

Emergent Quantum Mechanics 2013



Particles, Waves, and Trajectories: 210 Years After Young's Experiment

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Vienna, October 6, 2013

A year of celebrations!!

210 years of Young's celebrated two-slit experiment (1803)



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But, what do we know about quantum systems so far?

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But, what do we know about quantum systems so far?



Don't look! Don't ask! Don't tell!

 \Rightarrow Only measures of "observables"

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We have experiments resolved in real time

⇒ Phenomena directly related to the quantum phase

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... but the quantum phase is NOT an observable!!

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... but the quantum phase is NOT an observable!!

Let's try to find a practical tool to deal with the phase!!

WARNING!!

I won't talk, I won't tell anything about the Mathematics and numerics involved in the simulations that will be shown ... but you are free to ask!!



Outlook of this talk

What do I mean by Bohmian mechanics?

Bohmian mechanics and quantum hydrodynamics

Applications of Bohmian mechanics

Dissipative Bohmian dynamics

"Light" trajectories

Some matter-wave (related) outcomes

Concluding remarks





Juffmann et al., Nat. Nano. 7, 297 (2012)

Particle distributions behave as waves ...

(Born's statistical interpretation of quantum mechanics)





Juffmann *et al.*, Nat. Nano. **7**, 297 (2012)

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QUANTUM PROBABILITY DENSITY \checkmark





Juffmann *et al.*, Nat. Nano. **7**, 297 (2012)

Particle distributions behave as waves ...

(Born's statistical interpretation of quantum mechanics)

QUANTUM PROBABILITY DENSITY \checkmark

... but individual particles behave as individual point-like particles!





Juffmann et al., Nat. Nano. 7, 297 (2012)

Particle distributions behave as waves ...

(Born's statistical interpretation of quantum mechanics)

QUANTUM PROBABILITY DENSITY \checkmark

QUANTUM PROBABILITY CURRENT DENSITY ?

What's Bohmian mechanics?

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\Psi$$



What's Bohmian mechanics?



What's Bohmian mechanics?

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \Psi \qquad \longrightarrow \qquad \begin{cases} \frac{\partial R^2}{\partial t} + \nabla \cdot \left(R^2 \frac{\nabla S}{m} \right) = 0 \\ \frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + V - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} = 0 \end{cases}$$





$$\begin{cases} i\hbar \frac{\partial \Psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \Psi \\ v = \dot{r} = \frac{\nabla S}{m} \end{cases}$$

Bohmian mechanics ...



PHYSICAL REVIEW

VOLUME 85, NUMBER 2

JANUARY 15, 1952

A Suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables. I

DAVID BOHM* Palmer Physical Laboratory, Princeton University, Princeton, New Jersey (Received July 5, 1951)

The usual interpretation of the quantum theory is self-consistent, but it involves an assumption that cannot be tested experimentally, viz., that the most complete possible specification of an individual system is in terms of a wave function that determines only probable results of actual measurement processes. The only way of investigating the truth of this assumption is by trying to find some other interpretation of the quantum theory in terms of at present "hidden" variables, which in principle determine the precise behavior of an individual system, but which are in practice averaged over in measurements of the types that can now be carried out. In this paper and in a subsequent paper, an interpretation of the quantum theory in terms of just such "hidden" variables is suggested. It is shown that as long as the mathematical theory retains its present general form, this suggested interpretation leads to precisely the same results for all

physical processes as does the usual interpretation. Nevertheless, the suggested interpretation provides a broader conceptual framework than the usual interpretation, because it makes possible a precise and continuous description of all processes, even at the quantum level. This broader conceptual framework allows more general mathematical formulations of the theory than those allowed by the usual interpretation. Now, the usual mathematical formulation seems to lead to insoluble difficulties when it is extrapolated into the domain of distances of the order of 10^{-13} cm or less. It is therefore entirely possible that the interpretation suggested here may be needed for the resolution of these difficulties. In any case, the mere possibility of such an interpretation proves that it is not necessary for us to give up a precise, rational, and objective description of individual systems at a quantum level of accuracy.

... the pilot wave ...

