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Path Integral and Aharonov-Bohm effect

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Contents

1	Introduction	1
2	Classical Electrodynamics and Gauge Transformations	3
3	Path integral approach to Quantum Mechanics	5
3.1	Canonical Transformation in Classical and Quantum Mechanics . . .	5
3.2	Path integral	8
3.3	Equivalence of the Path Integral and the Schrödinger Equation . . .	11
3.4	The Classical Limit	13
4	Path Integrals as Determinants	15
4.1	Gaussian integrals	15
4.2	Computation of the Feynman Propagator	16
4.3	Free Particle Propagator and Normalization Constant	18
5	Interaction with an External Electromagnetic Field and Quantum Gauge Invariance	21
5.1	Quantum Gauge Invariance	21
6	The Aharonov-Bohm effect	23
6.1	The Thought Experiment and Topological Properties of the Space .	23
6.2	The Aharonov Bohm Effect	25
7	Conclusions	27
	Bibliography	28

1 Introduction

Classical electrodynamics can be expressed by equations which involve only the world-line of the charged particles $y^\mu(s)$ and the electric and magnetic fields $F^{\mu\nu}$. It is convenient, however, to introduce a 4-potential A^μ , as it simplifies problems and the formulation of the theory. For example, Maxwell equations in vacuum (which means that the 4-current J^μ is zero), written in terms of the 4-potential, assume the form of a wave equation and this yields a simple and elegant description of the electromagnetic waves. However, the A^μ overdetermines the system as two 4-potentials connected by a gauge transformation are equivalent: from a physical point of view, this means that A^μ cannot be measured. As the 4-potential is a convenient mathematical tool, but still not needful, and it cannot be measured, one concludes that in classical electrodynamics it has no independent physical meaning. The quantum mechanical description of electrodynamics is given by quantizing the classical theory; this can be done either through the canonical quantization or with the path integral approach (the latter is the one used in this thesis). In both cases a variational formulation of the classical theory is required and, as we will show in Section (2), this can be obtained only using the 4-potential as Lagrangian field: for a quantum mechanical description A^μ is needful.

In Section (3) and (4) the path integral approach to quantum mechanics will be presented. With this aim, we will start from Dirac's original idea to construct a formulation of quantum mechanics based on the Lagrangian formulation of classical mechanics; since one cannot expect to find a quantum analog of the Euler-Lagrange equations in a very direct way (no immediate meaning can be given to such equations in quantum theory, as they involve partial derivatives with respect to the coordinates and velocities), he proposed some observations concerning the analogies between the role of Hamilton principal function in classical mechanics and some operator rules in computing the transition amplitudes. Feynman extended this analogy adding the integral over all possible trajectories the quantum particle can follow and proposed the path-integral formulation of quantum mechanics.

In Section (5) it will be showed that the gauge transformation is also a physical symmetry of the quantum theory, which acts on the wave function as a local phase transformation. The fact that those two transformations act conjointly, gives A^μ an independent physical meaning in quantum mechanics, as we will show in Section (6). Through a thought experiment, proposed by Bohm and Aharonov in 1959 and later tested by Chambers (1960) and, more consistently, by Tonomura (1984), we will prove that a quantum charged particle in a multiply connected field free region feels an electromagnetic interaction, if we ask $F^{\mu\nu} \neq 0$ in some region of the space which the particle cannot enter.

In order to avoid non-local interactions between $F^{\mu\nu}$ and the particle (since it is problematic from a relativistic point of view) one can interpret this effect assum-

ing that the electromagnetic interaction occurs between A^μ and the charge. This conclusion gives the 4-potential a more fundamental physical role than the one it has in classical mechanics.

2 Classical Electrodynamics and Gauge Transformations

As it is commonly known, the three fundamental laws which control classical electrodynamics are

$$\epsilon_{\mu\nu\rho\sigma}\partial^\nu F^{\rho\sigma} = 0 \quad (1)$$

$$\partial_\mu F^{\mu\nu} = J^\nu \quad (2)$$

$$\frac{dp^\mu}{ds} = eF^{\mu\nu}(y)u_\nu \quad (3)$$

written in the explicitly covariant form. The first one is Bianchi's Identity, it constrains the form of the electromagnetic field $F^{\mu\nu}$; the second one is Maxwell's Equation and it is the equation of motion of the field, it defines how a generic current density J^μ generates a field. The last one is Lorentz's Equation and establishes how a charge behaves in an electromagnetic field. If one tries to solve this set of equations at the same time, meets some pathologies: according to Maxwell's equation, the field is singular on the world-line of the charge, while the last equation states, according to the principle of locality, that in order to compute the variation of momentum of the charge, $F^{\mu\nu}$ has to be evaluated on the world-line of the particle. From a theoretical point of view, at least one of these equations has to be modified. However, we will not worry about this issue, as we will assume that $F^{\mu\nu}$ is an external field, ignoring the radiation reaction. If the domain is topologically trivial,¹ eq. (1) can be identically solved, introducing the 4-potential $A^\mu = (A^0, \vec{A})$ and setting

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu \implies \epsilon_{\mu\nu\rho\sigma}\partial^\nu(\partial^\rho A^\sigma - \partial^\sigma A^\rho) = 0 \quad (4)$$

since $\partial^\mu\partial^\nu$ is symmetric while $\epsilon_{\mu\nu\rho\sigma}$ is antisymmetric under the exchange of two indices. All the electro-dynamical equations can be expressed in terms of the potential, simply using the substitution of the first equation in (4).

While the field $F^{\mu\nu}$ is univocally determined once A^μ is given, it is not true the opposite. If we consider the gauge transformation

$$A^\mu(x) \rightarrow A'^\mu(x) = A^\mu(x) + \partial^\mu\Lambda(x) \quad (5)$$

¹Topologically trivial means that the domain has to be contractible:

A subset \mathcal{C} of a topological space is contractible to the point $y \in \mathcal{C}$ if it exists a continuous map $F : [0, 1] \times \mathcal{C} \rightarrow \mathcal{C}$, $F : (\lambda, x) \rightarrow F(\lambda, x)$ such that $F(0, x) = x \forall x \in \mathcal{C}$ and $F(1, x) = y \forall x \in \mathcal{C}$.

where $\Lambda(x)$ is a generic scalar field, the fields remain unchanged: $F'^{\mu\nu} = F^{\mu\nu}$. Since all the electro-dynamical equations can be written and solved in terms of the gauge invariant field $F^{\mu\nu}$ and the potential is not gauge invariant, one concludes that A^μ is not a real physical quantity: it can be regarded as a mathematical tool which simplifies (and, indeed, it does) problems, but still it is not needful. Things change if we want to derive our theory from a variational principle and, therefore, interpret eq. (1), (2) and (3) as Euler-Lagrange equations. Since (1) and (2) correspond to 8 equations, we cannot hope to use $F^{\mu\nu}$ as a lagrangian field because it corresponds to the 6 independent fields \vec{E} and \vec{B} (or, equivalently, since it is a 4×4 antisymmetric tensor, it has 6 degrees of freedom). Therefore an alternative strategy is required: once Bianchi identity is solved introducing A^μ (4 fields), the potential can be used as a lagrangian field in order to derive Maxwell's equation (4 equations). Once again, classically, a variational formulation of the theory is useful but not necessary. On the other hand, it is the starting point for the quantization of the theory: from a quantistical point of view, A^μ is needful and its presence in the equations formally unavoidable.

Since it will be used later on in this thesis, here is reported the non relativistic lagrangian for a charged particle in an external electromagnetic field

$$L = \frac{1}{2}m\vec{v}^2 - eA^0(t, \vec{r}) + e\vec{A} \cdot \vec{v} \quad (6)$$

and the corresponding action for a path joining the space-time events $A = (t_1, \vec{x}_1)$ and $B = (t_2, \vec{x}_2)$

$$S = S_0 + S_{int} = \int_{t_1}^{t_2} dt \frac{1}{2}m\vec{v}^2 - e \int_A^B A_\mu dx^\mu \quad (7)$$

A gauge transformation adds a 4-divergence to the Lagrangian

$$L \rightarrow L' = L + \partial_\mu \Lambda(x)$$

and the action only changes by boundary terms

$$S \rightarrow S' = S - e \int_A^B \partial_\mu \Lambda(x) dx^\mu = S - e(\Lambda(B) - \Lambda(A)) \quad (8)$$

This is not a coincidence. Since a gauge transformation leaves physics unchanged, *i.e.* it does not affect Euler-Lagrange equations, the variations of the actions S and S' must be equal

$$\delta S = \delta S'$$

This is a general case: two Lagrangians which differ by a 4-divergence are physically equivalent.

