The Foundations of Path Integration in Quantum Mechanics: From de Broglie to Feynman

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M. Oltean, Waterloo Mathematics Review **1**, 1 (2011).

Outline

The World Before 1900

"In a few years, all great physical constants will have been approximately estimated, and the only occupation which will be left to men of science will be to carry these measurements to another place of decimals."

— J. C. Maxwell (*Scientific Papers*, 1871)

Classical physics. Mechanics, electrodynamics, statistical thermodynamics:

$$\nabla^2\Phi = 4\pi G\rho, \quad m\ddot{\mathbf{x}} = -\nabla\Phi.$$

$$\nabla\cdot\mathbf{B} = 0, \;\; \nabla\cdot\mathbf{E} = \rho/\varepsilon_0, \;\; \nabla\times\mathbf{E} = -\partial_t\mathbf{B}, \;\; \nabla\times\mathbf{B} = \mu_0\mathbf{J} + \mu_0\varepsilon_0\partial_t\mathbf{E}.$$

$$S = k\ln\Omega.$$

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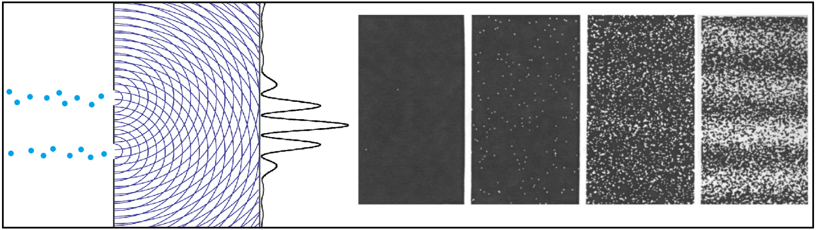
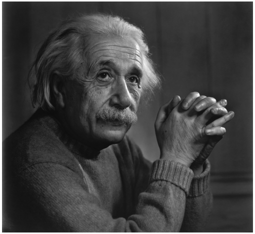
Dawn of the 20th Century: Particle or Wave?

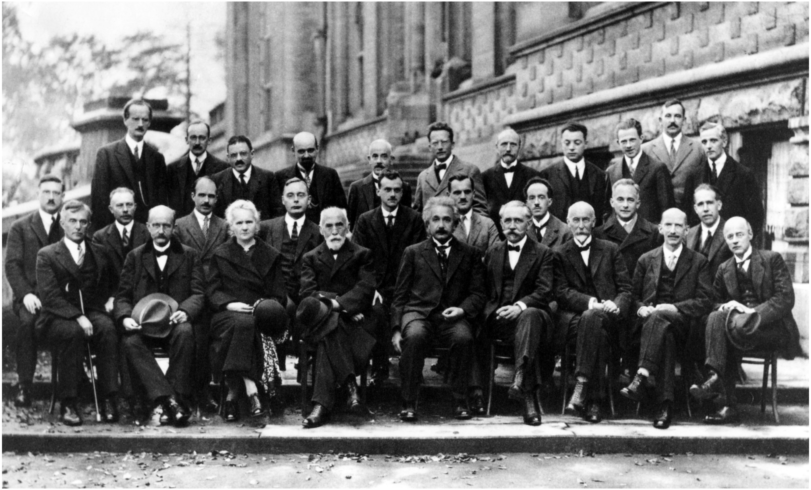




"It was as if the ground had been pulled out from under one, with no firm foundation to be seen anywhere, upon which one could have built."

— A. Einstein (*Philosopher-Scientist*, 1949)

The 1927 Solvay Conference



Axioms of Orthodox Quantum Theory

Complete Description. For a system of N particles:

$$\psi : \mathbb{R}^{3N} \times \mathbb{R} \to \mathbb{C}$$
$$(q, t) = (\mathbf{q}_1, ..., \mathbf{q}_N, t) \mapsto \psi(q, t)$$

Axiom 1. The Schrödinger equation:

When no ‘measurement’ is being performed, the wavefunction evolves via

$$i\hbar \frac{\partial \psi}{\partial t} = \sum_{j=1}^{N} \frac{-\hbar^2}{2m_j} \nabla_j^2 \psi + V\psi.$$

Axiom 2. The von Neumann projection postulate:

Upon ‘measurement’, the wavefunction randomly ‘collapses’ onto one of all the possible outcomes (eigenfunctions of the Hilbert space operator corresponding thereto), which have p.d.f. $\rho(q, t) = |\psi(q, t)|^2$.