SÉANCE DU 23 AOUT 1926.

447

PHYSIQUE MATHÉMATIQUE. – Sur la possibilité de relier les phénomènes d'interférence et de diffraction à la théorie des quanta de lumière. Note de M. Louis de Broglie, transmise par M. M. de Broglie.

La propagation des ondes lumineuses est régie par l'équation

(1)
$$\Delta u = \frac{1}{c^2} \cdot \frac{\partial^2 u}{\partial t^2} \cdot$$

Pour chaque problème d'interférence ou de diffraction, l'optique classique cherche une solution de la forme

(2)
$$u = a(x, y, z) e^{i\omega[t-\varphi(x, y, z)]}$$

satisfaisant aux conditions aux limites imposées par la présence des écrans ou autres obstacles rencontrés par l'onde. La nouvelle optique des quanta de lumière envisage une solution à amplitude variable de la forme

(3) $u = f(x, y, z, t) e^{i\omega [t - \varphi(x, y, z)]},$

où φ est la même fonction que dans (2). La fonction f comporte des singularités mobiles le long des courbes normales aux surfaces $\varphi = \text{const.}$; ces singularités constituent les quanta d'énergie radiante. La vitesse du quantum passant au point M à l'instant t est nécessairement

(4)
$$\mathbf{U} = \left(-\frac{\frac{\partial f}{\partial t}}{\frac{\partial f}{\partial n}}\right)_{\mathbf{M},t}$$

la variable n étant comptée le long de la trajectoire et les dérivées étant prises en M à l'instant t.



... and quantum hydrodynamics



Quantentheorie in hydrodynamischer Form.

Von E. Madelung in Frankfurt a. M.

(Eingegangen am 25. Oktober 1926.)

Es wird gezeigt, daß man die Schrödingersche Gleichung des Einelektronenproblems in die Form der hydrodynamischen Gleichungen transformieren kann.

Physical system

$$\begin{cases} i\hbar \frac{\partial \Psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \Psi \\ v = \dot{r} = \frac{\nabla S}{m} \end{cases}$$

Quantum hydrodynamics

$$\rho = R^{2} = \Psi^{*}\Psi$$
$$J = \rho v = R^{2} \frac{\nabla S}{m}$$
$$\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0$$

Hydrodynamics: streamlines and tracer particles

Continuum media: hydrodynamics

gas - smoke

liquid { tinny floating particles (e.g., pollen, charcoal) other liquids (e.g., ink)

Universe as a fluid – galaxies, stars, etc.







Quantum Dynamics of the Collinear (H, H₂) Reaction*

EDWARD A. McCULLOUGH, JR., † AND ROBERT E. WYATT Department of Chemistry, The University of Texas at Austin, Austin, Texas 78712 (Received 21 March 1969)

J. Chem. Phys. 51, 1253 (1969)



FIG. 1. Saddle point region, time step 85, showing the saddle point (SP), reaction path (---), and symmetric stretch line (---). Region is 1.28 a.u. square. (a) Probably density. (b) Flux. Length of largest vector is $1.70 \times 10^{44} \text{ a.u}^{-1} \text{ sec}^{-1}$. The four vectors closest to the "sink" are magnified by 2.5.

(h)





THE JOURNAL OF CHEMICAL PHYSICS

VOLUME 54, NUMBER 8

15 APRIL 1971

Dynamics of the Collinear $H + H_2$ Reaction. I. Probability Density and Flux*

EDWARD A. MCCULLOUGH, JR.† AND ROBERT E. WYATT Department of Chemistry, The University of Texas at Austin, Austin, Texas 78712 (Received 13 November 1970)

The time evolution of the collinear $H+H_2$ reaction as given by classical mechanics and by time-dependent quantum mechanics has been studied. The calculations employed the Porter-Karplus potential surface. The relevant equations of motion were solved to high accuracy by direct numerical integration. The evolution of the quantal probability density in the interaction region of the potential surface is shown in a series of perspective plots. Classical mechanics gives an amazingly good description of the probability density and flux patterns during most of the reaction; however, the classical and quantal descriptions begin to diverge near the end of the reaction. Essentially, the classical reaction terminates before the quantal reaction. The dynamic behavior of the reaction is hydrodynamically turbulent, as shown by transient whirlpool formation on the inside of the reaction path. All results reported in this paper are for one average system energy, namely, 0.65 eV (initial average translational energy=0.38 eV).



