Stability Properties of $|\Psi|^2$ in Bohmian Dynamics

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According to Bohmian dynamics, the particles of a quantum system move along trajectories, following a velocity field determined by the wave-function $\Psi(x,t)$. We show that for simple one-dimensional systems any initial probability distribution of a statistical ensemble approaches asymptotically $|\Psi(x,t)|^2$ if the system is subject to a random noise of arbitrarily small intensity.

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According to the de Broglie-Bohm quantum theory of motion [1-3], the $n$ particles of a quantum system described by a wavefunction

$$
\Psi(\vec{X}, t) = R(\vec{X}, t)e^{[i/\hbar]S(\vec{X},t)}, \quad \vec{X} \equiv \{\vec{x}_1, \vec{x}_2, \ldots \vec{x}_i, \ldots, \vec{x}_n\}
$$

that obeys the Schrödinger equation, follow trajectories whose velocity is given by the equation

$$
\vec{v}(\vec{X}, t) = \nabla S(\vec{X}, t)/\hbar.
$$
\[ \ddot{x}_i = \frac{1}{m} \frac{\partial S(\{x_1, x_2, \ldots, x_i, \ldots, x_n\}, t)}{\partial \dot{x}_i} \bigg|_{\dot{x}=\ddot{x}(t)}, \quad i = 1, \ldots, n \] (2)

which can be solved knowing the initial conditions \( \vec{X}(t = 0) \). Note that in this equation the actual value of the velocity (in configuration space) is the realization of a particular value of the velocity field \( 1/m \nabla_x S(\vec{X}, t) \) at the actual position \( \vec{X}(t) \) of the system.

Consider now an ensemble of systems, associated with a probability distribution in configuration space, \( \rho(\vec{X}, t) \). Both \( \rho \) and the quantum distribution probability, \( |\Psi|^2 \), obey a continuity equation \[ \frac{\partial g(\vec{X}, t)}{\partial t} + \nabla_X \cdot (g(\vec{X}, t) \dot{\vec{X}}) = 0, \quad g = \rho, |\Psi|^2. \] (3)

It is clear that if \( \rho \) and \( |\Psi|^2 \) coincide at a given time \( t_o \), they coincide at all times (that is called the equivariance property) so that the predictions of quantum mechanics are reproduced. The condition \( \rho(\vec{X}, t_o) = |\Psi(\vec{X}, t_o)|^2 \) is then sometimes taken as a postulate of the Bohmian quantum theory of motion (cf. e.g. \[3\]). However, this restriction of the theory to particular ensembles is not logically justified, since in the theory trajectories have an independent reality of their own \[4\], and in fact there have been attempts to deduce the quantal distribution from the dynamics of the system. Precisely because of the existence of trajectories this problem can be considered to be akin to that of classical statistical mechanics \[5\]. Valentini \[6,7\] has deduced a "subquantal" H-theorem, which involves hypothesis similar to those adopted in the demonstration of the H-theorem in classical mechanics, assuming that the orbits of the system are sufficiently complicated, so that they sample all the accessible regions of configuration space. Indeed, many recent studies deal with the chaotic features of the deBroglie and Bohm trajectories for systems with several degrees of freedom (cf. e.g. \[8\]).

We shall follow a different line of thought, inspired by the original paper by Bohm \[9\], who studied the consequences of random collisions among the electrons inside atoms or molecules, on the electron distribution.
Let us suppose that the electrons of a given statistical sub-ensemble of molecules are initially described by the stationary wavefunction of the ground state, $\psi_a(x_1, t)$, and by a distribution of particles, not necessarily corresponding to $|\psi_a|^2$. Let us further suppose that, during some amount of time, these molecules interact with a second set of uncontrolled molecules, described by the wavefunction $\phi_b(x_2, t)$.