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Two Conceptions of Science

"Physics is to be regarded not so much as the study of something a priori given, but rather as the development of methods of ordering and surveying human experience."

— N. Bohr (*The Unity of Human Knowledge*, 1960)

"If one renounces the assumption that what is present in different parts of space has an independent, real existence, then I do not at all see what physics is supposed to describe."

— A. Einstein (note to Born, 1948)

What is Wrong with Orthodox Quantum Theory?

- *As a phenomenological formalism*: Nothing at all – Axioms 1 and 2 have proven enormously successful in the prediction of experimental regularities in a wide range of atomic phenomena.

- *As a theory of fundamental physics*: A great deal – recall:

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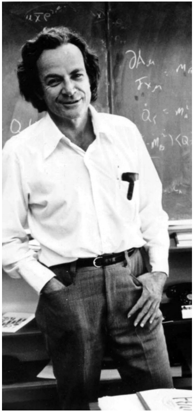
The Measurement Problem

One possible formulation: If orthodox quantum theory is correct, then why are the laws of physics contingent upon the act of 'measurement' (which is, in any event, a very vaguely defined concept)?



> "Does this mean that my observations become real only when I observe an observer observing something as it happens? This is a horrible viewpoint. Do you seriously entertain the thought that without observer there is no reality? Which observer? Any observer? Is a fly an observer? Is a star an observer? Was there no reality before 10^9 B.C. before life began? Or are you the observer? Then there is no reality to the world after you are dead? [...] By what philosophy will the Universe without man be understood?"

— R. Feynman (*Feynman Lectures on Gravitation*)

The Parting of the Ways

Conclusion: Orthodox quantum theory must be abandoned.
But what other options are there?

Alternative, empirically equivalent formulations of quantum mechanics

- Pilot-wave theory
- Objective collapse theories
- Many worlds theories
- Quantum Bayesianism
- Ensemble interpretation
- and so on...

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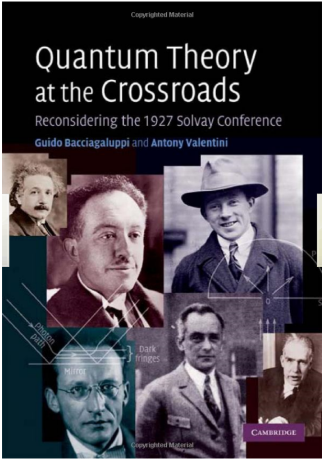
What's in a Name?

$$\left|\text{de Broglie}\right\rangle = \mathcal{N}\Big(\left|\text{/dəˈbrɔɪ/}\right\rangle + \left|\text{/dəˈbrɔɪl/}\right\rangle + \left|\text{/dəˈbroglɪə/}\right\rangle + \left|\text{/dəˈbrɔglɪɛ/}\right\rangle + \ldots\Big)$$

Discoverer of pilot-wave theory, also known as: de Broglie-Bohm theory, Bohmian mechanics, the causal interpretation of quantum mechanics, the ontological interpretation of quantum mechanics etc.