Quantum mechanical streamlines. I. Square potential barrier*

Joseph O. Hirschfelder and Albert C. Christoph

Theoretical Chemistry Institute, University of Wiconsin-Madison, Madison, Wisconsin 53706

William E. Palke

Department of Chemistry, University of California-Santa Barbara, Santa Barbara, California 93106 (Received 24 July 1974)



J. Chem. Phys. 61, 5435 (1974)

This paper has resulted from an effort to get a better understanding of quantum mechanics by making a thorough study of a very simple problem, the reflection and transmission of a beam of particles hitting a two-dimensional square potential barrier. The mathematics is simple, but the analysis is far-reaching.





X ---

(d)

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, Vol. XXV, 929-940 (1984)

Singularities of Magnetic-Field Induced Electron Current Density: A Study of the Ethylene Molecule

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A representation of the electron flow induced by the external field can be extremely useful to understand molecular magnetism. To this end, maps reporting modulus and trajectory of quantum-mechanical current density revealed a fundamental tool [1–3], whose importance could be hardly overestimated.





Figure 1. (a) Trajectory of the current density in the σ_h plane perpendicular to the magnetic field. Diamagnetic circulations are clockwise. (b) Modulus of the current density in the same plane as (a). Curves are marked according to the correspondence: 1 = 0.1, 2 = 0.03, 3 = 0.01, 4 = 0.003, 5 = 0.0015, 6 = 0.001, 7 = 0.0008, 8 = 0.0005, 9 = 0.0005, 11 = 0.0001 (in a.u.).

Stagnation Graphs and Topological Models of Magnetic-Field Induced Electron Current Density for Some Small Molecules in Connection With Their Magnetic Symmetry

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Dipartimento di Chimica, Università degli Studi di Modena e Reggio Emilia, Via Campi 183, 41100 Modena, Italy

Received 14 December 2009; accepted 9 February 2010 Published online 2 June 2010 in Wiley Online Library (wileyonlinelibrary.com). DOI 10.1002/qua.22658

ABSTRACT: Spatial models of magnetic-field induced electronic currents have been constructed for a series of small molecules of different point group symmetry via stagnation graphs and current density maps. These tools provide fundamental help for rationalization of magnetic response properties, such as magnetizability and nuclear magnetic shielding. © 2010 Wiley Periodicals, Inc. Int J Quantum Chem 111: 356–367, 2011

Int. J. Quantum Chem. 111, 356 (2011)



FIGURE 4. Perspective view of the current density vector field in H₃BO₃, with magnetic symmetry C_{3h} . The uniform external magnetic field **B** is perpendicular to the plane of the atoms. The figure shows diatropic streamlines spiralling about $(3, \pm 1)$ foci at the boron and oxygen nuclei, above and below the σ_h symmetry plane, which cannot crossed by the flow. Diatropic limit cycles, separating upper and lower spirals, lie on σ_h . Two pairs of arrows indicate the direction of the local eigenvectors corresponding to the real eigenvalue of the Jacobian matrix at the boron nucleus. [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]



Math. Ann. 47, 317 (1896)



Fig. 11.12 Amplitude contours of H_z (amplitude of incident wave is taken as unity) for diffraction of a normally incident *H*-polarized plane wave by a perfectly conducting half-plane. (After W. Braunbek and G. Laukien, *Optik*, **9** (1952), 174.)



Fig. 11.13 Phase contours of H_z for diffraction of a normally incident *H*-polarized plane wave by a perfectly conducting half-plane. (After W. Braunbek and G. Laukien, *Optik*, **9** (1952), 174.)



Optik **9**, 174 (1952)



Fig. 11.14 Lines of average energy flow for diffraction of a normally incident *H*-polarized plane wave by a perfectly conducting half-plane. (After W. Braunbek and G. Laukien, *Optik*, **9** (1952), 174.)