3 Path integral approach to Quantum Mechanics

Consider a classical system of N degrees of freedom. The dynamics of the system is governed by the Hamiltonian $H(p, q)$, which is a function of the coordinates $\{q_i\}$ and the conjugate momenta $\{p_i\}$. The coordinates and the conjugate momenta satisfy a set of Poisson Bracket relations

$$\{p_i, p_j\} = \{q_i, q_j\} = 0 \quad \{q_i, p_j\} = \delta_{ij} \quad (9)$$

There are two different ways to quantize the system

- The canonical quantization
- The path integral procedure

The first one consists in demanding that to the classical canonical pair (p, q) we associate the pair of operators \hat{p}_i and \hat{q}_i , which we require to obey to the canonical commutation relations

$$[\hat{q}_i, \hat{q}_j] = [\hat{p}_i, \hat{p}_j] = 0 \quad [\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij} \quad (10)$$

obtained by the formal correspondence $\{A, B\} \rightarrow -\frac{i}{\hbar}[A, B]$. The relations (10) allow to implement the uncertainty principle, since it is a consequence of the non-commutativity of two conjugate operators. By following this prescription, we can promote the function $H(p, q)$ to the operator $\hat{H}(\hat{p}, \hat{q})$ by replacing the dynamical variables with the corresponding operators. The latter procedure, which is the one that will be used in this thesis, is described in the following sections.

3.1 Canonical Transformation in Classical and Quantum Mechanics

Let's consider a particle moving in one dimension with hamiltonian $H(p, q, t)$. The equations of motion are the Hamilton's equations

$$q = \frac{\partial H}{\partial p} \quad \dot{p} = -\frac{\partial H}{\partial q} \quad (11)$$

Eq. (11) can be derived from a variational principle

$$\delta \int_{t_1}^{t_2} dt (p\dot{q} - H) = 0 \quad (12)$$

where the independent variations δp and δq are taken to vanish at the boundaries.

We call canonical transformations the maps

$$p \rightarrow P = P(p, q, t) \quad q \rightarrow Q = Q(p, q, t) \quad (13)$$

which leaves Hamilton's equations form invariant, *i.e.* it exists a new hamiltonian $\tilde{H}(P, Q, t)$ such that

$$\dot{Q} = \frac{\partial \tilde{H}}{\partial P} \quad \dot{P} = -\frac{\partial \tilde{H}}{\partial Q} \quad (14)$$

In order that the new independent variables P and Q satisfy Hamilton's equations, the variational principle must remain valid

$$\delta \int_{t_1}^{t_2} dt \left(P\dot{Q} - \tilde{H} \right) = 0 \quad (15)$$

Since eq. (12) and (15) are equivalent only if the integrands differ, at most, by the total derivative of an arbitrary function G of time and any pair (q, Q) , (q, P) , (p, Q) or (p, P) treated as independent variables; it follows that

$$p\dot{q} - H = P\dot{Q} - \tilde{H} + \frac{dG}{dt} \quad (16)$$

Let's consider the case in which $G = G(q, Q, t)$, then eq. (16) becomes

$$\left(p - \frac{\partial G}{\partial q} \right) \dot{q} - \left(P + \frac{\partial G}{\partial Q} \right) \dot{Q} = \frac{\partial G}{\partial t} + H - \tilde{H}$$

which yields

$$p = \frac{\partial G}{\partial q} \quad P = -\frac{\partial G}{\partial Q} \quad \tilde{H} = \frac{\partial G}{\partial t} + H \quad (17)$$

Therefore the knowledge of the generating function G , through eq. (17), defines the relations between the old variables (p, q) , the new variables (P, Q) and the form of the new hamiltonian \tilde{H} .

Let's now consider the special case in which the canonical transformation maps the variables (p, q) to a new set which is time independent, so that $\dot{Q} = \dot{P} = 0$. From eq. (14) we read that the new hamiltonian \tilde{H} can only be constant, with or without time dependence. Let's take for simplicity $\tilde{H} = 0$. Once the canonical transformation is found and, equivalently, once the generating function is known, the dynamical problem reduces to the inversion problem

$$\begin{cases} Q = \text{const} = Q(p, q, t) \\ P = \text{const} = P(p, q, t) \end{cases} \implies \begin{cases} p = p(P, Q, t) \\ q = q(P, Q, t) \end{cases}$$

so that P, Q play the role of initial conditions. From eq. (16) we have that, in this case, the time derivative of the generating function, which we will call Hamilton Principal Function and denote by S

$$\frac{dS}{dt} = -H + p\dot{q}$$

is nothing but the Lagrangian. Integrating we get

$$S = \int_{t_0}^t dt L$$

and we recognize S to be the time integral of the Lagrangian regarded as a function of $q(t)$ and $Q = q(t_0)$.²

We arrived to the central result that in the classical theory the dynamical variables vary in such a way that their values $q(t)$ and $p(t)$ at any time t are connected with their values $q(T)$ and $p(T)$ at any other time T by a canonical transformation with $q = q(t)$, $p = p(t)$, $Q = q(T)$, $P = p(T)$ and $G \equiv S$, the generating function of this transformation, which transforms the dynamical variables from one time to another, is the action.

In this special case eq. (17) becomes

$$H = -\frac{\partial S}{\partial t} \quad p = \frac{\partial S}{\partial q}$$

and we shall write

$$p_\mu = -\partial_\mu S \tag{18}$$

Let's now try to make an analogy of this in quantum mechanics. The states of a quantum system can be taken to be the position states $|q\rangle$ which, in terms of the operators \hat{q} and \hat{p} that obey to the commutation relations (10), satisfy

$$\hat{q}|q\rangle = q|q\rangle \quad \langle q|q'\rangle = \delta(q - q') \quad \int dq |q\rangle\langle q| = \mathbb{I}$$

The quantum analog of the classical canonical transformation is a transformation between operators $(\hat{q}, \hat{p}) \rightarrow (\hat{Q}, \hat{P})$ which does not change the form of the fundamental commutation relations (10). The system can therefore be described in terms of $|q\rangle$ or $|Q\rangle$ states and there is a transformation function $\langle q|Q\rangle$ connecting the two representations.

²The time integral of the Lagrangian will be called generally "action". To be precise, however, it is called action when it is a functional of a path; when this path is the classical trajectory it should be called, more properly, Hamilton Principal Function.

It is straightforward to show that

$$\langle q|\hat{q}|Q\rangle = q\langle q|Q\rangle \quad \langle q|\hat{Q}|Q\rangle = Q\langle q|Q\rangle \quad (19)$$

Then, since $\hat{p}|q\rangle = -i\hbar\frac{\partial}{\partial q}|q\rangle$, we have

$$\langle q|\hat{p}|Q\rangle = i\hbar\frac{\partial}{\partial q}\langle q|Q\rangle \quad \langle q|\hat{P}|Q\rangle = -i\hbar\frac{\partial}{\partial q}\langle q|Q\rangle \quad (20)$$

note the difference in sign in the last two equations. The value of an arbitrary operator $F(\hat{q}, \hat{Q})$ in the mixed representation may not be well defined. However, if we consider $F(\hat{q}, \hat{Q})$ to be a well ordered function of \hat{q} and \hat{Q} (which means that it can be written as $F(\hat{q}, \hat{Q}) = f_1(\hat{q})f_2(\hat{Q})$), we have from eq. (19)

$$\langle q|F(\hat{q}, \hat{Q})|Q\rangle = \langle q|f_1(\hat{q})f_2(\hat{Q})|Q\rangle = f_1(q)f_2(Q)\langle q|Q\rangle = F(q, Q)\langle q|Q\rangle$$

Following Dirac, let's set

$$\langle q|Q\rangle = e^{\frac{i}{\hbar}G(q, Q)} \quad (21)$$

where G is some function of q and Q . From eq. (20) and (21), we get

$$\langle q|\hat{p}|Q\rangle = \frac{\partial G}{\partial q}\langle q|Q\rangle \quad \langle q|\hat{P}|Q\rangle = -\frac{\partial G}{\partial Q}\langle q|Q\rangle$$

If we assume $\frac{\partial G}{\partial q}$ and $\frac{\partial G}{\partial Q}$ to be well-ordered functions, the last equations can be read in terms of equalities between operators

$$\hat{p} = \frac{\partial \hat{G}}{\partial q} \quad \hat{P} = -\frac{\partial \hat{G}}{\partial Q}$$

We can therefore consider G , defined by (21), to be the quantum analog of the classical generating function.

