Contextuality, decoherence and quantum trajectories

A. S. Sanz\textsuperscript{1},\textsuperscript{*} and F. Borondo\textsuperscript{2},\textsuperscript{†}

\textsuperscript{1}Instituto de Física Fundamental, Consejo Superior de Investigaciones Científicas, Serrano 123, 28006 Madrid, Spain

\textsuperscript{2}Instituto Mixto de Ciencias Matemáticas CSIC–UAM–UC3M–UCM, and Departamento de Química, C–IX, Universidad Autónoma de Madrid, Cantoblanco – 28049 Madrid, Spain

(Dated: August 24, 2009)

Abstract

Here we analyze the relationship between quantum contextuality and decoherence in interference experiments with matter particles by means of a simple reduced quantum-trajectory model, which attempts to simulate the behavior of the projections of multi-dimensional, system-plus-environment Bohmian trajectories onto the subspace of the reduced system. This model allows us to understand the crossing of the subsystem trajectories as a combined effect of interference quenching and erasure of “which-way” information, which can be of utility to interpret decoherence effects in many-dimensional systems where full Bohmian treatments become prohibitive computationally.

PACS numbers: 03.65.Ta, 03.65.Ca, 03.65.-w, 03.65.Yz

\textsuperscript{*}Electronic address: asanz@imaff.cfmac.csic.es

\textsuperscript{†}Electronic address: fborondo@uam.es
I. INTRODUCTION

Quantum physics is characterized by striking properties which puzzle and challenge our understanding of the physical world. One of them is contextuality, the unavoidable dependence of the description of a system on the experimental (or contextual) setup, which strongly determines the wave function describing the quantum state of that system [1]. This strongly contrasts with the behavior displayed by classical systems, whose dynamics is only governed by the eventual external forces. The interference of separate diffracted beams of matter particles [2, 3, 4, 5, 6, 7, 8] constitutes a nice scenario where this property becomes very apparent. Consider, for instance, a two-slit diffraction experiment. If no “which-way” information is demanded, the diffracted projectiles will distribute beyond the slits at a time $t$ according to the probability density

$$
\rho_t(r) = |\psi_{1,t}(r) + \psi_{2,t}(r)|^2 = \rho_{1,t}(r) + \rho_{2,t}(r) + \rho_{\text{int},t}(r).
$$

(1)

Here, $\psi_{i,t}(r)$ ($i = 1, 2$) is the wave function describing the particle after only passing through slit $i$ and $\rho_{i,t}(r) = |\psi_{i,t}(r)|^2$ is the probability corresponding to finding that particle at $r$. The particular fringe-like features observed in the interference pattern arise from the interference term $\rho_{\text{int},t}(r)$, which is associated with the contextual or experimental information “both slits are open simultaneously when the particle beam reaches them”. Otherwise, if we choose our context to be one slit open at a time, particles will distribute according to the classical-like probability distribution

$$
\rho_t(r) = |\psi_{1,t}(r)|^2 + |\psi_{2,t}(r)|^2 = \rho_{1,t}(r) + \rho_{2,t}(r),
$$

(2)

which obviously does not contain the interference term. Thus, for the same physical system, two different contexts provide two different answers — note that in classical mechanics we would only have the case described by Eq. (2), since the (conditional) probability (density) to pass through one of the slits when the other is also open is just zero.

In the literature it is common to associate the two contexts described above with either the duality principle (with the two slits open simultaneously, the system behaves as a wave; with only one, as a corpuscle) or the uncertainty principle (determining the particle position is the same as to determine which slit the particle passed through, while letting it pass through both slits open allows us to determine its momentum). However, we can also find
a relationship between the change of context and the problem of decoherence. As is well known, decoherence is nowadays the most widespread mechanism used in the literature to explain the appearance of classical-like behaviors in quantum systems due to their dynamical interaction with an environment. If system plus environment are initially described by a separable total wave function, their coupling makes this wave function to become entangled in time. When we “look” at the reduced system dynamics, this entanglement translates into a partial or even total loss of the system coherence. In the case of the two slits, this process could be seen as a sort of smooth transition from a context where both slits are open simultaneously, to another in which only one slit is open at a time, because of the gradual screening of the information which establishes that both were open when the particle got diffracted. In other words, as the entanglement becomes stronger, the effect is similar to assume that the particle track becomes more localized in time.