Initially (for $t \to -\infty$) the wavefunction of the two colliding molecules is

$$
\Psi_a(x_1, x_2, r_{12}; t) = \psi_a(x_1; t)\phi_b(x_2; t)d_o(r_{12}; t),
$$

while during the collision the wave function must be written as the linear combination

$$
\Psi(x_1, x_2, r_{12}; t) = \sum_{\alpha,\beta,\gamma} C_{\alpha,\beta,\gamma} \Psi_{\alpha,\beta,\gamma}(x_1; \{x_2, r_{12}; t\})
$$

with

$$
\Psi_{\alpha,\beta,\gamma}(x_1, x_2, r_{12}; t) = \psi_\alpha(x_1; t)\phi_\beta(x_2; t)d_\gamma(r_{12}; t)
$$

where $\psi_\alpha(x_1, t)$ represents a stationary state of molecule-1, $\psi_\beta(x_2, t)$ represents a stationary state of molecule-2, and $d_\gamma(r_{12}, t)$ represents a state of relative motion of the center of mass of the colliding molecules (typically a wave-packet). The details of the initial state, that is $\psi_\alpha(x_1), \phi_\beta(x_2)$ and $d_o(r_{12})$, determine, via the Schrödinger equation, the amplitudes $C_{\alpha,\beta,\gamma}$ of the different stationary states of the compound wave function.

Note that, in order to calculate the velocity of electron-1, this wave function may be rewritten as the linear combination of eigenstates of molecule-1

$$
\Psi(x_1, t) = \sum_{\alpha} \mathcal{X}_{\alpha}(x_2(t), r_{12}(t); t)\psi_\alpha(x_1; t),
$$

in which the coefficients $\mathcal{X}_{\alpha}(x_2(t), r_{12}(t); t)$ incorporate the dependence in $x_2$ and $r_{12}$, and the summation over the indices $\beta$ and $\gamma$. The velocity of the electron in the interior of molecule-1
is obtained using this wave function by means of Eq.(2), being thus sensitive to all the initial conditions, including, the positions of the electrons of molecule-2, \( (x_2(t = -\infty)) \) and the relative positions. Similar expressions may be adopted for the velocities associated to \( x_2 \) and \( r_{12} \).

After the collision (for \( t \to +\infty \)) the linear combination in Eq.(5) may be simplified, for all practical purposes, by retaining only one component, for example that of \( \alpha = \beta = a \) in the case of elastic scattering. This is a kind of ”natural” wave function collapse (see [2,10]), and guarantees that after the collision process the system is left in a stationary state. The question one would like to address is how the collision process affects the original distribution.

In order to find an answer, we shall study the evolution of the particle distribution of one of the subensembles, that of coordinate \( x_1 \), replacing the detailed description of the other variables (\( x_2 \) and \( r_{12} \)) during the collision process by the action of a random noise. The stochastic noise will represent the effect of the deviation of all those other degrees of freedom from their average value.

We shall solve the equations of motion, studying numerically the resulting distribution function of the electrons, instead of making the strong statistical assumptions adopted by Bohm\(^1\). Our aim will be to show that the system tends to a distribution described by \( |\Psi|^2 \), starting from an arbitrary initial distribution.

We first study some properties of the time evolution of the distribution of particles governed by Bohmian dynamics, in relation with its response to a stochastic perturbation.

\(^1\)Bohm’s proof was based on the assumption of a continuity equation (Eq.(3) in [9]), even if the random perturbation acting on the electrons inside the molecules would require the more general Fokker-Planck equation, including sources and diffusion terms.
In particular we consider the effects of stochastic noise on one-dimensional, non-degenerate systems in non-stationary states. Starting from arbitrary initial ensemble distributions, we will show that they tend to the quantal distribution.

In a realistic calculation, the noise intensity should be determined in accordance to the coefficients of the linear combination (7), and as a consequence should be dependent on the position along the trajectory. It would be natural to expect that during the reaction the noise will reach a peak value around the distance of closest approach between the colliding molecules, tending to zero for $t \to \pm \infty$. In the following, we shall limit ourselves to a very simplified description, solving the equations of motion (the one-dimensional equivalent of Eq.(2))

$$\dot{x}_i = \frac{1}{m} \nabla S(x_i, t) + C \eta_i, \quad i = 1, 2, \ldots N$$

where $i$ labels the $N$ elements of the statistical ensemble of one-particle systems, initially distributed according to a given function $\rho_0(x) \equiv \rho(x, t = 0)$, and subject to a random white noise $\eta_i(t)$, whose intensity is controlled by the parameter $C$ (in what follows $C$ will be measured in hundredths of the speed of light, which is a natural scale for the studied systems). The $x$-independent character of the noise that we use, would produce a complete diffusion in the whole space. This is avoided by confining the system in a box with infinite, perfectly reflecting walls.