3.2 Path integral

The states of a quantum system are described by a state vector ψ of a complex Hilbert space \mathcal{H} : $\psi \in \{ \alpha\varphi \mid \varphi \in \mathcal{H}, \alpha \in \mathbb{C} \setminus \{0\} \}$. In the coordinates representation we have $\langle x|\psi\rangle = \psi(x) \in \mathbb{C}$, this is the probability amplitude of the system. According to the Copenhagen interpretation of quantum mechanics, it represents the maximum information available about the system and, as first proposed by Max Born, its modulus squared represents a probability density.

In the path integral formulation of quantum mechanics (formulation due to Feynman and Dirac), a probability amplitude is associated with an entire motion of a particle as a function of time, rather than just with a position at a particular time.

Before continuing, it is important to keep in mind that in quantum mechanics time is not an observable: it plays the role of a parameter.

Let's consider a quantum system made of a single particle (in order to fix the ideas, we shall limit to a single degree of freedom, as the generalization is obvious) with amplitude $\psi(q, t) \equiv \psi(q_t)$. In order to solve the dynamical problem of how $\psi(q, t)$ develops in time, consider two fixed times t_1 and t_2 . $\psi(q_1, t_1)$ and $\psi(q'_2, t_2)$ are respectively the amplitude of finding the particle in q_1 at t_1 and in q'_2 at t_2 . Let $K(q'_2, t_2; q_1, t_1)$ denote the amplitude associated to the event that a particle in q_1 at t_1 is observed in q'_2 at t_2 . $K(q'_2, t_2; q_1, t_1)$ is the Feynman Propagator. Now, suppose we observe the particle in q'_2 at t_2 , it must have been somewhere at time t_1 . Here lays the core of quantum mechanics (and, in particular, of Feynman formulation): unless we measure the position of the particle, the statement "the position of the particle at time t_1 had some well defined value" could be meaningless: it was everywhere (or nowhere, it depends on the point of view). $\psi(q'_2, t_2)$ is composed of two individual contributions: the particle was in q_1 at t_1 (amplitude = $\psi(q_1, t_1)$) and the particle moved from q_1 at t_1 to q'_2 at t_2 (amplitude = $K(q'_2, t_2; q_1, t_1)$).

Hence we shall write

$$\psi(q'_2, t_2) = \int dq_1 K(q'_2, t_2; q_1, t_1) \psi(q_1, t_1) \quad (22)$$

This is the basic dynamical equation of the theory.

In order to determinate the Feynman propagator let's derive eq. (22) following another point of view. In particular we shall proceed to apply the analogy suggested by Dirac, eq. (21), using Hamilton's principle function with $q = q_{t_1}$ at t_1 and $Q = q'_{t_2}$ at t_2 . Using the completeness relation

$$\mathbb{I} = \int dq |q\rangle\langle q| \quad (23)$$

we have

$$\psi(q'_{t_2}) = \langle q'_{t_2} | \int dq_{t_1} |q_{t_1}\rangle \langle q_{t_1} | \psi \rangle = \int dq_{t_1} \langle q'_{t_2} | q_{t_1} \rangle \psi(q_1, t_1) \quad (24)$$

Comparing eqs. (22) (24) we see that the transformation function $\langle q'_{t_2} | q_{t_1} \rangle$, connecting the representations at the two different times t_1 and t_2 , is the Feynman propagator. From the analogy between classical and quantum canonical transformations, following Dirac, we say that there is the following correspondence

$$\langle q_{t_1} | q'_{t_2} \rangle \sim e^{-\frac{i}{\hbar} \int_{t_1}^{t_2} dt L} \quad (25)$$

It is important to stress that, for the sake of the analogy, the classical Lagrangian L should be considered a function of the spatial coordinates at time t_1 and at time

t_2 , rather than a function of the coordinates and velocities. One could be tempted to replace the \sim sign in eq. (25) with an equality sign, but this cannot be correct in general. In fact, if we split the time interval $[t_1, t_2]$ into N time intervals $[t'_k, t'_{k+1}]$, with $t'_k = t_1 + k\epsilon$ and $N\epsilon = t_2 - t_1$, and we set $q_a \equiv q_{t_a}$, eq. (23) leads to

$$\langle q_{t_1} | q'_{t_2} \rangle = \int dq_1 dq'_2 \cdots dq_{N-1} \langle q_{t_1} | q_1 \rangle \langle q_1 | q_2 \rangle \cdots \langle q_{N-1} | q'_{t_2} \rangle \quad (26)$$

This is an exact quantum mechanical equation. On the other hand, if in eq. (25) we replace an equality sign, splitting the integral into N integration regions we get

$$\langle q_{t_1} | q'_{t_2} \rangle = \langle q_{t_1} | q_1 \rangle \langle q_1 | q_2 \rangle \cdots \langle q_{N-1} | q'_{t_2} \rangle \quad (27)$$

which cannot be correct. The problem does not lie in the equality sign per se, but in having used it when the time interval $t_2 - t_1$ is finite: in this hypothesis we have been able to split the integration region and we occurred in the contradiction of eq. (26) and (27). However, if we postulate eq. (25) to hold as an equality, up to a constant, for an infinitesimal time interval δt

$$\langle q'_{t+\delta t} | q_t \rangle = A e^{\frac{i}{\hbar} L(q_t, q_{t+\delta t}) \delta t} \quad (28)$$

we run into no conflict with eq. (26).

The need of a constant A is clear from dimensional considerations. Since the wave function has the dimension of $[\text{length}^{-\frac{1}{2}}]$, the Feynman propagator must have the dimension of $[\text{length}^{-1}]$. In order to fix it, let's ask that, according to the orthonormality in the sense of δ -function

$$\lim_{\delta t \rightarrow 0} \langle q'_{t+\delta t} | q_t \rangle = \delta(q' - q)$$

We shall assume $A = A(\delta t)$, which means that it depends only on the time interval and not on the particular system considered. We are, therefore, legitimated to consider specifically the free partical case $L = \frac{1}{2} m \frac{(q' - q)^2}{\delta t^2}$

$$\delta(q' - q) = \lim_{\delta t \rightarrow 0} A(\delta t) e^{\frac{i}{\hbar} \frac{m}{2} \frac{(q' - q)^2}{\delta t}} \implies A(\delta t) = \sqrt{\frac{m}{2\pi i \hbar \delta t}} \quad (29)$$

where we have used the gaussian representation of the δ

$$\lim_{\delta t \rightarrow 0} \sqrt{\frac{m}{2\pi i \hbar \delta t}} e^{\frac{i}{\hbar} \frac{m}{2} \frac{(x)^2}{\delta t}} = \delta(x)$$

By eqs. (26) (28), taking the limit for $N \rightarrow \infty$ in order to make the time intervals $[t'_k, t'_{k+1}]$ infinitesimal, we get

$$\begin{aligned} \langle q'_{t_2} | q_{t_1} \rangle &= \lim_{\substack{N \rightarrow \infty \\ N\epsilon \text{ fixed}}} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} \int \prod_{i=1}^{N-1} dq_i e^{\frac{i}{\hbar} \int_{t_1}^{t_2} dt L(q, \dot{q})} \\ &\equiv \int_{q(t_1)=q}^{q(t_2)=q'} D[q(t)] e^{\frac{i}{\hbar} S(t_1, t_2, [q(t)])} \end{aligned} \quad (30)$$

which is the Feynman Path Integral. Eq. (30) states that the transition amplitude $\langle q'_{t_2} | q_{t_1} \rangle$ is given by the sum over all possible paths linking q at time t_1 with q' at time t_2 : each path contributes equally in magnitude, but the phase of its contribution is the action, evaluated on that path, in units of \hbar . To be more precise the paths are defined only by the succession of points q_i through which the particle passes at times t'_i . However, to compute $S = \int dt L(q, \dot{q})$ we need to know the path at each point, not just at q_i , since the Lagrangian is a function of the position and the velocity. We shall therefore assume that the path followed by the particle in the n -th infinitesimal time interval is the one followed by a classical particle, with Lagrangian L . If the Lagrangian does not depend on higher time derivatives of the position than the first (as it is usually the case, according to the newtonian determinism) the starting and ending points are sufficient to define the classical path.