Advertisement Break



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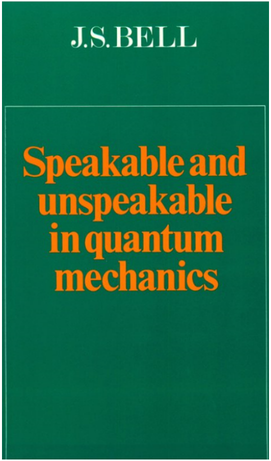
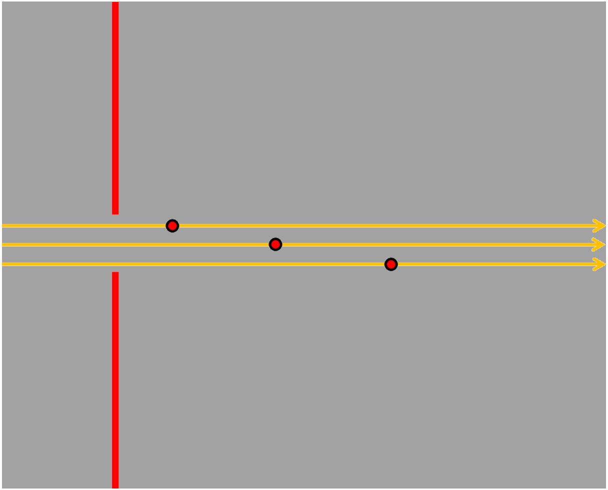
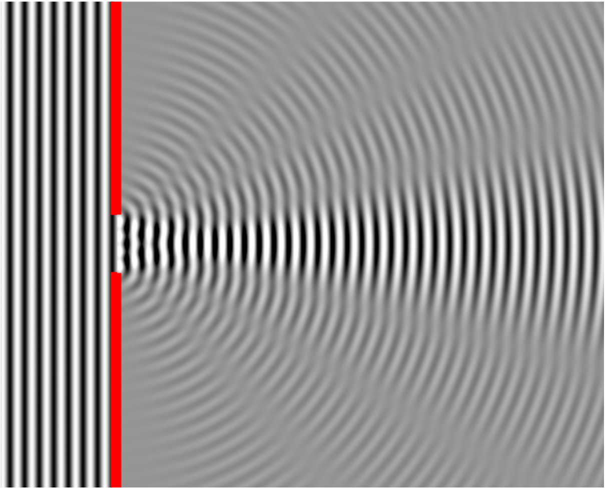


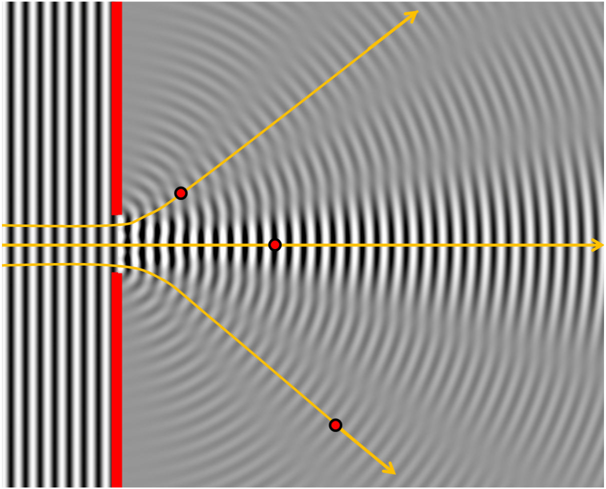
Photons Passing Through a Slit: Newtonian Prediction



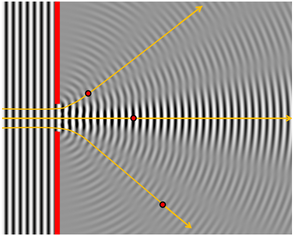
What Actually Happens: Diffraction



Diffraction of Light Quanta



The Inspiration for Pilot-Wave Theory



De Broglie hypothesized that

$$\mathbf{v} \propto \nabla S,$$

where $\mathbf{v}$ is the particle's velocity and S is the phase of the 'guiding' wave passing through the slit.

> "Guided by the idea of a deep unity between the principle of least action and that of Fermat, [...] I was led to *assume* that, for a given value of the total energy of the moving body and therefore of the frequency of its phase wave, the dynamically possible trajectories of the one coincided with the possible rays of the other."

