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A generalization of Fermat's principle for classical and quantum systems

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A B S T R A C T

The analogy between dynamics and optics had a great influence on the development of the foundations of classical and quantum mechanics. We take this analogy one step further and investigate the validity of Fermat's principle in many-dimensional spaces describing dynamical systems (i.e., the quantum Hilbert space and the classical phase and configuration space). We propose that if the notion of a metric distance is well defined in that space and the velocity of the representative point of the system is an invariant of motion, then a generalized version of Fermat's principle will hold. We substantiate this conjecture for time-independent quantum systems and for a classical system consisting of coupled harmonic oscillators. An exception to this principle is the configuration space of a charged particle in a constant magnetic field; in this case the principle is valid in a frame rotating by half the Larmor frequency, not the stationary lab frame.

1. Introduction

An important lesson that has been emphasized throughout the history of physics is that illuminating new aspects of the interwoven connections between geometry and physics leads to paradigm shifts in physics. Typically, novel geometric considerations of physical quantities lead to new variational principles which assign the natural evolution of physical systems with an extremum of some functional or a geodesic curve in some hyperspace. The oldest of these variational principles is the Fermat principle of least time, which became a fundamental principle in geometric optics. The principle was introduced by Fermat, who also called it *the principle of natural economy* [1], and it states that light rays travel in a general medium along the path that minimizes the time taken to travel between the initial and final destinations. The concept of natural economy inspired Maupertuis to introduce the principle of least action in analytical mechanics, which later evolved through the work of Euler, Lagrange, Hamilton, and Jacobi to become a fundamental concept in classical mechanics. By 1887, it had become clear that the least action is a universal concept in physics when Helmholtz expanded its domain of validity by applying it to two regimes beyond the standard problems of classical mechanics, namely, thermodynamics and electrodynamics [2]. Since then, the pursuit of new variational principles in physics has not relented [3].

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The mathematical formulation of Fermat's principle states that the time functional $\mathcal{T}$, defined as

$$\mathcal{T} = \int \frac{ds}{v(s)}, \qquad (1)$$

where $v(s)$ is the speed of light and ds is the distance element along the light trajectory, is minimized [4]. In other words, if $\mathcal{T}$ is computed along all possible trajectories between fixed initial and final positions, $\mathcal{T}$ will always be minimum along the actual path traveled by the light rays (the physical path). The modern version of Fermat's principle is written in terms of the index of refraction $n(s) = \frac{c}{v(s)}$, where c is the speed of light in free space, and states that the optical path length $\int n(s)ds$ is a minimum. In that sense, Fermat's principle is the optical analog of Jacobi's principle of least action [5], which states that for a conservative classical system at energy E, with potential function V between its constituent particles, the action functional

$$I = \int \sqrt{E - V(s)}\,ds \qquad (2)$$

is an extremum.

The remarkable property of this action that distinguishes it from other variational principles in analytical mechanics, i.e., Hamilton and Lagrange's variational principles, is that it represents a purely geometric quantity. This quantity is computed along different trajectories in the configuration space between fixed points without referring to any time evolution. Therefore, Eq. (2) can be used to define a new Riemannian space, whose metric

$ds' = \sqrt{E - V(s)}ds$, where the natural evolution of the representative point of the system is along geodesic curves.

In this work, we set out to seek how far the analogy between dynamics and optics applies as far as the Fermat principle is concerned. In particular, we investigate the validity of Fermat's principle for a generic many-body classical and quantum system, and pose the following question: If the state of a conservative dynamical system is represented in some metric space $\mathbb{S}$ by a point, and the velocity field $\nu(s)$ is computed everywhere in $\mathbb{S}$ from the equations of motion using the proper metric of that space, will the motion of this point be along a path that extremizes the time functional $\mathcal{T}$?

2. The generalized Fermat principle

We answer the question posed above by proposing the *generalized Fermat principle* (GFP): Whenever the speed of the representative point of a conservative dynamical system, $\nu(s)$, is an integral of motion in a metric space $\mathbb{S}$, the path followed during the dynamical evolution of that system in $\mathbb{S}$ between fixed initial and final states makes the time functional $\mathcal{T}$ stationary against small variations of the path. In contrast to light rays, where $\mathcal{T}$ is an extremum even when the speed of light is not constant (i.e., in an inhomogeneous medium), this conjecture considers only the case when $\nu(s)$ is invariant during the time evolution. A corollary that follows from this conjecture is that the length of the physical path $\int ds$ is stationary (e.g., the path can be a geodesic) on the submanifold of a given value of $\nu(s)$ embedded in $\mathbb{S}$ when the above condition is fulfilled.

Mathematically speaking, the GFP states that if $\nu(s)$ is a constant of motion along the physical path (not necessarily in the whole space), then among all possible trajectories between initial and final states, only those which make $\mathcal{T}$ invariant under an infinitesimal variation of the path, i.e.,

$$\delta\mathcal{T} = 0, \tag{3}$$

are possible candidates for the dynamical evolution. The value of $\mathcal{T}$ corresponding to the physical path is not necessarily the global minimum between all paths connecting the initial and final states. We emphasize here that we are not aiming to derive the equations of motion from the time action, because we have to use them to find $\nu(s)$ in the first place. We rather propose that they necessarily lead to a stationary time action when $\nu(s)$ is an integral of motion. Unlike the original Fermat principle, not every pair of states are connected by a physical path. Rather, the principle proposed here gives a geometrically appealing argument to explain why the evolution of the system followed a certain trajectory between a given pair of initial and final states which we know a priori are connected by some physical path.