International Journal of Theoretical Physics, Vol. 15, No. 3 (1976), pp. 169-180

The Interpretation of Diffraction and Interference in Terms of Energy Flow

R. D. PROSSER

Physics Department, University of Stirling, Stirling, Scotland

Received: 20 December 1974

Abstract

Solutions to Maxwell's equations at a semi-infinite plane and a double slit are used to construct lines of constant amplitude, constant phase and energy flow. The lines of energy flow show how the electromagnetic boundary conditions necessitate a particular undulation in the path of the light energy and that the consequent redistribution of energy corresponds with a diffraction or interference pattern. This interpretation complements the interpretation in terms of the interaction of secondary wavelets due to Huygens.







Figure 3c.

Energy streamlines of a sound source

R. V. Waterhouse,^{a)} T. W. Yates,^{b)} D. Feit, and Y. N. Liu David W. Taylor Naval Ship Research & Development Center, Bethesda, Maryland 20084-5000

(Received 17 February 1985; accepted for publication 8 April 1985)

A method is presented for computing the energy streamlines of a sound source. This enables charts to be plotted showing, as continuous lines, the flow paths of the sound energy from the vibrating surface to the nearfield and beyond. Energy streamlines appear to be a new construct; they have some similarities to the velocity streamlines used in fluid dynamics. Examples of the energy streamlines are given for the point-driven plate in water.

J. Acoust. Soc. Am. 78, 758 (1985)

Intensity meters have been commercially available for the last year or two, and several papers^{1,2} have appeared giving measured intensity data for various sound sources. Generally, the data have been presented in a plot similar to those shown in Figs. 1 and 2, where the arrows show the directions of the intensity vectors at a number of points uniformly spaced on a rectangular grid. The vectors may be adjusted to have the same length, to focus attention on the directions of the energy flow, or they may have lengths proportional to the magnitudes of the intensities at the various points. Similar plots have been used to present the theoretical results of intensity calculations.^{3,4}

The purpose of this paper is to present a development of the above scheme, which enables continuous streamlines of intensity (i.e., energy flow) to be calculated and plotted. These streamlines make it easier for the eye to follow the energy flow from the source into the nearfield and beyond. These paths are complicated, in some cases, but are of considerable interest from several points of view.

To demonstrate the method, examples are given of the energy streamlines for a point-driven plate in water.



FIG. 1. Intensity vectors in the rz plane for a point-driven plate in water. The axis z is normal to the plate. The lengths of the vectors are not to scale, but have been made all the same. The point drive is at 0 and λ is the wavelength of bending waves on the plate *in vacuo*.



FIG. 3. Energy streamlines in the nearfield of a point-driven plate in water, derived from the data shown in Figs. 1 and 2. Here, 32 grid points per λ were used.

Hydrodynamics: streamlines and tracer particles

Do real quantum particles move along Bohmian trajectories?

A Bohmian particle is a particle that obeys a Bohmian dynamics, i.e., according to a (local) average drift momentum, which provides the particle with nonlocal (global) hydrodynamic-like information

Such a particle allows us to infer dynamical properties of the quantum fluid, which are usually "hidden" when studied by means of the wave function formulation

Bohmian particles are the quantum equivalent of classical tracer particles

Schrödinger's wave mechanics

Heisenberg's (matrix) quantum mechanics

Dirac's (interaction) representation

Feynman's path integral representation

Wigner-Moyal (phase space) representation

Madelung-Bohm (quantum fluid dynamics) representation (Bohmian mechanics)

What's going on in the quantum world?