— L. de Broglie (Ph.D. thesis, 1924)

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Axiom 2. The de Broglie guiding equation:

The position of the j-th particle is determined by the equation of motion

$$\frac{d\mathbf{Q}_j}{dt}=\frac{\hbar}{m_j}\Im\left(\frac{\nabla_j\psi}{\psi}\right)\Bigg|_{\mathcal{Q}(t)}.$$

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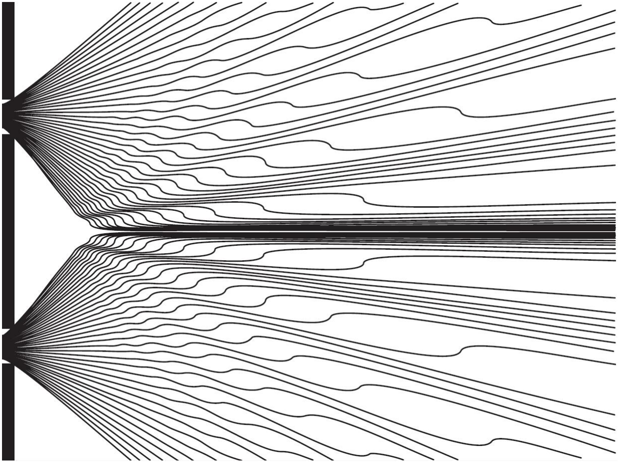
Example of Trajectories: The Double-Slit Experiment



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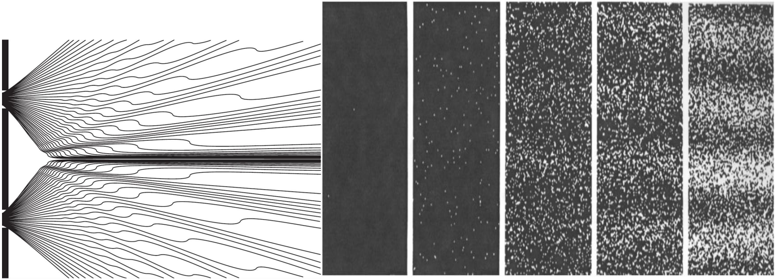

"While the founding fathers agonized over the question 'particle' *or* 'wave', de Broglie in 1925 proposed the obvious answer 'particle' *and* 'wave'. Is it not clear from the smallness of the scintillation on the screen that we have to do with a particle? And is it not clear, from the diffraction and interference patterns, that the motion of the particle is directed by a wave? [...] This idea seems to me so natural and simple, to resolve the wave-particle dilemma in such a clear and ordinary way, that it is a great mystery to me that it was so generally ignored."

— J.S. Bell (*Speakable and Unspeakable in QM*, 1987)

The Continuity and Quantum Hamilton-Jacobi Equations

Choosing a suitable phase function $S : \mathbb{R}^{3N} \times \mathbb{R} \to \mathbb{R}$, we can rewrite the wavefunction in the polar form

$$\psi = |\psi| \exp\left(\frac{i}{\hbar} S\right).$$

Inserting this into the Schrödinger equation, we get

The continuity equation for $|\psi|^2 : \mathbb{R}^{3N} \times \mathbb{R} \to \mathbb{R}$:

$$\frac{\partial |\psi|^2}{\partial t} + \sum_{j=1}^{N} \nabla_j \cdot \left(|\psi|^2 \frac{\nabla_j S}{m_j} \right) = 0.$$

The quantum Hamilton-Jacobi equation for N particles:

$$\frac{\partial S}{\partial t} + \sum_{j=1}^{N} \frac{\|\nabla_j S\|^2}{2m_j} + V + \sum_{j=1}^{N} \frac{-\hbar^2}{2m_j} \left(\frac{\nabla_j^2 |\psi|}{|\psi|} \right) = 0.$$

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(One Possible) Justification for the Guiding Equation

The continuity equation for $|\psi|^2 : \mathbb{R}^{3N} \times \mathbb{R} \to \mathbb{R}$:

$$\frac{\partial |\psi|^2}{\partial t} + \sum_{j=1}^{N} \nabla_j \cdot \underbrace{\left(|\psi|^2 \frac{\nabla_j S}{m_j} \right)}_{\boldsymbol{\mathcal{J}}_j^{\psi} = \frac{i\hbar}{2m_j}\left(\psi \nabla_j \psi^* - \psi^* \nabla_j \psi\right)} = 0.$$