The transition from one context to the other due to decoherence can be very well visualized in terms of quantum trajectories, since they offer a clear interpretational advantage by making possible to follow the system dynamics and to (intuitively) understand the underlying physics of the process at the same level that classical trajectories do in classical mechanics. It is well known that the standard version of quantum mechanics (Copenhagen interpretation) can be reformulated in an exact fashion in terms of a trajectory-based theory, namely Bohmian mechanics, which has been widely used, precisely, to describe quantum interference and diffraction among many other different applications. However, and as it also happens in standard quantum mechanics, Bohmian mechanics cannot be directly applied to decoherence problems with a large number of degrees of freedom because any calculation becomes numerically prohibitive. This inconvenience can be avoided, nevertheless, by following the same philosophy as in standard quantum mechanics when Markovian conditions apply. In such cases, the effects of the environment on the system dynamics appear through some dissipative terms (dissipators) in the system equations of motion, as can be seen in different approaches based on solving either master equations for the reduced density matrix or stochastic wave equations. This allows one to devise simple, phenomenological models to understand the way how the coherence damping takes place. Similarly, one can also devise simple quantum trajectory models grounded on Bohmian mechanics, such as the reduced quantum trajectory formalism, where the environment effects appear
in the system equations of motion through some dissipative terms and, therefore, it is not necessary to deal with the dynamics of the whole system-plus-environment set of degrees of freedom. In this regard, we would like to mention that former analyses of decoherence by means of quantum trajectories were carried out by Na and Wyatt [30, 31], where a coherent superposition was coupled to a harmonic bath.

Finally, it is worth pointing out that the questions addressed here, i.e. entanglement and decoherence, have recently received a great deal of attention from the theoretical chemistry community. This arises from the feasibility of using excited vibrational states as a basis for quantum computing [32, 33, 34]. Then problems such as entanglement dynamics [35, 36, 37, 38], or the role of the different characteristics of the corresponding potential energy surfaces [39] have been addressed in molecular states in $\text{H}_2\text{O}$, $\text{SO}_2$, $\text{O}_3$, and formaldehyde.

In this work we explore the properties of reduced quantum trajectory formalisms in connection with the problems of contextuality and decoherence. In particular, we propose a simple trajectory model which includes also a simple mechanism of information screening. Although approximate, the quantum trajectories within this model are able to reproduce satisfactorily the projection of the “true” Bohmian trajectories onto the subspace of the reduced system, since it can be expected that, due to entanglement, such projections violate the non-crossing property of Bohmian mechanics [40]. To make this paper self-contained, prior to the description of our model, we briefly analyze in Sec. II the problem of decoherence in two-slit experiments from the standard quantum-mechanical point of view. Then, in Sec. III we describe the reduced quantum trajectory model based on the screening mechanism mentioned above. Numerical simulations based on this model are presented and discussed in Sec. IV. A final discussion and the main conclusions derived from the present work are summarized in Sec. V.

II. DECOHERENCE IN THE DOUBLE-SLIT EXPERIMENT

Consider a particle beam after getting diffracted by two slits. In the absence of interactions with an environment, its time-evolution can be described at any time by