Quantum phase effects and quantum dynamics

Interference and non-crossing



Chem. Phys. Lett. 445, 350 (2007); J. Phys. A 41, 435303 (2008); Am. J. Phys. 80, 525 (2012)

Quantum phase effects and quantum dynamics

J. Phys. A 41, 435303 (2008)

Bohmian statistics and standard quantum mechanics



Pérez-Ríos & AS (in preparation)

$$m\ddot{x} + m\gamma\dot{x} + \partial_x V(x) = 0$$

classical context

 $P \equiv m e^{\gamma t} \dot{x} = p e^{\gamma t}$

X = x

$$\mathcal{H} = \dot{X}P - \mathcal{L} = \frac{P^2}{2m} e^{-\gamma t} + V(X)e^{\gamma t}$$
$$\dot{X} = \partial_P \mathcal{H}$$
$$\dot{P} = -\partial_X \mathcal{H}$$

quantum context

 $\hat{P} = -i\hbar\partial/\partial X$

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m} \ e^{-\gamma t} \ \partial_X^2 + V(X) e^{\gamma t}$$

$$\begin{split} [\hat{X}, \hat{P}] &= i\hbar \\ [\hat{x}, \hat{p}] &= i\hbar e^{-\gamma t} \qquad i\hbar \end{split}$$

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m} \ e^{-\gamma t}\partial_x^2\Psi + V(x)e^{\gamma t}\Psi$$

$$\dot{x} = \frac{\mathcal{J}}{\rho} = \frac{\partial_x S}{m} \ e^{-\gamma t}$$

arXiv:1306.6607

uniform motion



accelerated motion



arXiv:1306.6607

oscillatory motion



oscillatory motion



On the Schrödinger-Langevin Equation*

M. D. Kostin

Department of Chemical Engineering, Princeton University, Princeton, New Jersey 08540 (Received 16 June 1972)

It is shown that the Heisenberg-Langevin equation can be used to derive a Schrödinger equation for a Brownian particle interacting with a thermal environment. The equation derived is

 $i\hbar(\partial\psi/\partial t) = -(\hbar^2/2m)\nabla^2\psi + V\psi + V_R\psi + [(\hbar f/2im)\ln(\psi/\psi^*) + W(t)]\psi(\mathbf{r}, t),$

 $W(t) = -(\hbar f/2im) \int \psi^* \ln(\psi/\psi^*) \psi d\mathbf{r},$

where f is the friction constant and V_R is a random potential.

Kostin, J. Chem. Phys. 57, 3589 (1972)

oscillatory motion



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where f is the friction constant and V_R is a random potential.

Kostin, J. Chem. Phys. 57, 3589 (1972)



Garashchuk, Dixit, Gu & Mazzuca, J. Chem. Phys.. 138, 054107 (2013)

arXiv:1306.6607

oscillatory motion



Quantum mechanics in terms of discrete beables

Jeroen C. Vink

Department of Physics 0319, University of California at San Diego, La Jolla, California 92093 (Received 15 April 1993)

An interpretation of quantum mechanics in terms of classical concepts, "beables," due to de Broglie, Bohm, and Bell (BBB) is generalized and further developed. By assuming that all physical quantities take discrete values on sufficiently small scales, we can use this interpretation to give trajectories for all possible quantities, including the position of a particle, its spin, etc. When applied to position, it is shown that, in the continuum limit, this interpretation reduces to the causal one of Bohm. As an illustration, the BBB trajectories are computed explicitly in two simple models.

Phys. Rev. A 48, 1808 (1993)

arXiv:1306.6607

oscillatory motion



Quantum mechanics in terms of discrete beables

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Phys. Rev. A 48, 1808 (1993)



interference in free space



vibrational interference



interference in free space



arXiv:1306.6607

Lorenzen, da Ponte & Moussa, Phys. Rev. A 80, 032101 (2009)







Ann. Phys. **325**, 763 (2010); J. Russ. Laser Res. **31**, 117 (2010)

Observing the Average Trajectories of Single Photons in a Two-Slit Interferometer

Sacha Kocsis,^{1,2}* Boris Braverman,¹* Sylvain Ravets,³* Martin J. Stevens,⁴ Richard P. Mirin,⁴ L. Krister Shalm,^{1,5} Aephraim M. Steinberg¹†

A consequence of the quantum mechanical uncertainty principle is that one may not discuss the path or "trajectory" that a quantum particle takes, because any measurement of position irrevocably disturbs the momentum, and vice versa. Using weak measurements, however, it is possible to operationally define a set of trajectories for an ensemble of quantum particles. We sent single photons emitted by a quantum dot through a double-slit interferometer and reconstructed these trajectories by performing a weak measurement of the photon momentum, postselected according to the result of a strong measurement of photon position in a series of planes. The results provide an observationally grounded description of the propagation of subensembles of quantum particles in a two-slit interferometer.