We would expect, if the path integral approach is consistent, that eq. (24) and eq. (30) are equivalent to Schrödinger equation and this formulation of quantum mechanics has a coherent classical limit. Those problems will be analyzed in the next sections.

3.3 Equivalence of the Path Integral and the Schrödinger Equation

The aim of this section is to show that Schrödinger equation can be derived from the path integral approach. This will prove the equivalence of Feynman's formulation of quantum mechanics and the standard one. Let's consider the "trivial" statement that the path integral is invariant under an overall shift of the integration variable

$$q(t) \rightarrow q(t) + \delta q(t) \quad \text{with} \quad \delta q(t_1) = \delta q(t_2) = 0 \quad (31)$$

this yields

$$\int_{q(t_1)=q}^{q(t_2)=q'} D[q(t)] e^{\frac{i}{\hbar} S[q(t)]} = \int_{q(t_1)=q}^{q(t_2)=q'} D[q(t)] e^{\frac{i}{\hbar} S[q(t)+\delta q(t)]} \quad (32)$$

which follows from the (assumed) invariance of the measure under (31). If we take the variation $\delta q(t)$ infinitesimal, we have

$$S[q(t) + \delta q(t)] = S[q(t)] + \delta S[q(t)] \quad (33)$$

where $\delta S[q(t)]$ is the variation of the action; if $\delta q(t)$ vanishes at the boundaries, as required from eq. (31), we get the Euler-Lagrange equations
From

$$\delta S[q(t)] = \int_{t_1}^{t_2} dt \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \delta q(t) \quad (34)$$

eq. (32) and (33) yields

$$\int_{q(t_1)=q}^{q(t_2)=q'} D[q(t)] \delta S[q(t)] e^{\frac{i}{\hbar} S[q(t)]} = \int_{q(t_1)=q}^{q(t_2)=q'} D[q(t)] \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) e^{\frac{i}{\hbar} S[q(t)]} = 0 \quad (35)$$

This is the path integral version of Ehrenfest's theorem: the Euler-Lagrange equations must hold as an expectation value.

Before deriving Schrödinger equation we need another result: the momentum is given by a derivative with respect to the position. Let's take $\delta q(t)$ infinitesimal, but with boundary conditions $\delta q(t_1) = 0$ and $\delta q(t_2) \neq 0$. Under this variation the propagator $K(q', t_2 | q, t_1) = \langle q', t_2 | q, t_1 \rangle$ changes by

$$\langle q' + \delta q(t_2), t_2 | q, t_1 \rangle - \langle q', t_2 | q, t_1 \rangle = \frac{\partial}{\partial q'} \langle q', t_2 | q, t_1 \rangle \delta q(t_2) \quad (36)$$

and the path integral changes by

$$\int D[q(t)] e^{\frac{i}{\hbar} S[q(t) + \delta q(t)]} - \int D[q(t)] e^{\frac{i}{\hbar} S[q(t)]} = \int D[q(t)] \frac{i}{\hbar} \delta S[q(t)] e^{\frac{i}{\hbar} S[q(t)]} \neq 0 \quad (37)$$

Since the boundary conditions of the variation have changed, eq. (35) differs from eq. (37). In fact in this case we have

$$\delta S[q(t)] = \int_{t_1}^{t_2} dt \left(\frac{\partial L}{\partial q} \delta q(t) + \frac{\partial L}{\partial \dot{q}} \delta \dot{q}(t) \right) = \frac{\partial L}{\partial \dot{q}} \delta q(t) \Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} dt \left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \delta q(t) \quad (38)$$

The last term vanishes because of the Ehrenfest's theorem eq. (35), and we are left with

$$\delta S[q(t)] = \left. \frac{\partial L}{\partial \dot{q}} \right|_{t_2} \delta q(t_2) = p(t_2) \delta q(t_2)$$

From eq. (36), (37) and (38) we get

$$\frac{\partial}{\partial q'} \langle q', t_2 | q, t_1 \rangle = \int D[q(t)] e^{\frac{i}{\hbar} S[q(t)]} \frac{i}{\hbar} p(t_2)$$

which is precisely the momentum in the position representation

$$\hat{p}' = -i\hbar \frac{\partial}{\partial q'} \quad (39)$$

In the same way we can derive Schrödinger equation, by taking a variation with respect to t_2 .

$$\langle q', t_2 + \delta t_2 | q, t_1 \rangle - \langle q', t_2 | q, t_1 \rangle = \frac{\partial}{\partial t_2} \langle q', t_2 | q, t_1 \rangle \delta t_2$$

Then, from eq. (18) follows

$$\int D[q(t)] e^{\frac{i}{\hbar} (S[q(t)] + \frac{\partial S}{\partial t_2} \delta t_2)} - \int D[q(t)] e^{\frac{i}{\hbar} S[q(t)]} = \int D[q(t)] \left(-\frac{i}{\hbar} H(t_2) \right) e^{\frac{i}{\hbar} S[q(t)]} \delta t_2$$

Hence

$$\left(i\hbar \frac{\partial}{\partial t_2} - \hat{H}(\hat{q}', \hat{p}' = -i\hbar \frac{\partial}{\partial q'}) \right) \int_{q=q(t_1)}^{q'=q(t_2)} D[q(t)] e^{\frac{i}{\hbar} S[q(t)]} = 0 \quad (40)$$

3.4 The Classical Limit

In quantum mechanics, a particle is described in terms of a probability amplitude whose temporal evolution is given by Schrödinger equation. In classical mechanics, instead, a particle is treated as a material point, moving along a path which is completely and univocally determined by the Euler-Lagrange equations.

How can we combine together those two interpretations of the world? The need of combining them into a unique frame derives from the assumption that there are not two worlds, a classical and a quantum one, but, instead, quantum mechanics contains classical mechanics in the form of a certain limiting case. This is exactly what happens with Einstein's Special Relativity: performing the limit $c \rightarrow \infty$, we get back to Galileo's Relativity (and, therefore, to Newtonian mechanics).³

Before analyzing the meaning of a classical limit in the Path Integral formulation of quantum mechanics and, moreover, how the single classical path can emerge

³To be precise, the limit is $\frac{v}{c} \rightarrow 0$, *i.e.* small velocities compared to the speed of light.

from eq. (30), where the integral is performed over all possible paths, some clarifications are required. The problem of the classical limit in quantum mechanics is still debated and there are still many open questions: what is the classical limit of a quantum measure? How can the quantum probability calculus, which assigns nontrivial probabilities (between 0 and 1), degenerate into a probability calculus, which classically assigns trivial probabilities (either 0 or 1)? In which sense can the role that the time play in quantum and classical physics be compatible? The list could be much longer and, probably, an answer to those questions could lead to a deeper understanding of quantum mechanics.

Dirac suggested in "Principles of Quantum Mechanics" that "classical mechanics may be regarded as the limiting case of quantum mechanics where \hbar tends to zero". This is the limit performed in the semiclassical approximation (WKB approximation). In analogy with the classical limit of Special Relativity, we would like to perform the limit of an adimensional quantity (which could be something like $\frac{S}{\hbar} \rightarrow \infty$, where S , for the moment, is some physical quantity that has the dimension of an action). So, we might be tempted to characterize a classical problem as the one where the involved actions are large compared to \hbar , while a quantum mechanical problem as the one where the involved actions are smaller or comparable to \hbar . However, with this formulation we fall into a mistake: since the action is an integral, it is determined up to a constant and the action for a single path does not have an absolute meaning. Nonetheless, the difference of the actions for two different paths Γ_1 and Γ_2 does have it: $\Delta S = S(\Gamma_1) - S(\Gamma_2)$ has a unique meaning. Therefore the following formulation is allowed: a classical problem is one where the change of the action ΔS due to a small change in the path is such that $\Delta S \gg \hbar$ while a quantum problem is one in which $\Delta S \sim \hbar$ or smaller.

Now, in eq. (30) we sum over all possible paths, each one contributing with the phase $\frac{S}{\hbar}$, where S is the action of that path. Suppose we consider two paths Γ_1 and Γ_2 whose actions differ by $\pi\hbar$: their contributions will cancel each other, since

$$e^{\frac{i}{\hbar}S(\Gamma_1)} = -e^{\frac{i}{\hbar}S(\Gamma_2)}$$

and they do not contribute to the general sum because of the destructive interference.