$$|\Psi_t^{(0)}\rangle = c_1|\psi_{1,t}\rangle + c_2|\psi_{2,t}\rangle,$$  (3)
where \(|c_1|^2 + |c_2|^2 = 1\). In the coordinate representation, the element \((\mathbf{r}, \mathbf{r}')\) of the associate density matrix, \(\hat{\rho}_t^{(0)} = |\Psi_t^{(0)}\rangle \langle \Psi_t^{(0)}|\), will read as
\[
\rho_t^{(0)}(\mathbf{r}, \mathbf{r}') = \Psi_t^{(0)}(\mathbf{r}) \left( \Psi_t^{(0)}(\mathbf{r}') \right)^* ,
\]
and the diagonal terms giving the probability density as
\[
\rho_t^{(0)}(\mathbf{r}) = |c_1|^2 |\psi_{1,t}(\mathbf{r})|^2 + |c_2|^2 |\psi_{2,t}(\mathbf{r})|^2 + 2 |c_1| |c_2| |\psi_{1,t}(\mathbf{r})||\psi_{2,t}(\mathbf{r})| \cos \delta_t(\mathbf{r}),
\]
with \(\Psi_t^{(0)}(\mathbf{r}) = \langle \mathbf{r} | \Psi_t^{(0)} \rangle\). In this last expression, \(\delta_t\) is the space and time dependent phase-shift between the two partial waves.

In order to include the effects of an environment over the system, consider now the following simple model (though general enough to study other interference process than two-slit experiments). Under the presence of such an environment, Eq. (3) is no longer valid to describe the system dynamics. Assuming that system and environment are initially decoupled, the (initial) total wave function accounting for both can be expressed as a factorized product of the initial wave function describing each subsystem,
\[
|\Psi\rangle = |\Psi^{(0)}\rangle \otimes |E_0\rangle,
\]
with \(|\Psi^{(0)}\rangle\), as in Eq. (3). If the environment acts differently on each branch of the diffracted beam \([9, 23, 26, 27]\), at any subsequent time we will find
\[
|\Psi_t\rangle = c_1 |\psi_{1,t}(\mathbf{r})| \otimes |E_{1,t}\rangle + c_2 |\psi_{2,t}(\mathbf{r})| \otimes |E_{2,t}\rangle,
\]
i.e. the total wave function has become entangled. The reduced probability density associated with the system of interest is now obtained from (7) by tracing the full density matrix,
\[
\hat{\rho}_t = |\Psi_t\rangle \langle \Psi_t| ,
\]
over the environment states, which leads to
\[
\tilde{\rho}_t = \sum_{j=1,2} \langle E_{j,t} | \hat{\rho}_t | E_{j,t} \rangle .
\]
Note that, in the coordinate representation and for an environment constituted by \(N\) particles, Eq. (8) becomes
\[
\tilde{\rho}_t(\mathbf{r}, \mathbf{r}') = \int \langle \mathbf{r}, \mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N | \Psi_t \rangle \langle \Psi_t | \mathbf{r}', \mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N \rangle d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N .
\]
Substituting (7) into Eq. (8), rearranging terms and then expressing the final result in the reduced coordinate representation, we reach
\[
\tilde{\rho}_t(\mathbf{r}, \mathbf{r}') = (1 + |\alpha_t|^2) \sum_{j=1,2} |c_j|^2 |\psi_{j,t}(\mathbf{r})\rangle \langle \psi_{j,t}(\mathbf{r}')| + 2 \alpha_t c_1 c_2^* |\psi_{1,t}(\mathbf{r})\rangle \langle \psi_{2,t}(\mathbf{r}')| + c.c.,
\]
where \( \alpha_t = \langle E_{2,t} | E_{1,t} \rangle \) and c.c. indicates the complex conjugate of the second term on the r.h.s. Finally, the (reduced) probability density resulting from Eq. (10) is

\[
\tilde{\rho}_t = (1 + |\alpha_t|^2) \left[ |c_1|^2 |\psi_{1,t}|^2 + |c_2|^2 |\psi_{2,t}|^2 + 2\Lambda_t |c_1| |c_2| |\psi_{1,t}| |\psi_{2,t}| \cos \delta_t \right],
\]

with

\[
\Lambda_t = \frac{2|\alpha_t|}{(1 + |\alpha_t|^2)}
\]