If we adopt the usual interpretation of current as the product of density and velocity, then it takes no imagination to guess that the particle velocities might simply be determined by

$$\frac{d\mathbf{Q}_j}{dt} = \mathbf{v}_j^{\psi}\Big|_{\mathcal{Q}(t)}; \qquad \mathbf{v}_j^{\psi} = \frac{\boldsymbol{\mathcal{J}}_j^{\psi}}{|\psi|^2} = \frac{\nabla_j S}{m_j} = \frac{\hbar}{m_j} \Im \left(\frac{\nabla_j \psi}{\psi} \right).$$

The Quantum Lagrangian

The quantum Hamilton-Jacobi equation for N particles:

$$\frac{\partial S}{\partial t} + \underbrace{\overbrace{\sum_{j=1}^{N}\left(\frac{\left\|\nabla_j S\right\|^2}{2m_j}\right)}^{\frac{1}{2}m_j\left\|\mathbf{v}_j^{\psi}\right\|^2}}_{=T} + V + \underbrace{\sum_{j=1}^{N}\frac{-\hbar^2}{2m_j}\left(\frac{\nabla_j^2|\psi|}{|\psi|}\right)}_{:=V_q} = 0.$$

A standard result in classical mechanics is the classical Hamilton-Jacobi equation, which is identical to the above expression except for the term in red, with T representing the kinetic energy. This suggests the following:

Definition. The classical and quantum Lagrangians (respectively):

$$\mathcal{L}_c := T - V,$$
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The Dynamical Origin of Quantum Randomness

Randomness in classical statistical mechanics: The apparently random behaviour of large systems (as described, for instance, by the Maxwell-Boltzmann distribution of molecular velocities in a gas) emerges purely as a consequence of the underlying (deterministic) Newtonian dynamics governing the motions of the constituting particles.

Theorem. Subquantum H-Theorem:

Any N-particle system obeying pilot-wave dynamics that has an initial (epistemic) p.d.f. $\rho \neq |\psi|^2$ will, over time, eventually approach the 'equilibrium distribution' $\rho = |\psi|^2$ (with the exception of cases where there is no motion, and notwithstanding the time reversal invariance of the defining evolution equations).

Proof.

See A. Valentini, Phys. Lett. A **156**, 5 (1991). □

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Quantum Nonequilibrium in the Early Universe

Claim. A. Valentini, Phys. Rev. D **82**, 063513 (2010):

There is no a priori mathematical measure for any preferred distribution of the early Universe. Hence, the Universe probably started with some initial p.d.f. $\rho \neq |\psi|^2$, which then (by the H-Theorem) must have relaxed to the equilibrium distribution $\rho = |\psi|^2$ we observe today.

This offers the first possibility of an empirical distinction between pilot-wave theory and orthodox quantum theory, by observing either:

- a measurable signature in the spectrum of the CMB,
- 'relic' particles which, in the very early Universe, stopped interacting with other particles before they had enough time to reach equilibrium; if we can still find them around today, these should be seen to violate the Heisenberg uncertainty relation.

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Criticisms of Pilot-Wave Theory

- **Reasonable objections:** Essentially just one – finding relativistic/ quantum field theoretical generalizations. The issue arises from the fact that pilot-wave theory is explicitly nonlocal,

$$\frac{d\mathbf{Q}_j}{dt} = \frac{\hbar}{m_j}\Im\left(\frac{\nabla_j\psi}{\psi}\right)\bigg|_{\mathcal{Q}(t)} .$$

  For more, see J.S. Bell, *Speakable and Unspeakable in Quantum Mechanics* (1987), or W. Struyve, arXiv:1101.5819.

- **Silly objections:** Unfortunately too many – that the theory is 'complicated' or 'contrived,' that it constitutes a regression back to classical physics, that it does not postulate $\rho = |\psi|^2$, that quantum mechanics is inconsistent with determinism, and other assertions of this sort. If you really need a reply to any of these, see M. Kiessling, Found. Phys. **40**, 418 (2010), or O. Passon, quant-ph/0412119.

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Strategy for our Alternative Proof

Recall that we can write the wavefunction in the polar form

$$\psi(q,t) = |\psi(q,t)| \exp\left(\frac{i}{\hbar} S(q,t)\right).$$

So to find $\psi(q', t')$ we can proceed along the following lines:

- Firstly, propagate the modulus $|\psi|$.
- Secondly, propagate the phase S.
- Thirdly, put these together and thus propagate ψ.