Let us thus numerically study the case of a statistical ensemble of $N = 5000$ test systems, each of them representing an electron confined in a box of length $L = 2\,\text{Å}$ with wave-function

$$\Psi(x, t) = a_1 \phi_1(x) e^{-iE_1t/\hbar} + a_2 \phi_2(x) e^{-iE_2t/\hbar},$$

where $\phi_1$ and $\phi_2$ are the two first stationary states of the well, taken with amplitudes $a_1, a_2$, which in a more general case would represent typical values during the reaction process (cf.
Eq. (7)). Here for simplicity we shall use the constant values $a_1 = a_2 = 1/\sqrt{2}$. We have solved the stochastic differential equation (8) using Heun algorithm [11].

We shall compare the results obtained with two different initial distributions, a uniform one, $\rho_0(x) = \rho_{un}(x) \equiv 1/L$, and another coinciding, at $t = 0$, with the usual quantum distribution, $\rho_0(x) = \rho_q(x) \equiv |\Psi(x,0)|^2$. The time evolution of $\rho_0(x,t)$ starting from $\rho_{un}(x)$ is shown in Fig.1 for the case of $C = 0.1$, which is a rather large noise intensity, corresponding to about 2% of the average velocity. It is seen that the approach to $|\Psi(x,t)|^2$ is already significant after one oscillation of the distribution.

We shall measure the difference between the distribution $\rho(x,t)$ evolving from the initial one, $\rho_0(x)$, and the quantal distribution $|\Psi(x,t)|^2$ making use of the function

$$\chi^2_{\rho_0}(t) = \int |\rho(x,t) - |\Psi(x,t)|^2| dx.$$  \hspace{1cm} (10)

In Fig.2 we present the results for three different values of $C$. For each one we present the time evolution of $\chi^2$. To be noted that for both initial conditions ($\rho_{un}(x)$ and $\rho_q(x)$) the systems evolve under the influence of the random noise; therefore, even starting from $\rho_q$, $\chi^2_{\rho_q}$ is in general different from zero. Similar results are obtained using other measures of the difference between $\rho(x,t)$ and $\Psi(x,t)$, in particular the relative entropy used in [7,8].

It can be seen that $\chi^2_{\rho_{un}}$ decreases until it reaches a minimum value, around which it stabilizes. This value coincides (apart from statistical fluctuations arising from the finite number of particles) with the one attained by $\chi^2_{\rho_q}$. This feature is seen in all the three cases presented, although the time needed for $\chi^2$ to stabilize is longer ($\tau = 60, 600$ and 6000 periods) for smaller values of $C$ ($C = 0.01, 0.001$ and 0.0001). It is also important to note that the asymptotic value of $\chi^2$ becomes smaller for smaller $C$, which means that the obtained particle distribution is closer to the quantum mechanical value $|\Psi(x,t)|^2$ the smaller the value of $C$ is. This is illustrated by the distributions presented on the right side of Fig.2. It can
be seen that reducing the noise, $\chi^2$ tends to an asymptotic value that is not equal to zero, what is mainly (90%) due to the finite statistical sampling (5000 systems distributed over 200 $x$-subintervals), and in a much smaller extent to the unavoidable errors in the numerical integration of the equations of motion (performed with $\Delta t = 1/500$ of a period). In fact, we have verified that eliminating the noise, that is, putting $C$ equal to zero, the asymptotic value is equal to 0.20, very close to the value obtained for $C = 0.0001$.

In order to obtain some insight in the results discussed above, it is convenient to rewrite the Bohmian equation of motion as a second-order Newtonian equation for the acceleration[2],

$$m\ddot{x}_i = -\nabla U_{cl} - \nabla U_{qu},$$  \hspace{1cm} (11)

where $U_{cl}$ is the classical potential and

$$U_{qu} = -(\hbar^2 / 2m)\nabla^2 R/R$$  \hspace{1cm} (12)

is the so-called quantum potential.

In the case of the particle in the box $U_{cl} = 0$ and thus, aside from the stochastic noise, the trajectories are determined by the behavior of $U_{qu}$. This is a time dependent potential, which goes to infinity where $R = 0$, that is at the nodal points. Instead at the points where $R$ has maxima, $U_{qu}$ is almost flat.