being the coherence degree \([26, 27]\), which gives an idea of the fringe visibility of the interference pattern. For instance, if we consider \(|\alpha_t| = e^{-t/\tau_c}\), we find

\[
\Lambda_t = \text{sech}(t/\tau_c),
\]

where \( \tau_c \) is the coherence time, which is a function of different physical parameters (the system mass, temperature, etc.). In the literature one can find detailed models which allow one to get an estimation of coherence times in different physical situations \([24, 25, 28]\). Nevertheless, as can be seen in Eq. (11), if \( \tau_c \to \infty \), the decoherence process is very slow and the interference pattern is always well defined. On the contrary, for \( \tau_c \) finite we observe an asymptotic decay of the interference pattern to a classical-like one described by

\[
\tilde{\rho}_t = |c_1|^2 |\psi_{1,t}|^2 + |c_2|^2 |\psi_{2,t}|^2.
\]

That is, we observe a smooth transition from the context where both slits were open simultaneously to another one where only one slit is open at a time, not precisely because this was the case, but because the environment makes the information of simultaneity to become screened.

### III. A SIMPLE REDUCED QUANTUM TRAJECTORY MODEL FOR LOSS OF “WHICH-WAY” INFORMATION

In order to visualize and describe the action of the environment over the system in terms of trajectories, it is convenient to express the probability current density \( \mathbf{J}_t \) in terms of the system density matrix,

\[
\mathbf{J}_t = \frac{\hbar}{m} \text{Im}[\nabla_r \rho_t^{(0)}(r, r') \big|_{r'=r}],
\]

where \( \rho_t^{(0)} \) is the initial density matrix.
instead of starting from the standard Bohmian derivation in terms of $\Psi_t^{(0)}$ [40]. Thus, under the presence of the environment, Eq. (15) becomes

$$\tilde{J}_t \equiv \frac{\hbar}{m} \text{Im}[\nabla_r \tilde{\rho}_t(r, r')] \bigg|_{r'=r},$$  (16)

which satisfies the (reduced) continuity equation

$$\frac{\partial \tilde{\rho}_t}{\partial t} + \nabla \tilde{J}_t = 0.$$  (17)

After Eqs. (16) and (17), one can think of the reduced probability current density as a transport effect of the reduced probability density through a (reduced) velocity field, $\tilde{v}$, according to the relation

$$\tilde{J}_t = \tilde{\rho}_t \tilde{v}.$$  (18)

This field is the reduced analog of the Bohmian velocity field and we can obtain reduced quantum trajectories from it by defining [29], in analogy to Bohmian mechanics, the equation of motion

$$\tilde{v} = \dot{r}_t = \frac{\hbar}{m} \text{Im}[\nabla_r \tilde{\rho}_t(r, r')] \bigg|_{r'=r}.,$$  (19)

Due to the continuity equation (17) and definition (18), the dynamics described by Eq. (19) leads to the correct intensity pattern when the statistics of a large particle ensemble is considered [29], as also happens in standard Bohmian mechanics. However, despite the insight on decoherence processes provided by this equation as well as its computational advantages, a close analysis shows us that it still keeps the non-crossing property of Bohmian mechanics. If we consider the limit $t \gg \tau_c$ ($\alpha_t \to 0$), Eq. (19) becomes

$$\dot{r}_t = \frac{|c_1|^2 \rho_{1,t} \dot{r}_{1,t} + |c_2|^2 \rho_{2,t} \dot{r}_{2,t}}{\rho_{cl,t}},$$  (20)

where $\dot{r}_{j,t}$ and $\rho_{j,t}$ are, respectively, the velocity field and probability density associated with the wave $|\psi_{j,t}\rangle$, and

$$\rho_{cl,t} \equiv |c_1|^2 \rho_{1,t} + |c_2|^2 \rho_{2,t}.$$  (21)

Note that, in this limit, both $\rho_{cl,t}$ and the probability current density,

$$\textbf{J}_{cl,t} \equiv \rho_{cl,t} \dot{r}_t = |c_1|^2 \rho_{1,t} \dot{r}_{1,t} + |c_2|^2 \rho_{2,t} \dot{r}_{2,t},$$  (22)

are properly defined. However, Eq. (20) still contains information on both slits, which leads to the non-crossing of the reduced trajectories, while the expected behavior would be just a
crossing as will happen with the projection of the true Bohmian trajectories on the subspace of the reduced system \([41]\). In order to observe a full transition towards a classical-like regime within the theoretical framework of the model here described, it is therefore necessary the gradual screening of such an information.

