>
<td>207</td>
</tr>
<tr>
<td>( \bar{\rho}_4, \mu = 1, f_1 )</td>
<td>300</td>
<td>54</td>
</tr>
<tr>
<td>( \bar{\rho}_4, \mu = 2, f_1 )</td>
<td>300</td>
<td>21</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( t = 0 )</th>
<th>( t = 2\pi )</th>
<th>( t = 4\pi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \bar{\rho}_0, \mu = 0 )</td>
<td>54</td>
<td>39</td>
</tr>
<tr>
<td>( \bar{\rho}_0, \mu = \frac{1}{2}, f_2 )</td>
<td>54</td>
<td>23</td>
</tr>
<tr>
<td>( \bar{\rho}_0, \mu = 1, f_2 )</td>
<td>54</td>
<td>22</td>
</tr>
<tr>
<td>( \bar{\rho}_0, \mu = 1, f_3 )</td>
<td>54</td>
<td>5</td>
</tr>
<tr>
<td>( \bar{\rho}_0, \mu = 2, f_3 )</td>
<td>54</td>
<td>2</td>
</tr>
</tbody>
</table>

paper. Figures 2 and 3 display some trajectories for different possible guidance equations. The trajectory for \( f = f_2 \) and \( \mu = 1 \) circles around the node from time \( t = 0 \) to \( t = 4\pi \), unlike the trajectories corresponding to the other guidance equations, which tend to cover a bigger area of the box in that time. This might be a possible reason why the relaxation is not so good in this case. If the dynamics is such that initial positions that start near a node remain close to it for long periods of time and merely circle around it, one might expect that there is insufficient mixing-like behaviour for relaxation to occur efficiently.

In the case of the wavefunction without node, there is some convergence towards quantum equilibrium for the ordinary de Broglie–Bohm guidance equation. However, there is definitely not a good relaxation. It is unclear how much better the convergence would be for larger times. In the case of the guidance equation with \( \mu = 2 \) and \( f = f_1 \), there is an approximate relaxation...
Table 4. Values of $\tilde{H}$ (rounded to the nearest integer) for the densities plotted in figure 8.

<table>
<thead>
<tr>
<th></th>
<th>$t = 0$</th>
<th>$t = 6\pi$</th>
<th>$t = 12\pi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tilde{\rho}_0, \mu = 0$</td>
<td>17</td>
<td>16</td>
<td></td>
</tr>
<tr>
<td>$\tilde{\rho}_0, \mu = 2, f_1$</td>
<td>17</td>
<td>1</td>
<td>$-1$</td>
</tr>
</tbody>
</table>

to equilibrium. Presumably the more efficient relaxation in the latter case is related to possible chaotic behaviour induced by the vorticity. In the ordinary de Broglie–Bohm theory, there is probably no chaotic motion for this wavefunction, due to the absence of nodes.

5. Conclusion

We have considered non-equilibrium distributions and their relaxation properties for a class of de Broglie–Bohm-type theories and found that the relaxation time depends substantially on the form of the guidance equation. In particular, for the examples considered here of such theories, there was a faster relaxation compared to the ordinary de Broglie–Bohm theory.

Only non-relativistic quantum theory was considered, but similar results are expected to hold for relativistic quantum theory or quantum field theory. As such, these results might have potential implications for empirical predictions concerning non-equilibrium distributions, such as, for example, those of Valentini [11, 12] that were mentioned in the introduction. But, with this being said, Valentini’s predictions involve a field ontology for a scalar field, with a velocity field that is most natural. In support of his choice, Valentini actually proves the uniqueness of this velocity field for the vacuum state (the state of interest for his analysis) under certain natural assumptions [12].

Actually, when it comes to quantum field theory, there is, apart from the ambiguities in the velocity field, also a potential ambiguity in the choice of ontology. Some de Broglie–Bohm-type models, for example, suggest a field ontology, while others suggest a particle ontology (see for example [45, 46] for possible particle ontologies and see [47] for a review of possible field ontologies). Such ambiguities may potentially be relevant too for possible empirical predictions concerning non-equilibrium.

Note that similar ambiguities arise in, for example, the context of Nelson’s stochastic mechanics [48, 49]. Nelson’s mechanics [50, 51] can be regarded as a modification of the de Broglie–Bohm theory in which the deterministic de Broglie–Bohm dynamics is replaced by a diffusion process (although Nelson himself wanted to derive the wavefunction and Schrödinger’s dynamics from the stochastic process instead of assuming them independently). This diffusion process is expected to yield convergence to equilibrium for most distributions (see [52] for some rigorous results). As with the de Broglie–Bohm theory there are many ways in which a Nelsonian type of dynamics can be introduced that preserves the equilibrium distribution $|\psi|^2$. In particular, there are Nelsonian theories with arbitrary values of the diffusion constant [48]. In this case, relaxation time is expected to decrease with increasing diffusion constant.
Acknowledgments

SC acknowledges support from a PIAF (Perimeter Institute Australia Foundations) postdoctoral research fellowship and is grateful to Josh Combes, Indy Siva and Mike Towler for their help with some aspects of the numerical simulations. WS acknowledges support of the FWO-Flanders through a postdoctoral fellowship and is grateful to Lukas Maes and Ruben Stukken for their help with the initial exploration of this project and to Christian Maes for useful discussions. We further thank Antony Valentini, Hans Westman and Howard Wiseman for valuable discussions or comments. It is also a pleasure to thank Perimeter Institute for hospitality enjoyed during a stay when part of this work was completed (WS thanks Lucien Hardy for the invitation).

References


[38] Takabayasi T 1983 Prog. Theor. Phys. 69 1323