Let now Γ_c be the classical path, then, according to the Principle of Least Action, $S(\Gamma_c)$ is extremal and all the nearby paths will have almost the same action. Therefore the main contribution to the propagator comes from a "strip" around the classical path where the action varies slowly and its change is smaller than $\pi\hbar$. Since we have characterized a typical classical problem as one where $\Delta S \gg \hbar$, the strip of constructive interference is very thin while in a quantum problem it is very broad and, consequently, the classical path loses its significance.

4 Path Integrals as Determinants

In this section we will introduce an \hbar expansion for path integrals and show that the computation of the “leading” term in the expansion corresponds to the computation of the determinant of an operator.

4.1 Gaussian integrals

Before doing that, let’s itemize some basic results about Gaussian integrals

i) In one variable, with $\lambda > 0$, we have

$$\int dx e^{-\lambda x^2} = \sqrt{\frac{1}{\lambda}} \int dy e^{-y^2} = \sqrt{\frac{\pi}{\lambda}}$$

ii) Consider the following Gaussian integral in several variables, with $(\hat{\lambda})_{ij} = \lambda_{ij}$ real

$$\int \left(\prod_{i=1}^n dx_i \right) e^{-\sum_{i,j} \lambda_{ij} x_i x_j}$$

We can rotate the eigenbasis

$$x_i = O_{ij} \tilde{x}_j$$

by

$$O^T \hat{\lambda} O = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n) \quad O^T O = O O^T = \mathbb{I}$$

to get

$$\prod_{i=1}^n dx_i = |\det O| \prod_{i=1}^n d\tilde{x}_i = \prod_{i=1}^n d\tilde{x}_i$$

This yields

$$\int \left(\prod_{i=1}^n d\tilde{x}_i \right) e^{-\sum_i \lambda_i \tilde{x}_i^2} = \prod_{i=1}^n \sqrt{\frac{\pi}{\lambda_i}} = \left(|\det\left(\frac{\hat{\lambda}}{\pi}\right)| \right)^{-\frac{1}{2}}$$

iii) Consider an integral with imaginary exponent

$$\int dx e^{i\lambda x^2} = e^{i \text{sgn}(\lambda) \frac{\pi}{4}} \sqrt{\frac{\pi}{\lambda}}$$

iv) Generalizing (iii) with (ii) we get

$$\int \left(\prod_{i=1}^n dx_i \right) e^{i \sum_{i,j} \lambda_{ij} x_i x_j} = e^{i(n_+ - n_-) \frac{\pi}{4}} \left(|\det\left(\frac{\hat{\lambda}}{\pi}\right)| \right)^{-\frac{1}{2}} \quad (41)$$

where n_+ and n_- are the number of positive and negative eigenvalues of $\hat{\lambda}$, respectively.

4.2 Computation of the Feynman Propagator

Let's start by

$$\langle q_f, t_f | q_i, t_i \rangle = \int_{q(t_1)=q_i}^{q(t_2)=q_f} D[q(t)] e^{\frac{i}{\hbar} S([q(t)])} \quad (42)$$

Consider the change of variable

$$q(t) = q_c(t) + y(t) \quad \text{with} \quad y(t_i) = y(t_f) = 0 \quad (43)$$

where $q_c(t)$ is the classical path and the boundary conditions for $y(t)$ follow from $q_c(t_1) = q_i$ and $q_c(t_2) = q_f$. Since, as already noticed for eq. (32), $D[q(t)] = D[y(t)]$, we have

$$\langle q_f, t_f | q_i, t_i \rangle = \int_{y(t_i)=0}^{y(t_f)=0} D[y(t)] e^{\frac{i}{\hbar} S([q_c(t)+y(t)])} \quad (44)$$

We can Taylor expand the action in $y(t)$

$$\begin{aligned} S[q_c(t) + y(t)] &= S[q_c(t)] + \int dt_1 \frac{\delta S}{\delta q(t_1)} \Big|_{q=q_c} y(t_1) \\ &+ \frac{1}{2} \int dt_1 dt_2 \frac{\delta^2 S}{\delta q(t_1) \delta q(t_2)} \Big|_{q=q_c} y(t_1) y(t_2) + O(y^3) \end{aligned}$$

According to the Principle of Least Action, $q_c(t)$ extremizes the action

$$\int dt_1 \frac{\delta S}{\delta q(t_1)} \Big|_{q=q_c} y(t_1) = \int dt \left(\frac{\partial L}{\partial q} \Big|_{q=q_c} y + \frac{\partial L}{\partial \dot{q}} \Big|_{q=q_c} \dot{y} \right) = 0$$

and

$$\int dt_1 dt_2 \frac{\delta^2 S}{\delta q(t_1) \delta q(t_2)} \Big|_{q=q_c} y(t_1) y(t_2) = \int dt \left(\frac{\partial^2 L}{\partial q^2} \Big|_{q=q_c} y^2 + \frac{\partial^2 L}{\partial q \partial \dot{q}} \Big|_{q=q_c} y \dot{y} + \frac{\partial^2 L}{\partial \dot{q}^2} \Big|_{q=q_c} \dot{y}^2 \right) \quad (45)$$

Thus eq. (44) becomes

$$\langle q_f, t_f | q_i, t_i \rangle = \int D[y(t)] e^{\frac{i}{\hbar} [S([q_c(t)] + \frac{1}{2} \frac{\delta^2 S}{\delta q^2} y^2 + O(y^3))]} \quad (46)$$

where $\frac{\delta^2 S}{\delta q^2} y^2$ is just a short hand for the second variation of S , shown in eq. (45). The physical interpretation of eq. (46) is that the propagator can be decomposed into two pieces

- i) The classical trajectory $q_c(t)$ gives the exponential term $e^{\frac{i}{\hbar} S([q_c(t)])}$.
- ii) The fluctuation $y(t)$, over which we must integrate, represents the quantum fluctuations around the classical path.

Eq. (46) turns out to be an expansion of the path integral in \hbar , a semiclassical expansion. This can be shown more explicitly by the rescaling $y = \sqrt{\hbar} \tilde{y}$

$$\begin{aligned} \langle q_f, t_f | q_i, t_i \rangle &= N e^{\frac{i}{\hbar} S([q_c(t)])} \int D[\tilde{y}(t)] e^{\frac{1}{2} \frac{\delta^2 S}{\delta q^2} \tilde{y}^2 + O(\sqrt{\hbar} \tilde{y}^3)} \\ &= N e^{\frac{i}{\hbar} S([q_c(t)])} \int D[\tilde{y}(t)] e^{\frac{1}{2} \frac{\delta^2 S}{\delta q^2} \tilde{y}^2} \left(1 + \frac{i\sqrt{\hbar}}{3!} \frac{\delta^3 S}{\delta q^3} \tilde{y}^3 + O(\hbar) \right) \\ &= N e^{\frac{i}{\hbar} S([q_c(t)])} \int D[\tilde{y}(t)] e^{\frac{1}{2} \frac{\delta^2 S}{\delta q^2} \tilde{y}^2} (1 + O(\hbar)) \end{aligned} \quad (47)$$

where N is the Jacobian of the rescaling and we have used the fact that the leading $\hbar^{\frac{1}{2}}$ correction vanishes because the integrand is odd under $\tilde{y} \rightarrow -\tilde{y}$.

For a general system, an exact evaluation of eq. (42) is certainly too much to hope for. Indeed, even in the finite dimensional case, integrals of exponentials of elementary functions can typically be evaluated exactly only in purely quadratic (Gaussian, Fresnel) cases; while more general integrals are then evaluated ‘‘perturbatively’’.

Let’s focus now on a special case: the quadratic Lagrangian.

$$L(q, \dot{q}, t) = a(t)\dot{q}^2 + b(t)q\dot{q} + c(t)q^2 + d(t)\dot{q} + e(t)q + f(t)$$

which still covers many interesting systems: the free particle, the harmonic oscillator, the forced oscillator, etc.