In order to observe such a behavior, we can further proceed with our model as follows. If, from a trajectory point of view, a particle does not pass through one slit, we will call this the empty slit. Thus, in analogy to \(\alpha_t\), assume that the influence of the empty slit on the particle motion decreases exponentially due to the increasing entanglement with the environment. At the same time, the loss of information about the empty slit strengthens the information about the traversed one. In other words, the weight or influence of the empty slit decreases with time in the corresponding trajectory evolution, while that of the traversed slit increases. Consider that the decay of information goes exponentially. That is, if the particle passes through, say, slit 1, we assume that the coefficient associated with \(|\psi_{2,t}\rangle\) is given by \(c'_2 = c_2 e^{-t/\tau_s}\), where \(\tau_s\) is the screening time, in analogy to the coherence time \(\tau_c\). Here, note that \(\tau_s\) gives a timescale related to how fast the information provided by the empty slit is screened or decoupled from the particle motion due to the environment. On the other hand, for the coefficient of \(|\psi_{1,t}\rangle\) we choose

\[
c'_1 = c_1 \sqrt{1 - |c_2|^2 e^{-2t/\tau_s}} / |c_1|^2,
\]

indicating the increasing role of the traversed slit in the quantum motion. Now, the evolution of the system is then described by Eq. (19), but replacing the \(c_i\) by their respective time-dependent counterparts, \(c'_i\).

Since there are two characteristic times, \(\tau_s\) and \(\tau_c\), we can define the ratio \(\eta \equiv \tau_s/\tau_c\). Thus, if \(\eta \ll 1\), the screening of the empty-slit information takes place much faster than the process that leads to the quenching or damping of the interference fringes. In this case, if the screened slit is, say, 2, Eq. (19) reduces to

\[
\dot{\mathbf{r}}_t = \dot{\mathbf{r}}_{1,t}
\]

and the trajectories will evolve like if there was no other slit at all, i.e. like in a context where there is only one slit open at a time. This means that particles are allowed to cross the symmetry axis of the experiment because, at a given time, the momentum can have two different values on the same space point, as in classical mechanics. In next section we illustrate this processes by means of some numerical simulations.
FIG. 1: a) Intensity obtained from the statistics of reduced quantum trajectories (full circles) and standard quantum mechanics (solid line) with $\tau_c = 2.26 \times 10^{-2}$ s. b) Sample of reduced quantum trajectories illustrating the dynamics associated with the results shown in part (a).

IV. NUMERICAL SIMULATIONS

The parameters (dimensions of the two-slit assembly, particle masses and wavelengths) utilized in the simulations that we will present here refer to the two-slit experiment with cold neutrons carried out by Zeilinger et al. [3], which we will utilize as a working model. Thus, in Fig. I(a), we show the excellent agreement between the statistics over reduced quantum trajectories (full circles) and the corresponding standard quantum mechanical calculations (solid line), in accordance to the continuity equation (17) and definition (18) for the reduced field. A sample of reduced trajectories illustrating the dynamics associated with the results of Fig. I(a) is displayed in part (b) of the same figure. Here, we see that as the outgoing neutron beams start to interfere (at a distance of $\sim 1$ m from the two slits), some trajectories (mainly those closer to the symmetry axis of the experiment) start to show a conspicuous change of direction, which is typical in the Bohmian description of interference processes [15, 17, 18]. However, due to the interference quenching, the extent of this behavior is reduced in both space and time: in space because the interference effects are stronger for the innermost trajectories [which give rise to the central peaks in Fig. I(a)] and in time because the time-of-flight of the neutrons ($\tau_f = 2.33 \times 10^{-2}$ s) is slightly larger than $\tau_c$.

