Generalized Fermat Principle for Classical and Quantum Systems

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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 classical phase 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 of coupled harmonic oscillators.

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 reconsiderations of geometric quantities in physics 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 \([3]\).

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

\[
\mathcal{T} = \int_{s_i}^{s_f} \frac{ds}{\nu(s)},
\]

where \(\nu(s)\) 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 initial and final positions \(s_i, s_f\), \(\mathcal{T}\) 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 \(n(s) = \frac{c}{\nu(s)}\), where \(c\) is the speed of light in free space and states that the optical path length \(\int_{s_i}^{s_f} n(s)\,ds\) 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

\[
I = \int_{s_i}^{s_f} \sqrt{E - V(s)}\,ds
\]

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 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 \(S\) by a point, and the velocity field \(\nu(s)\) is computed everywhere in \(S\) 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 \(\mathcal{T}\)? We answer this question by proposing the following conjecture: Whenever the speed of the representative point of a conservative dynamical system, \(\nu(s)\), is an integral of motion in a metric space \(S\), the path followed during the dynamical evolution of that system in \(S\) extremizes the time functional \(\mathcal{T}\).

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 an extremum (e.g., the path is geodesic) on the sub-manifold of a given value of \(\nu(s)\) embedded in \(S\).

Mathematically speaking, the conjecture 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 \(s_i\) and \(s_f\), only those which make
\( T \) invariant under an infinitesimal variation of the path, i.e.,
\[
\delta T = 0, \tag{3}
\]
are possible candidates for the dynamical evolution. The value of \( T \) corresponding to the physical path is not necessarily the global minimum between all paths connecting \( s_i \) and \( s_f \). 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.

We illustrate the validity of this conjecture by considering two 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 single classical harmonic oscillator or a system of coupled harmonic oscillators in the phase space consisting of all the generalized coordinates and momenta \( \{q_i, p_i\} \) and equipped with an Euclidean metric. 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).

**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 \( \Delta E = \left( \langle H^2 \rangle - \langle H \rangle^2 \right)^{1/2} \) via
\[
ds = \Delta E \frac{dt}{h}, \tag{4}
\]
where \( ds \) is the infinitesimal distance in \( \mathbb{P} \) given by the Fubini-Study (FS) metric \( ds^2 = \frac{(\delta \omega(\delta \psi))}{\langle \psi | \psi \rangle} - \frac{|(\delta \omega(\psi))|^2}{\langle \psi | \psi \rangle^2} \). On the unit sphere, \( ds = \langle \psi | 1 - \hat{P} | \psi \rangle \frac{d\tau}{\tau} \), where \( \hat{P} \) is the projection operator \( | \psi \rangle \langle \psi | \). The trajectory traversed by a ray in \( \mathbb{P} \) under unitary evolution is 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 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 \( \Delta E / h \) is invariant for time-independent Hamiltonians, the simple answer to this problem suggested by the present paper is to consider \( T = \int \frac{d\tau}{\Delta E} \) as a geodesic quantity, i.e., *Fermat’s principle in Hilbert space*. 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. 1-a).

To show that \( T \) is stationary along the physical path through \( \mathbb{P} \), let us parametrize the evolution along any path connecting \( | \psi_i \rangle \) and \( | \psi_f \rangle \) by some arbitrary parameter \( \tau \). We can write Eq. (1) as
\[
T = \int_{| \psi_i \rangle}^{| \psi_f \rangle} d\tau \frac{\langle \psi | 1 - \hat{P} | \psi \rangle^{\frac{1}{2}}}{\sqrt{\langle \psi | H^2 | \psi \rangle - \langle \psi | H | \psi \rangle^2}}, \tag{5}
\]
where \( | \dot{\psi} \rangle = \frac{| \delta \psi \rangle}{\delta \tau} \). Taking the variational derivative of \( T \) with respect to \( | \dot{\psi} \rangle \) subject to the constraints of normalization and fixed initial and final states, we arrive at the Euler-Lagrange (EL) equation,
\[
\frac{\delta L}{\delta \dot{\psi}} - \frac{d}{d\tau} \frac{\delta L}{\delta \dot{\psi}} = 0, \tag{6}
\]
where \( L \) is the integrand in Eq. (5) added to the Lagrange multiplier term \( \lambda(\tau) (| \psi \rangle | \psi \rangle - 1) \) that ensures the conservation of the norm of \( | \psi \rangle \). Calling the numerator and denominator in Eq. (5), \( A \) and \( B \) respectively, Eq. (6) reads