We investigate the validity of this conjecture by considering three cases: (i) The evolution of quantum systems in the projective Hilbert space $\mathbb{P}$, where wavefunctions are defined up to an overall phase factor. (ii) The evolution of a system of coupled harmonic oscillators in the phase space consisting of coordinates and momenta and equipped with a Euclidean metric. (iii) The motion of a charged particle in a constant magnetic field, which turns out to be an exception. Similar to the Jacobi's principle, the principle proposed here represents a geometric variational principle in the phase and Hilbert spaces. In both cases, the velocity field $\nu(s)$ is defined completely by the Hamiltonian of the problem, and is obtained from the equations of motion of the system that will drive its evolution along the physical path (i.e., Schrödinger equation in quantum systems and Hamilton's equations of motion in classical systems).

2.1. Generalized Fermat principle in Hilbert space

The development of the concept of geometric phase in quantum mechanics triggered the interest of many physicists to look for more connections between quantum mechanics and geometry [6]. Anandan and Aharonov investigated the nature of the geometry of quantum evolution in the projective Hilbert space $\mathbb{P}$ through a series of papers in the late 80s [7–9]. They have shown [8] that the speed of quantum evolution in $\mathbb{P}$ is related to the energy uncertainty $\Delta E = (\langle H^2\rangle - \langle H\rangle^2)^{1/2}$ via

$$ds = \Delta E\, dt/\hbar, \tag{4}$$

where ds is the infinitesimal distance in $\mathbb{P}$ given by the Fubini–Study (FS) metric $ds^2 = \frac{\langle\delta\psi|\delta\psi\rangle}{\langle\psi|\psi\rangle} - \frac{|\langle\delta\psi|\psi\rangle|^2}{\langle\psi|\psi\rangle^2}$. On the unit sphere, $ds = \langle\delta\psi|1 - \hat{P}|\delta\psi\rangle^{\frac{1}{2}}$, where $\hat{P}$ is the projection operator $|\psi\rangle\langle\psi|$. The trajectory traversed by a ray in $\mathbb{P}$ under unitary evolution is generally not a geodesic, i.e., $\delta\int ds \neq 0$. This can be easily conceived by considering a system composed of a single quantum spin-1/2. In this case, $\mathbb{P}$ is simply the Bloch sphere and the precession motion of the spin on Bloch sphere off the equator is not a geodesic.

Several attempts [10,11] have been made to find new formulations where the quantum evolution is a geodesic flow. Noticing that the speed of quantum evolution $\Delta E/\hbar$ is invariant for time-independent Hamiltonians, the simple answer to this problem suggested by the present paper is to consider $\mathcal{T} = \int \frac{ds}{\Delta E}$ as a geodesic quantity, i.e., *Fermat's principle in Hilbert space* (here and in what follows, we set $\hbar = 1$). This issue should be distinguished from the quantum brachistochrone problem [12], where the Hamiltonian that leads to optimal time evolution between an initial and final state is sought. The above proposition, however, states that the unitary evolution generated by any time-independent Hamiltonian is optimal, with respect to all other possible trajectories connecting the initial and final states (Fig. 1a).

To show that $\mathcal{T}$ is stationary along the physical path through $\mathbb{P}$, let us parameterize the evolution along any path connecting the initial and final states $|\psi_i\rangle$ and $|\psi_f\rangle$ by some arbitrary parameter τ. We can write Eq. (1) as

$$\mathcal{T} = \int_{|\psi_i\rangle}^{|\psi_f\rangle} d\tau \frac{\langle\dot{\psi}|1 - \hat{P}|\dot{\psi}\rangle^{\frac{1}{2}}}{(\langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2)^{\frac{1}{2}}}, \tag{5}$$

where $|\dot{\psi}\rangle = \frac{|\delta\psi\rangle}{\delta\tau}$. Taking the variational derivative of $\mathcal{T}$ with respect to $\langle\delta\psi|$ subject to the constraints of normalization and fixed initial and final states, we arrive at the Euler–Lagrange (EL) equation,

$$\frac{\delta L}{\langle\delta\psi|} - \frac{d}{d\tau}\frac{\delta L}{\langle\delta\dot{\psi}|} = 0, \tag{6}$$

where L is the integrand in Eq. (5) added to the Lagrange multiplier term $\lambda(\tau)(\langle\psi|\psi\rangle - 1)$. Although we have already imposed the normalization condition in the Fubini–Study metric, we use the Lagrange-multiplier method here to ensure that the variations of the path will respect the conservation of the norm of $|\psi\rangle$. Calling the numerator and denominator in Eq. (5), A and B respectively, Eq. (6) reads

$$\begin{aligned}
&\left[\frac{-1}{2AB}\langle\dot{\psi}|\psi\rangle|\dot{\psi}\rangle - \frac{A}{2B^3}\big(H^2|\psi\rangle - 2\langle H\rangle H|\psi\rangle\big)\right] \\
&\quad - \frac{1}{2AB}\big[|\ddot{\psi}\rangle - \langle\psi|\dot{\psi}\rangle|\dot{\psi}\rangle - \big(\langle\dot{\psi}|\dot{\psi}\rangle + \langle\psi|\ddot{\psi}\rangle\big)|\psi\rangle\big] \\
&\quad - \frac{1}{2}\big(|\dot{\psi}\rangle - \langle\psi|\dot{\psi}\rangle|\psi\rangle\big)
\end{aligned}$$