In Fig. II we show the results for the extreme case of maximal decoherence, that takes place for $\tau_c = 0$. Similarly to what we did in Fig. I, the statistical results obtained by
FIG. 2: a) Intensity obtained from reduced quantum trajectory (full circles) and standard quantum mechanics (solid line) calculations for a double-slit experiment with cold neutrons and $\tau_c = 0$ (no coherence). b) Sample of reduced quantum trajectories illustrating the dynamics associated with the results shown in part (a).

means of quantum trajectories and standard quantum mechanics (a), as well as a sample of representative trajectories (b) are plotted. Notice that despite there is no coherence (in the sense that the interference terms of the reduced density matrix have been damped out), trajectories do not cross the symmetry axis between the two slits because they obey Eq. (20), which contains information about the two slits open simultaneously. The absence of interference only prevents the particles from undergoing the typical “wiggling” motion leading to the different diffraction peaks [18].

In order to illustrate how the additional mechanism leading to the screening of the information provided by the empty slit works, we show in Fig. 3 results for several values of the parameter $\eta$ once the $c_i$ coefficients have been replaced by the $c'_1$ ones in Eq. (19). The statistics of reduced-screened quantum trajectories are given in the top row and samples of quantum trajectories illustrating the corresponding dynamics are displayed in the bottom one. As can be noticed in Fig. 3(a), for small values of $\eta$ the screening is very slow screening and the non-crossing dominates the system dynamics. However, as we move to higher values of $\eta$ (from left to right in the figure), the screening starts to increase in importance over the interference quenching and trajectories start to cross the axis between the two slits. In the extreme case, where the screening is very strong, the trajectories display a classical-like behavior because the information about the two slits open simultaneously initially is lost
FIG. 3: Top: Intensity obtained after counting of the corresponding pseudo-reduced quantum trajectories for: a) $\eta = \infty$, b) $\eta = 10$, c) $\eta = 1$, and d) $\eta = 0.1$. The results from the counting (full circles) have been joined by means of B-splines (solid line) in order to facilitate their understanding. Bottom: Samples of trajectories illustrating the dynamics of the results shown in the upper part.

The transition from one regime to the other one is also interesting both from the dynamical and the statistical points of view. As $\eta$ increases an order of magnitude, a set of trajectories densely concentrates along the symmetry axis, a region where before there was a strong quantum force preventing the approach of trajectories. Thus, the central intensity maximum is remarkably enhanced, as can be seen in Fig. 3(b), when compared with the same peak in Fig. 3(a). This enhancement occurs at the expense of the intensity of the other maxima. That is, there is a transfer of trajectories from the outermost to the innermost diffraction channels. Dynamically, once the strong boundary imposed by the quantum potential along the symmetry axis (which is stronger than along the directions separating the different diffraction channels [18]) is suppressed, the “quantum pressure” [18, 19] pushes the trajectories towards the region covered by the empty slit, and favors their transfer from one diffraction channel to the nearby one.

As $\eta$ is further increased, quantum trajectories are also able to penetrate more across the symmetry axis, as it is apparent in Fig. 3(c). The availability of a wider accessible region
in the other side of the symmetry axis makes the concentration of trajectories along this direction to decrease, and they distribute more homogeneously. This causes a remarkable decrease of the coherence degree in the measured intensity, although the central peaks are still relatively intense. This trend continues until the interference pattern completely disappears when the decoupling is maximum [see Fig. 3(d)]. In this case, the trajectories are unaffected by the presence of the other slit, i.e. they display a totally classical-like behavior. Moreover, a full transition from a dynamics characterized by single-valuedness of the momentum to another where it is bi-valued is observed, taking place this process within the system subspace.