Strategy for our Alternative Proof

Recall that we can write the wavefunction in the polar form

$$\psi(q,t) = |\psi(q,t)| \exp\left(\frac{i}{\hbar} S(q,t)\right).$$

So to find $\psi(q',t')$ we can proceed along the following lines:

- Firstly, propagate the modulus $|\psi|$.
- Secondly, propagate the phase S.
- Thirdly, put these together and thus propagate ψ.

Propagation of the Modulus

Lemma. Propagation of the modulus:

The wavefunction modulus is propagated according to

$$\left|\psi\left(q',t'\right)\right| = \left[\exp\left(-\frac{1}{2}\sum_{j=1}^{N}\int_{t}^{t'}\nabla\cdot\mathbf{v}_j^{\psi}\,dt\right)\right]\left|\psi\left(q,t\right)\right|,$$

where $\mathbf{v}_j^{\psi} = \nabla_j S/m_j$ is the velocity function.

Proof.

The continuity equation can be rewritten as follows:

$$\frac{\partial|\psi|^2}{\partial t} + \sum_{j=1}^{N}\nabla_j\cdot\left(|\psi|^2\frac{\nabla_j S}{m_j}\right) = 0 \Longrightarrow \ln\left|\frac{\psi\left(q',t'\right)}{\psi\left(q,t\right)}\right| = -\frac{1}{2}\sum_{j=1}^{N}\int_{t}^{t'}\nabla\cdot\mathbf{v}_j^{\psi}\,dt.$$

Taking the exponential of both sides thus yields the desired result. $\square$

Propagation of the Phase

Lemma. Propagation of the phase:

The phase function is propagated according to

$$S\left(q', t'\right) = S\left(q, t\right) + \int_{t}^{t'} \mathcal{L}_q \, dt,$$

where $\mathcal{L}_q := T - \left(V + V_q\right)$ is the quantum Lagrangian.

Proof.

Using the Chain Rule, the quantum Hamilton-Jacobi equation implies

$$\frac{\partial S}{\partial t} + T + V + V_q = 0 \Longrightarrow \frac{dS}{dt} = \sum_{j=1}^{N} \overbrace{\frac{\partial S}{\partial \boldsymbol{q}_j}}^{\nabla_j S} \cdot \overbrace{\frac{d\boldsymbol{q}_j}{dt}}^{\mathbf{v}_j^{\psi}} + \frac{\partial S}{\partial t} = \mathcal{L}_q,$$

which, in the form of an integral equation, gives the desired expression. $\square$

Proof for the de Broglie-Bohm Path Integral

Proof.

So far, we have by the two previous lemmas, respectively,

$$\left|\psi\left(q', t'\right)\right| = \left[\exp\left(-\frac{1}{2}\sum_{j=1}^{N}\int_{t}^{t'} \nabla \cdot \mathbf{v}_j^{\psi}\, dt\right)\right] \left|\psi\left(q, t\right)\right|,$$

$$\exp\left[\frac{i}{\hbar}S\left(q', t'\right)\right] = \exp\left(\int_{t}^{t'} \frac{i}{\hbar}\mathcal{L}_q\, dt\right) \exp\left[\frac{i}{\hbar}S\left(q, t\right)\right].$$

Putting these together, we get

$$\psi\left(q', t'\right) = \left|\psi\left(q', t'\right)\right| \exp\left[\frac{i}{\hbar}S\left(q', t'\right)\right]$$

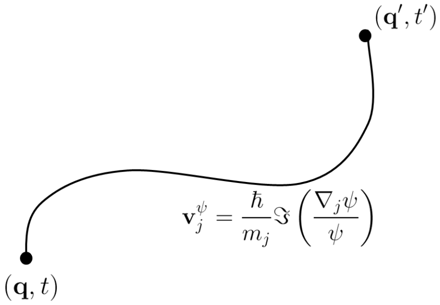
$$= \exp\left(\int_{t}^{t'} \frac{i}{\hbar}\mathcal{L}_q\, dt\right) \exp\left(-\frac{1}{2}\sum_{j=1}^{N}\int_{t}^{t'} \nabla \cdot \mathbf{v}_j^{\psi}\, dt\right) \left|\psi\left(q, t\right)\right| \exp\left[\frac{i}{\hbar}S\left(q, t\right)\right].$$