3 JUNE 2011 VOL 332 SCIENCE www.sciencemag.org







Phys. Scr. **T153**, 014015 (2013); Europhys. News **44**(6), 36 (2013)



J. Phys.: Condens. Matter 14, 6109 (2002), J. Chem. Phys. 126, 234106 (2007)

PHYSICAL REVIEW A 79, 053823 (2009)

Poisson's spot with molecules

Thomas Reisinger,^{1,*} Amil A. Patel,² Herbert Reingruber,³ Katrin Fladischer,³ Wolfgang E. Ernst,³ Gianangelo Bracco,⁴ Henry I. Smith,² and Bodil Holst¹

¹Department of Physics and Technology, University of Bergen, Allégaten 55, 5007 Bergen, Norway ²NanoStructures Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA ³Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria ⁴Department of Physics and CNR-IMEM, University of Genova, V. Dodecaneso 33, 16146 Genova, Italy (Received 6 December 2008; published 14 May 2009)

In the Poisson-spot experiment, waves emanating from a source are blocked by a circular obstacle. Due to their positive on-axis interference an image of the source (the Poisson spot) is observed within the geometrical shadow of the obstacle. In this paper we report the observation of Poisson's spot using a beam of neutral deuterium molecules. The wavelength independence and the weak constraints on angular alignment and position of the circular obstacle make Poisson's spot a promising candidate for applications ranging from the study of large molecule diffraction to patterning with molecules.







PHYSICAL REVIEW A 79, 053823 (2009)

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¹Department of Physics and Technology, University of Bergen, Allégaten 55, 5007 Bergen, Norway ²NanoStructures Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA ³Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria ⁴Department of Physics and CNR-IMEM, University of Genova, V. Dodecaneso 33, 16146 Genova, Italy (Received 6 December 2008; published 14 May 2009)

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0.05





Wheeler, The past and the delayed-choice double-slit experiment, in *Mathematical Foundations of Quantum Theory*, Marlow (Ed.) (Academic Press, New York, 1978)

Hiley & Callaghan, Phys. Scr. 74, 336 (2006)

Cassinello & Sánchez-Gómez, La Realidad Cuántica (Crítica, Barcelona, 2013)



















Choque & AS (in preparation)

























Choque & AS (in preparation)













Rather than an alternative interpretation TO, Bohmian mechanics seems to constitute al anternative representation OF quantum mechanics

This representation stresses the role of the quantum phase, which can be monitored by means of weak measures

Bohmian trajectories help us to understand and analyze the flow of quantum phase in quantum systems

The same "philosophy" can be (has been) transferred to other fields of physics with similar purposes

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Interesting (practical) analytical and computational working tool in many degree-of-freedom (= many-body) problems

Suitable candidate to "explore" how quantum dynamics emerges from a non-equilibrium particle dynamics

In the end of the day ... we need a working model

Quantum phase analysis with quantum trajectories: A step towards the creation of a Bohmian thinking

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(Received 21 October 2011; accepted 13 March 2012)

We introduce a pedagogical discussion on Bohmian mechanics and its physical implications in connection with the important role played by the quantum phase in the dynamics of quantum processes. In particular, we focus on phenomena such as quantum coherence, diffraction, and interference, due to their historical relevance in the development of the quantum theory and their key role in a myriad of fundamental and applied problems of current interest. © 2012 American Association of Physics Teachers.

[http://dx.doi.org/10.1119/1.3698324]



Acknowledgements

Laura Choque (PhD student) (Instituto de Física Fundamental)

Jesús Pérez Ríos (Purdue University)

Salvador Miret (Instituto de Física Fundamental), Ruth Martínez-Casado (Imperial College)

Mirjana Bozic, Milena Davidovic (Institute of Physics, Belgrade)





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