In the absence of noise, the Bohmian trajectories may be thought as those of classical particles moving in the time dependent potential $U_{qu}$, with the condition that the initial velocities, needed for integrating Eq.(11), must be those determined by the wave-function of the system (cf. Eq.(2)).

In our case, with only two eigenstates in the linear combination of $\Psi$ (cf. Eq.(9)), the density oscillates in time with Bohr’s period $T = 2\pi\hbar/(E_2 - E_1)$, and thus the potential
$U_{qu}(x,t)$ and the trajectories are also periodic (see Fig.3 and Figs. 4a,b). The trajectories near to the nodal points are compressed and re-expanded periodically by the strongly varying quantum potential. Such a compression-expansion is instead very soft for the trajectories close to maxima of $R$ (note $R$ in the denominator in Eq.(12)).

The effect of the stochastic noise is to break this periodic pattern (see Fig.4c). This breaking can be very effective, because any slight perturbation in the coordinate during the compressed phase makes the particle dramatically change its subsequent trajectory in the re-expansion process. The net effect of all these changes of trajectory is a higher residence time around the maxima of $R$, that produces a distribution of particles resembling $|\Psi|^2$ in spite of the initial distribution. We then see why the distribution $|\Psi|^2$ displays the remarkable stability against random perturbations of the system found above (cf. Fig.2).

We have checked that the above results are neither a special feature of the chosen potential, nor of the particular considered wave-function, by repeating the calculation with potentials of different shapes inside the walls and with different linear combinations of eigenstates, obtaining always a similar behaviour for the density distribution. In the case of the parabolic potential we have also analyzed the classically forbidden region, that is the region where the classical potential is larger than the average energy of the considered wave function, and found again that the density distribution approaches $|\Psi|^2$ as the noise intensity is set to smaller values. Let us however make some specific comments on the case of stationary states.

According to Bohmian dynamics, in the case of a stationary state ($\Psi(x,t) = \phi(x)e^{-iEt/\hbar}$)

\[2\text{In general, for more complex linear combination of states of the box, the periodicity will be controlled by the ground state frequency, of which all the other frequencies are multiples.}\]
the electrons are at rest (cf. Eq.(2)), and the addition of a stochastic noise would give rise to a pure diffusion process, leading inevitably to a uniform distribution inside the box. However this situation is not physically meaningful since, as stated above, the stochastic noise represents the (random) deviations of the single-particle like wave-function in eq.(7) from its average linear combination, which for a pure stationary state is just zero. In other words, the non-stationary character of the wave-function and the stochastic noise go together.

We conclude that under the action of random noise, at least for very simple, one-dimensional systems, an ensemble of particles, initially arbitrarily distributed, and governed by Bohmian dynamics progressively loses the "memory" of the initial distribution as time proceeds, and approaches the distribution \( |\Psi(x,t)|^2 \), a process which is based on the different stability of the underlying Bohmian trajectories. The origin of the random noise may be naturally found in the uncontrollable character of the position of the particles in Bohm's theory.

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Figure captions

Fig. 1
Evolution of the particles distribution during the first oscillation corresponding to an initially uniform distribution subject to a noise intensity of $C = 0.1$ (continuous line) and the corresponding $|\Psi(x)|^2$ (dashed line).

Fig. 2
On the left hand side the evolution of $\chi_{\rho_{un}}^2(t)$ (solid line) and $\chi_{\rho_q}^2(t)$ (dashed line) is shown as a function of time for three different values of $C$ (0.01, 0.001 and 0.0001). On the right hand side the distribution $\rho(x, \tau)$ evolving from $\rho_{un}$ (solid line) for the three different $C$ values at a fixed values of time ($\tau = 60, 600$ and 6,000 periods, respectively), is compared to $|\Psi(x, \tau)|^2$ (dashed line).

Fig. 3
The periodic, time-dependent quantum potential $U_{qu}(x, t)$ (in eV) is shown as a function of $x$ (in Å) and $t$ (in periods). Note the nodal point appearing as peaks in $U_{qu}(x, t)$.

Fig. 4
a) Trajectories of a set of particles initially distributed according to $|\Psi(x, t = 0)|^2$, and without any noise. b) Trajectories of a set of particles initially uniformly distributed ($\rho_o = \rho_{un} \equiv 1/L$) without any noise. c) The same as in b) but under the action of the stochastic noise ($C = 0.1$ in this example).
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