A quadratic Lagrangian can be defined by the property

$$\frac{\delta^{(n)} S}{\delta q^{(n)}} = 0 \quad \text{for} \quad n > 2$$

For these Lagrangians, eq. (47) becomes exactly

$$\langle q_f, t_f | q_i, t_i \rangle = e^{\frac{i}{\hbar} S[q_c(t)]} \int D[y(t)] e^{\frac{i}{2\hbar} \frac{\delta^2 S}{\delta q^2} y^2} = \text{const} e^{\frac{i}{\hbar} S[q_c(t)]} \left(\left| \det \frac{\delta^2 S}{\delta q^2} \right| \right)^{-\frac{1}{2}} \quad (48)$$

where the last equality comes from eq. (41).

4.3 Free Particle Propagator and Normalization Constant

Let's compute the propagator for a free particle: $L = \frac{1}{2}m\dot{q}^2$

$$\langle q_f, t_f | q_i, t_i \rangle = e^{\frac{i}{\hbar} S_{cl}} \int D[y(t)] e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt \frac{1}{2} m \dot{y}^2}$$

The action for the classical path is

$$S_{cl} = S[q_c(t)] = \frac{1}{2} m \frac{(q_f - q_i)^2}{t_f - t_i}$$

In order to solve the integral, we note that

$$i \int_{t_i}^{t_f} dt \frac{m}{2\hbar} \dot{y}^2 = i \int_{t_i}^{t_f} dt \frac{m}{2\hbar} \frac{d}{dt} (y\dot{y}) - i \int_{t_i}^{t_f} dt \frac{m}{2\hbar} y \left(\frac{d^2}{dt^2} \right) y = i \int_{t_i}^{t_f} dt y \hat{O} y$$

where $\hat{O} = -\frac{m}{2\hbar} \frac{d^2}{dt^2}$ and the last equality follows from the boundary conditions (43). We shall solve the eigenvalue problem for the operator \hat{O}

$$\begin{aligned} \hat{O} y_n = \lambda_n y_n & \implies y_n = \sqrt{\frac{2}{T}} \sin\left(\frac{n\pi}{T}(t - t_i)\right) \\ \lambda_n &= \frac{m n^2 \pi^2}{2\hbar T^2} \\ \int_{t_i}^{t_f} dt y_n y_m &= \delta_{nm} \end{aligned}$$

where $T = t_f - t_i$ and $n \in \mathbb{N} \setminus \{0\}$; notice that all the eigenvalues are positive. The $\{y_n\}$ form a complete basis of the Hilbert space $L^2([t_i, t_f])$, with $y(t_i) = y(t_f) = 0$, thus a generic path $y(t)$ can be expanded as $y(t) = \sum_{n=1}^{\infty} a_n y_n(t)$, which yields

$$\int_{t_i}^{t_f} dt y \hat{O} y = \sum_{n,m} a_n a_m \int_{t_i}^{t_f} dt y_m \hat{O} y_m = \sum_n \lambda_n a_n^2$$

The integration over all possible paths $y(t)$ can thus be performed using the a_n as a discrete set of integration variables, and we can write

$$D[y(t)] = c \prod_{n=1}^{\infty} a_n \quad (49)$$

where c is a normalization factor (it plays the role of a kind of Jacobian). It is important to stress that c cannot depend on the particular system considered (it

will be fixed later and it will be shown that it depends just on m , t_i and t_f). Finally we can write

$$\langle q_f, t_f | q_i, t_i \rangle = e^{\frac{i}{\hbar} S_{cl}} c \int \left(\prod_{n=1}^{\infty} da_n \right) e^{i \sum_n \lambda_n a_n^2} = e^{\frac{i}{\hbar} S_{cl}} c \left(\det \left(\frac{\hat{O}}{\pi i} \right) \right)^{-\frac{1}{2}} \quad (50)$$

The determinant of an operator is the product of its eigenvalues, so we get

$$\det \left(\frac{\hat{O}}{\pi i} \right) = \prod_{n=1}^{\infty} \frac{m n^2 \pi}{2i\hbar T^2}$$

This is clearly infinite, and thus $(\det(\frac{\hat{O}}{\pi i}))^{-\frac{1}{2}}$ is zero, but this will be compensated by the infinite normalization constant c : its presence in eq. (49) is essential. In order to fix the normalization constant, and, therefore, to find the expression of the propagator for the free particle, let's consider the following equality, given by eqs. (30), (49), and (41)

$$\begin{aligned} \int_{y(t_i)=0}^{y(t_f)=0} D[y(t)] e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt \frac{1}{2} m \dot{y}^2} &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} \int \left(\prod_{k=1}^{N-1} dy_k \right) e^{\frac{i}{\hbar} \frac{m}{2} \sum_{k=0}^{N-1} \frac{(y_{k+1} - y_k)^2}{\epsilon}} \\ &= c \int \left(\prod_{k=1}^{\infty} da_k \right) e^{i \sum_{k=1}^{\infty} \lambda_k a_k^2} = c \left(\det \left(\frac{\hat{O}}{\pi i} \right) \right)^{-\frac{1}{2}} \end{aligned} \quad (51)$$

Noting that $y_N = y_0 = 0$, we can write

$$\sum_{k=0}^{N-1} (y_{k+1} - y_k)^2 = y_N^2 + 2y_N y_{N-1} + y_{N-1}^2 + \cdots + y_1^2 + 2y_1 y_0 + y_0^2 = \sum_{j,k=1}^{N-1} y_j A_{jk} y_k$$

where A_{jk} are the elements of the $(N-1) \times (N-1)$ matrix \hat{A}

$$\hat{A} = \begin{pmatrix} 2 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & -1 & 2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 2 & -1 \\ 0 & 0 & 0 & \dots & -1 & 2 \end{pmatrix}$$

Thus the second expression in eq. (51) can be solved as a Gaussian integral

$$\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N}{2}} \int \left(\prod_{k=1}^{N-1} dy_k\right) e^{i\frac{m}{2\epsilon\hbar} \sum_{j,k=1}^{N-1} y_j A_{jk} y_k} = \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N}{2}} \left(\det\left(\frac{\hat{A}m}{2\pi i\hbar\epsilon}\right)\right)^{-\frac{1}{2}} \quad (52)$$

In order to evaluate $\det(\hat{A})$ it is straightforward to prove the following recursive formula

$$\det(\hat{a}_n) = 2 \det(\hat{a}_{n-1}) - \det(\hat{a}_{n-2})$$

where \hat{a}_n is the n^{th} leading principal minor of the matrix \hat{A} . Using $\det(\hat{a}_1) = 2$ and $\det(\hat{a}_2) = 3$, one gets $\det(\hat{a}_n) = n + 1$.

By $\hat{A} = \hat{a}_{N-1}$

$$\det(\hat{A}) = N$$

The normalization constant is fixed by eq. (51) and (52)

$$c = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N}{2}} \left(\det\left(\frac{\hat{A}m}{2\pi i\hbar\epsilon}\right)\right)^{-\frac{1}{2}} \left(\det\left(\frac{\hat{O}}{\pi i}\right)\right)^{\frac{1}{2}} = \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} \left(\det\left(\frac{\hat{O}}{\pi i}\right)\right)^{\frac{1}{2}} \quad (53)$$

As already mentioned, the normalization constant c does not depend on the particular system (free particle) from which it has been derived: now that it has been fixed, expression (53) can be used to derive the propagator for a generical system using the determinant method, through eq. (50). Finally, the Feynman propagator for the free particle is

$$\langle q_f, t_f | q_i, t_i \rangle = \sqrt{\frac{m}{2\pi i\hbar(t_f - t_i)}} e^{i\frac{m}{\hbar} \frac{(q_f - q_i)^2}{2(t_f - t_i)}} \quad (54)$$

5 Interaction with an External Electromagnetic Field and Quantum Gauge Invariance

The quantum mechanics of a charged non-relativistic particle interacting with an external electromagnetic field (that is, a field produced by some macroscopic system whose quantum fluctuation are negligible), in the path integral formalism, is obtained by substituting in the Feynman Propagator (30) the action (7)

$$K(x_f, t_f; x_i, t_i) = \int_{x_i}^{x_f} D[x(t)] e^{\frac{i}{\hbar}(S_0 + S_{int})} = \int_{x_i}^{x_f} D[x(t)] e^{\frac{i}{\hbar}(\int_{t_i}^{t_f} \frac{1}{2}m\dot{x}^2 - \int_{(x_i, t_i)}^{(x_f, t_f)} A_\mu dx^\mu)} \quad (55)$$

We shall now study what happens to gauge invariance upon quantization.