V. FINAL DISCUSSION AND CONCLUSIONS

Trajectory-based approaches have received much attention in the last years as a potential tool to handle and study high-dimensional complex quantum systems \[42\]. Nowadays the design of new numerical tools highly relies on this kind of formalisms rather than using other approaches based on the time-dependent Schrödinger equation \[20\]. In the particular case of Bohmian mechanics, this computational power combines with its capability to provide causal interpretations to quantum phenomena within a purely quantum-mechanical framework, unlike other semiclassical or classical approaches. These two interesting features have brought Bohmian mechanics from the field of the Foundations of Physics to the most applied fields in physics and chemical physics, attracting the interest of many different communities within. Similarly, the model proposed here to study decoherence and the process of going from one context to another one in quantum mechanics provides an understandable and intuitive insight into dynamics involved. In particular, regarding the mechanism that leads a linear theory with single-valued momenta to an “apparent” non-linear one, where the momentum can be multi-valued.

Here we have dealt with the problem of the damping or quenching of the interference fringes produced by decoherence in a two-slit experiment under the presence of an environment, which yields as a result a classical-like pattern. This effect is, to some extent, similar to consider the transition from a context where both slits are open simultaneously to another one where only one slit is open at a time and, therefore, the particle track is localized (i.e. the particle has passed through one slit or the other). In order to elucidate and understand
decoherence without taking into account explicitly the dynamics of the environment degrees of freedom, we have considered some simple reduced quantum-trajectory models. Though limited because of their simplicity, one can infer from them that, unless there is a sort of screening of the empty-slit information, the patterns affected by decoherence can be well reproduced, but keeping still a sort of internal coherence which makes the trajectories to avoid their crossing, as in standard Bohmian mechanics. Only when the empty-slit information is gradually screened, the trajectories start to cross, as one would expect when using Bohmian mechanics and projecting the true $3(N+1)$-dimensional quantum trajectories onto the subspace of the reduced system. Thus, though simple and approximate —more refined and precise models, which are out of the scope of this work, but that are being currently developed in order to go beyond the analysis presented here—, this model allows us to study the properties of decoherence at a relatively cheap computational cost and providing, at the same time, a physical insight on the way how the contextual dependence and nonlocal correlations are gradually suppressed.

### Acknowledgements

This work has been supported by the Ministerio de Ciencia e Innovación (Spain) under Projects MTM2006-15533, CONSOLIDER 2006-32, and FIS2007-62006; Comunidad de Madrid under Project S-0505/ESP-0158; and Agencia Española de Cooperación Internacional under Project A/6072/06. A.S. Sanz also acknowledges the Consejo Superior de Investigaciones Científicas for a JAE-Doc Contract.