$\square$

The de Broglie-Bohm Path Integral

More succinctly,

$$\psi\left(q',t'\right)=\left\{\exp\left[\int_{t}^{t'}\left(\frac{i}{\hbar}\mathcal{L}_q-\frac{1}{2}\sum_{j=1}^{N}\nabla_j\cdot\mathbf{v}_j^{\psi}\right)dt\right]\right\}\psi\left(q,t\right).$$



The Feynman Path Integral (Single Particle Case)

Theorem. The single particle Feynman path integral:

Consider a single particle with some wavefunction $\psi(\mathbf{q}, t)$. Let $[t, t'] \subset \mathbb{R}$ be divided into n infinitesimal slices $\{[t_k, t_{k+1}] | t_{k+1} - t_k = \Delta t, \forall k\}_{k=0}^{n-1}$ with $t_0 = t$ and $t_n = t'$; furthermore, let each t_k correspond to position coordinate $\mathbf{q}_k \in \mathbb{R}^3$ with $\mathbf{q}_0 = \mathbf{q}$ and $\mathbf{q}_n = \mathbf{q}'$. Then, if $\mathcal{L}_c := T - V$,

$$\psi(\mathbf{q}', t') = \int_{\mathbb{R}^3} \left[\lim_{n\to\infty} \int \cdots \int_{\mathbb{R}^{3(n-1)}} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{3}{2}n} \times \exp\left(\frac{i}{\hbar}\int_t^{t'} \mathcal{L}_c \, dt\right) \prod_{k=1}^{n-1} d^3\mathbf{q}_k \right] \psi(\mathbf{q}, t)\, d^3\mathbf{q}.$$

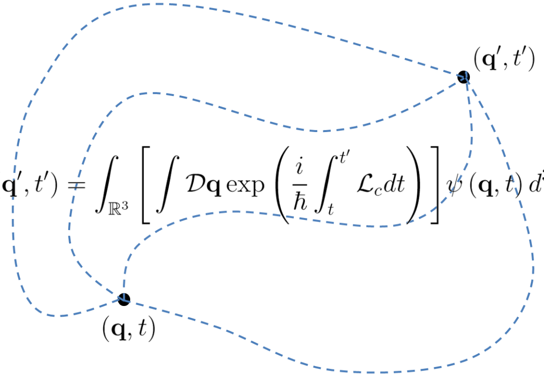
Proof.

Follows from the de Broglie-Bohm path integral.
For the full proof, see M. Oltean, Waterloo Mathematics Review **1**, 1 (2011).

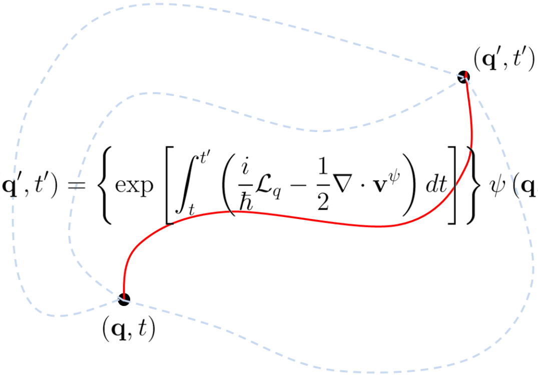
□

Conclusion

$$\psi\left(\mathbf{q}', t'\right) = \int_{\mathbb{R}^3} \left[\int \mathcal{D}\mathbf{q} \exp\left(\frac{i}{\hbar} \int_t^{t'} \mathcal{L}_c dt \right) \right] \psi\left(\mathbf{q}, t\right) d^3\mathbf{q}.$$



Conclusion



$$\psi(\mathbf{q}', t') = \left\{ \exp\left[\int_t^{t'} \left(\frac{i}{\hbar}\mathcal{L}_q - \frac{1}{2}\nabla \cdot \mathbf{v}^{\psi} \right) dt \right] \right\} \psi(\mathbf{q}, t)$$

Thank you for your attention.