5.1 Quantum Gauge Invariance

Performing a gauge transformation, the action changes by eq. (8), and eq. (55) gives

$$\begin{aligned} K(x_f, t_f; x_i, t_i) \rightarrow K'(x_f, t_f; x_i, t_i) &= \int_{x_i}^{x_f} D[x(t)] e^{\frac{i}{\hbar}S - \frac{ie}{\hbar} \int_{(x_i, t_i)}^{(x_f, t_f)} \partial_\mu \Lambda dx^\mu} \\ &= e^{-\frac{ie}{\hbar} \Lambda(x_f, t_f)} K(x_f, t_f; x_i, t_i) e^{\frac{ie}{\hbar} \Lambda(x_i, t_i)} \end{aligned} \quad (56)$$

Consequently the Feynman Propagator is not gauge invariant. Imposing the gauge covariance of eq. (24), the probability amplitude has to change

$$\psi(x, t) \rightarrow \psi'(x, t)$$

Under a gauge transformation, by eqs. (24) (56) we get

$$\begin{aligned} \psi'(x_f, t_f) &= \int K'(x_f, t_f; x_i, t_i) \psi'(x_i, t_i) dx_i \\ &= \int e^{-\frac{ie}{\hbar} \Lambda(x_f, t_f)} K(x_f, t_f; x_i, t_i) e^{\frac{ie}{\hbar} \Lambda(x_i, t_i)} \psi'(x_i, t_i) dx_i \end{aligned}$$

which can be expressed as

$$e^{\frac{ie}{\hbar} \Lambda(x_f, t_f)} \psi'(x_f, t_f) = \int K(x_f, t_f; x_i, t_i) e^{\frac{ie}{\hbar} \Lambda(x_i, t_i)} \psi'(x_i, t_i) dx_i \quad (57)$$

Comparing eq. (24) and eq. (57)

$$\psi(x, t) = e^{\frac{ie}{\hbar} \Lambda(x, t)} \psi'(x, t)$$

Therefore the wave function transforms as

$$\psi(x, t) \rightarrow \psi'(x, t) = e^{-\frac{ie}{\hbar}\Lambda(x, t)}\psi(x, t) \quad (58)$$

The square of the norm $|\psi(x, t)|^2$ which, according to the Copenhagen interpretation, represents a probability density and is the only physically measurable quantity associated to the wave function, remains unchanged by a gauge transformation. Hence, quantum mechanically too, all 4-potentials, differing by a gauge transformation, represent the same physical state.

In order to study the transformations of the generalized momentum p and the hamiltonian H , we shall proceed recalling eq. (18) since it holds within the path integral formalism, as shown in Section 3.3. Considering (x_i, t_i) fixed, under a gauge transformation the action transforms as

$$S \rightarrow S' = S - e\Lambda(x, t)$$

being the term $\Lambda(x_i, t_i)$ constant it is inessential and it has not been reported. From eq. (18) we get

$$p'_\mu = -\partial_\mu S'$$

and thus

$$p'^i = p^i - e\partial_i\Lambda(x, t) \quad H' = H + e\partial_t\Lambda(x, t) \quad (59)$$

The canonical commutation relations are preserved

$$[\hat{x}, \hat{p}] \rightarrow [\hat{x}', \hat{p}'] = [\hat{x}', \hat{p} - e\partial_i\Lambda(\hat{x}, t)] = i\hbar\mathbb{I} \quad (60)$$

Finally we shall note that while the generalized momentum p is not gauge invariant the kinetic momentum Π

$$\Pi^i = \frac{\partial S_0}{\partial x_i} = p^i - eA^i$$

(where S_0 is the free particle action given by (7)) is gauge invariant

$$\Pi^i = p^i - eA^i \rightarrow \Pi'^i = p'^i - eA'^i = p^i - eA^i - e\partial_i\Lambda + e\partial_i\Lambda = \Pi^i$$

6 The Aharonov-Bohm effect

In classical electrodynamics the 4-potential A^μ is introduced as a convenient, but still not needful, mathematical tool, as all the fundamental equations can be expressed in terms of $F^{\mu\nu}$. In quantum mechanics, as established before, this is no more the case: potentials cannot be eliminated from the basic equations. The gauge transformation is a physical symmetry both in quantum mechanical and classical electrodynamics: according to this analogy, one could suggest that also in quantum mechanics the 4-potential itself has no independent physical meaning. Such conclusion is not completely correct, as firstly suggested by Aharonov and Bohm, because the analogy between classical and quantum-mechanical electrodynamics cannot be extended much further. Let's consider a charged particle moving in a field free region of the space, and impose $F^{\mu\nu} \neq 0$ in some region of the space R which the particle cannot enter. Classically, the particle moves freely because, according to eq. (3), no force acts on it. For a quantum mechanical description, instead, we have to look at the 4-potential. Since $F^{\mu\nu} \neq 0$ in R , A^μ , for continuity, is different from zero even in regions which the particle can enter. In this situation, as it will be shown in this Section, the quantum charge does not behave as a free particle any more. This measurable effect, which has no classical analog, is the Aharonov-Bohm effect.

6.1 The Thought Experiment and Topological Properties of the Space

Let's consider the following thought experiment (Figure 1): a double slit experiment with a solenoid beyond the slits.

The solenoid is modeled as an infinitely long and empty cylindrical shell, such that particles do not have access to its interior (let M be the space between B and C which the particle can enter). Inside the solenoid there is a constant magnetic field $\vec{B} \neq 0$. Outside, instead, $\vec{B} = 0$: this is a consequence of having taken an infinitely long solenoid. Since $\nabla \cdot \vec{B} = 0$, the magnetic field lines have to be closed. If the cylinder is finite the field lines, in order to shut, make edge effects and we have $\vec{B} \neq 0$ outside the solenoid. If we take it infinitely long, instead, this does not happen because the field lines shut at infinite.

Stoke's theorem implies $\vec{A} \neq 0$ outside the solenoid, in fact

$$\int_{\partial\Sigma} \vec{A} \cdot d\vec{x} = \Phi_B := \int_{\Sigma} \vec{B} \cdot d\vec{\Sigma}$$

where Σ is a surface that intersects the cylinder, $\partial\Sigma$ is its border and Φ_B is the total magnetic flux in the solenoid. The electric field is zero everywhere, so we take $A^0 = 0$. For the presence of the infinitely long solenoid, the topology of M

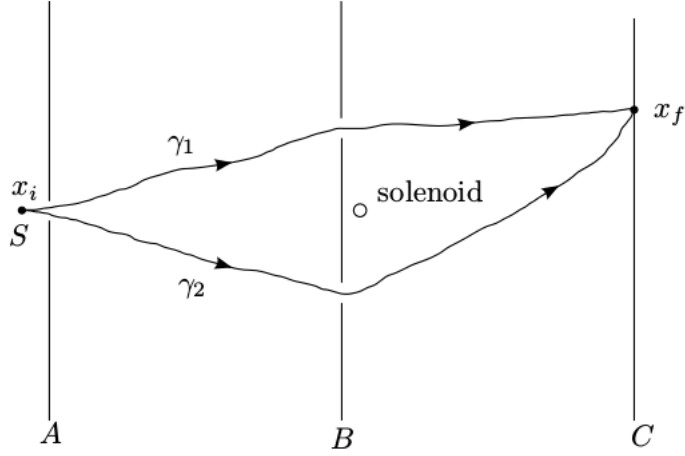


Figure 1: Double slit apparatus, with a solenoid beyond the slits.

is not trivial: it is multiply connected, since a closed curve around the solenoid is not homotopic⁴ to a point of M .

The condition that the electrons are confined in M , in the path integral approach, corresponds to summing only on the paths that do not pass through the interior of the cylinder. The topology of M implies that different paths may belong to different homotopy classes: a path encircling the solenoid n numbers of times cannot be continuously deformed into one encircling it m numbers of times ($n \neq m$). For each slit, the various non-homotopic configurations can be classified with the winding number n ($n \in \mathbb{Z}$): $K_n^i(x_f, t_f; x_i, t_i)$ is the partial amplitude, referred to the i -th slit ($i \in \{1, 2\}$), calculated by summing over all possible paths within the n -th homotopy class.