[1] A. Clemente de la Torre, Am. J. Phys. 62 (1994) 808.
[2] C.J. Davison, L.H. Germer, Phys. Rev. 30 (1927) 705.
[3] A. Zeilinger, R. Gähler, C.G. Shull, W. Treimer, W. Mampe, Rev. Mod. Phys. 60 (1988) 1067.
[4] A. Tonomura, J. Endo, T. Matsuda, T. Kawasaki, H. Ezawa, Am. J. Phys. 57 (1989) 117.
[5] F. Shimizu, K. Shimizu, H. Takuma, Phys. Rev. A 46 (1992) R17.
[6] B. Brezger, L. Hackermüller, S. Uttenthaler, J. Petschinka, M. Arndt, A. Zeilinger, Phys. Rev. Lett. 88 (2002) 100404.
[7] J.O. Cáceres, M. Morato, A. González Ureña, J. Phys. Chem. A Lett. 110 (2006) 13643.
[8] A. González Ureña, A. Requena, A. Bastida, J. Zúñiga, Eur. Phys. J. D 49 (2008) 297.
[9] D. Giulini, E. Joos, C. Kiefer, J. Kupsch, I.-O. Stamatescu, H.D. Zeh (Eds.), Decoherence and the Appearance of a Classical World in Quantum Theory, Springer, Berlin, 1996.
[10] E. Schrödinger, Proc. Cam. Phil. Soc. 31 (1935) 555.
[11] E. Schrödinger, Proc. Cam. Phil. Soc. 32 (1936) 446.
[12] D. Bohm, Phys. Rev. 85 (1952) 166.
[13] D. Bohm, Phys. Rev. 85 (1952) 180.
[14] P.R. Holland, The Quantum Theory of Motion, Cambridge University Press, Cambridge, 1993.
[15] C. Philippidis, C. Dewdney, B.J. Hiley, Nuovo Cimento B 52 (1979) 15.
[16] C. Philippidis, D. Bohm, R.D. Kaye, Nuovo Cimento B 71 (1982) 75.
[17] A.S. Sanz, F. Borondo, S. Miret-Artés, Phys. Rev. B 61 (2000) 7743.
[18] A.S. Sanz, F. Borondo, S. Miret-Artés, J. Phys.: Condens. Matter 14 (2002) 6109.
[19] R. Guantes, A.S. Sanz, J. Margalef-Roig, Miret-Artés, Surf. Sci. Rep. 53 (2004) 199.
[20] R.E. Wyatt, Quantum Dynamics with Trajectories: Introduction to Quantum Hydrodynamics, Springer, Berlin, 2005.
[21] H.-P. Breuer, F. Petruccione, The Theory of Open Quantum Systems, Oxford University Press, Oxford, 2002.
[22] I. Percival, Quantum State Diffusion, Cambridge University Press, Cambridge, 1998.
[23] S.M. Tan, D.F. Walls, Phys. Rev. A 47 (1993) 4663.
[24] C.M. Savage, D.F. Walls, Phys. Rev. A 32 (1985) 2316.
[25] C.M. Savage, D.F. Walls, Phys. Rev. A 32 (1985) 3487.
[26] A.S. Sanz, F. Borondo, M. Bastiaans, Phys. Rev. A. 71 (2005) 42103.
[27] A.S. Sanz, F. Borondo, Phys. Rev. A 77 (2008) 057601.
[28] T. Qureshi, A. Venugopalan, Int. J. Mod. Phys. B 22 (2008) 981.
[29] A.S. Sanz, F. Borondo, Eur. Phys. J. D 44 (2007) 319.
[30] K. Na, R.E. Wyatt, Phys. Lett. A 306 (2002) 97.
[31] K. Na, R.E. Wyatt, Phys. Scr. 67 (2003) 169.
[32] C.M. Tesch, R. de Vivie-Riedle, Phys. Rev. Lett. 89 (2002) 157901.
[33] D. Babikov, J. Chem. Phys. 121 (2004) 7577.
[34] T. Cheng, A. Brown, J. Chem. Phys. 124 (2006) 34111.
[35] X.W. Hou, J.H. Chen, Z.Q. Ma, Phys. Rev. A 74 (2006) 62513.
[36] X.W. Hou, J.H. Chen, M.F. Wan, Z.Q. Ma, Eur. Phys. J. D 49 (2008) 37.
[37] X.W. Hou, M.F. Wan, Z.Q. Ma, Opt. Commun. 281 (2008) 3587.
[38] X.W. Hou, M.F. Wan, Z.Q. Ma, Entanglement dynamics of Coriolis coupling vibrations to rotations in a polyatomic molecule: A case study of formaldehyde (preprint).
[39] C. Gollup, U. Troppmann, R. de Vivie-Riedle, New J. Phys. 8 (2008) 48.
[40] A.S. Sanz, S. Miret-Artés, J. Phys. A 41 (2008) 435303.
[41] E. Guay, L. Marchildon, J. Phys. A 36 (2003) 5617.
[42] D. Micha, I. Burghardt (Eds.), Quantum Dynamics of Complex Molecular Systems, Springer, Berlin, 2006.