The Feynman propagator is given by

$$K(x_f, t_f; x_i, t_i) = \sum_n K_n^1(x_f, t_f; x_i, t_i) + \sum_n K_n^2(x_f, t_f; x_i, t_i) \quad (61)$$

⁴Let $\alpha, \beta: [a, b] \rightarrow \mathbb{R}^n$ be two circuits. We say that α and β are *homotopic* if there exists a continuous map $h: [a, b] \times [0, 1] \rightarrow \mathbb{R}^n$ such that

- $h(t, 0) = \alpha(t), h(t, 1) = \beta(t) \forall t \in [a, b]$
- $h(a, \lambda) = h(b, \lambda) \forall \lambda \in [0, 1]$

6.2 The Aharonov Bohm Effect

According to eq. (61), the Feynman Propagator is given by a sum over all possible homotopy classes. As established in Section (3.4), however, the main contribution will be given by some of the paths belonging to the homotopy class with winding number $n = 0$. The other homotopy classes, in fact, contribute with paths that are exotic from a semi-classical point of view and their probability amplitude is negligible; for simplicity we will take into account only $K_0^1(x_f, t_f; x_i, t_i) \equiv K^1(x_f, t_f; x_i, t_i)$ and $K_0^2(x_f, t_f; x_i, t_i) \equiv K^2(x_f, t_f; x_i, t_i)$ and eq. (61) will be approximated as

$$K(x_f, t_f; x_i, t_i) = K^1(x_f, t_f; x_i, t_i) + K^2(x_f, t_f; x_i, t_i) \quad (62)$$

When the solenoid is off, $\vec{A} = 0$: the action of the system is the free particle action S_0

$$K(x_f, t_f; x_i, t_i) = \int_1 D[x] e^{\frac{i}{\hbar} S_0} + \int_2 D[x] e^{\frac{i}{\hbar} S_0} = \phi_0^1(x_f) + \phi_0^2(x_f)$$

For the symmetry of the problem, $\phi_0^1(x_f)$ and $\phi_0^2(x_f)$ can differ only for a phase

$$\phi_0^1(x_f) = C e^{\frac{i}{\hbar} \theta_1} \quad \phi_0^2(x_f) = C e^{\frac{i}{\hbar} \theta_2}$$

The interference pattern on the screen is given by the modulus squared of the propagator, *i.e.* from the probability

$$\begin{aligned} |K(x_f, t_f; x_i, t_i)|^2 &= |\phi_0^1(x_f) + \phi_0^2(x_f)|^2 = |\phi_0^1(x_f)|^2 + |\phi_0^2(x_f)|^2 + 2\text{Re}(\overline{\phi_0^1(x_f)} \phi_0^2(x_f)) \\ &= 2C^2 \left(1 + \cos\left(\frac{\theta_2 - \theta_1}{\hbar}\right) \right) = 4C^2 \cos^2\left(\frac{\theta_2 - \theta_1}{2\hbar}\right) \end{aligned} \quad (63)$$

If we light on the solenoid, the system is described by the action eq.(7). The propagator is

$$\begin{aligned} K(x_f, t_f; x_i, t_i) &= \int_1 D[x] e^{\frac{i}{\hbar} S_0 - \frac{i}{\hbar} e \int_1 A^\mu dx^\mu} + \int_2 D[x] e^{\frac{i}{\hbar} S_0 - \frac{i}{\hbar} e \int_2 A^\mu dx^\mu} \\ &= e^{\frac{i}{\hbar} e \int_1 A^i dx^i} \phi_0^1(x_f) + e^{\frac{i}{\hbar} e \int_2 A^i dx^i} \phi_0^2(x_f) \end{aligned} \quad (64)$$

where the last term is a consequence of Stoke's theorem: $\int A^i dx^i$ is the same for every trajectory in a given homotopy class.

The phase difference introduced by the interaction with A^μ is

$$\Delta\varphi = \frac{e}{\hbar} \left(\int_2 A^i dx^i - \int_1 A^i dx^i \right) = \frac{e}{\hbar} \oint_{2-1} A^i dx^i = \frac{e}{\hbar} \Phi_B$$

thus we have

$$K(x_f, t_f; x_i, t_i) = e^{\frac{i}{\hbar}e \int_1 A^i dx^i} (\phi_0^1(x_f) + e^{i\frac{e}{\hbar}\Phi_B} \phi_0^2(x_f)) \quad (65)$$

and the probability is

$$\begin{aligned} |K(x_f, t_f; x_i, t_i)|^2 &= |\phi_0^1(x_f)|^2 + |\phi_0^2(x_f)|^2 + 2\text{Re}(\overline{\phi_0^1(x_f)} e^{i\frac{e}{\hbar}\Phi_B} \phi_0^2(x_f)) \\ &= 2C \left(1 + \cos\left(\frac{\theta_2 - \theta_1}{\hbar} + \frac{e}{\hbar}\Phi_B\right) \right) = 4C \cos^2\left(\frac{\theta_2 - \theta_1}{2\hbar} + \frac{e}{2\hbar}\Phi_B\right) \end{aligned} \quad (66)$$

Comparing eq. (63) and eq. (66), it follows that the effect of the solenoid on the charge is a shift of the interference pattern, as the phase difference transforms as

$$\frac{\theta_2 - \theta_1}{\hbar} \rightarrow \frac{\theta_2 - \theta_1}{\hbar} + \frac{e}{\hbar}\Phi_B$$

therefore as Φ_B varies, the peaks of the interference pattern are shifted and this is an observable effect. This effect is periodic in the flux Φ_B , with period Φ_0 given by

$$\frac{e}{\hbar}\Phi_0 = 2\pi \implies \Phi_0 = \frac{2\pi\hbar}{e} \quad (67)$$

7 Conclusions

The previous discussion leads to the conclusion that a quantum charged particle can feel an electromagnetic interaction even though it has no access to regions in which $F^{\mu\nu} \neq 0$: in a field free multiply connected region the physical properties of the system depend on the 4-potential.

The Aharonov-Bohm effect is purely quantum mechanical. Classically, as the particle can never enter the region in which $F^{\mu\nu} \neq 0$, the Lorentz force is identically zero and the particle moves freely. The reason is that the 4-potential contributes with a phase factor, as in eq. (65), and this can be described only taking into account the quantum nature of the system. In quantum mechanics the essential difference is that the equations of motion of the particle are replaced by the Feynman Propagator, as in eq. (55). The Lorentz equation is not anymore a fundamental equation, but is an approximation holding in the classical limit.

Observe that the phase difference due to the 4-potential occurs only if we consider two paths belonging to different homotopy classes; as already established in eq. (64), according to Stoke's theorem, the integral $\int A^\mu dx_\mu$ is the same for two paths which can be continuously deformed into each other. In this sense, the Aharonov-Bohm effect is a topological effect: it occurs if the topology of the space is not trivial.

Aharonov and Bohm proposed two possible interpretation of this effect. One may explain it by introducing a non-local interaction between the charge and $F^{\mu\nu}$, however this analysis leads to inconsistencies from a relativistic point of view because, according to Einstein Special Relativity, all field interactions must be local. The second one, which is the best accredited in literature, gives an independent physical meaning to A^μ , interpreting its presence in the Lagrangian (6) not as a purely mathematical need, but as a physical symptom of the fact that the charge interacts with A^μ rather than with $F^{\mu\nu}$. In this way the particle interacts locally with the 4-potential and there is no contradiction with Einstein Relativity.

The gauge invariance of the theory implies that, even if the physical state of a system is fully specified, the 4-potential is not univocally determined, *i.e.* A^μ and $A'^\mu = A^\mu + \partial^\mu \Lambda$ are equivalent. This means that A^μ cannot be measured itself, but we can measure only gauge invariant combination of the 4-potential: certainly $F^{\mu\nu}$ is an example of this, but it is not the only one. According to eq. (65), the interference pattern depends on a phase difference given by the integral of the 4-potential $\oint A^\mu dx_\mu$. This integral, being gauge invariant, is measurable and it is not subject to arbitrariness. To be precise, just as $F^{\mu\nu}$ underdescribes quantum mechanical electrodynamics (different physical situation in a region may have the same $F^{\mu\nu}$ in that region), the phase $\Delta\varphi = \frac{e}{\hbar} \oint A^\mu dx_\mu$ overdescribes it since, according to eq. (67), the Aharonov Bohm effect is periodic. A complete description is given by the term $e^{i\Delta\varphi} = e^{i\frac{e}{\hbar} \oint A^\mu dx_\mu}$

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