\[
\begin{align*}
\left[ -\frac{1}{2AB} & \langle \psi | H^2 | \psi \rangle - \frac{A}{2B^3} \left( \langle H^2 | \psi \rangle - 2 \langle H | H | \psi \rangle \right) \right] - \frac{1}{2AB} \left[ | \dot{\psi} \rangle - | \psi \rangle | \dot{\psi} \rangle - \left( \langle \dot{\psi} | \psi \rangle + \langle \psi | \dot{\psi} \rangle \right) | \psi \rangle \right] - \frac{1}{2} \left( | \dot{\psi} \rangle - | \psi \rangle | \dot{\psi} \rangle \right) \lambda(\tau) | \psi \rangle = 0.
\end{align*}
\]

Although Eq. (7) is a highly nonlinear equation, it is easy to verify that the Schrödinger equation \( | \dot{\psi} \rangle = \pm iH | \psi \rangle \) satisfies this equation with a vanishing Lagrange multiplier, and therefore extremizes the time functional when
\( \tau \) equals the real time \( t \). The sign ambiguity can be considered a reminiscence of the non-unique mapping between \( \tau \) and \( t \). In cases where quantum ergodicity applies, i.e., when “all states, within a given energy range can be reached from all other states within the range” \([13]\), the opposite sign can be related to the other route to reach \( |\psi_f\rangle \) starting from \( |\psi_i\rangle \), i.e., backward in time.

The above discussion provokes several interesting issues. First, it is intriguing to question whether there is a nonlinear Schrödinger equation that would satisfy Eq. \((7)\) as a force that drives its evolution. The potential function responsible for this force is \( \log(\nu(s)) \).

Second, it has to be emphasized that Eq. \((6)\) is satisfied only for time-independent Hamiltonians. A very interesting problem is how to generalize this concept to time-dependent Hamiltonians as we shall do in the classical domain below. Finally, we expect the Fermat principle to be equally valid for the unitary evolution of a density matrix with the FS metric replaced by the Hilbert-Schmidt metric. It would be interesting, though, to investigate whether the non-unitary evolution of the density matrix of an open quantum system described by a master equation follows a Fermat principle. We present no further details on these issues in this paper.

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**Generalized Fermat Principle in Phase Space**—In optics, the Euler-Lagrange equation for the functional \( \frac{1}{2} \int n(s) ds \) reduces to the ray equation \([14]\)

\[
\frac{d}{ds}(n(s)\hat{t}) - \nabla n(s) = 0, \quad (9)
\]

where \( \hat{t} \) is a unit tangent vector defined in terms of the position vector \( r \) as \( \hat{t} = d\vec{r}/ds \) (the length of the path \( s \) plays the role of time in this derivation). When \( n(s) \) is constant along the path (i.e., independent of \( s \)), Eq. \((9)\) can be rewritten as

\[
\frac{d}{ds}(\hat{t}) = -\frac{\nabla \nu(s)}{\nu(s)}. \quad (10)
\]

The left hand side of this equation represents a curvature vector \( \kappa \) whose magnitude equals the curvature of the path and direction is orthogonal to the direction of motion. Therefore, for the case of an Euclidean space \( S \), the above conjecture is equivalent to stating that \( \kappa \) equals \( -\nabla \nu(s)/\nu(s) \) for a dynamical system that has invariable speed \( \nu(s) \) along its evolution in \( S \). On the other hand, since \( \kappa \) is the acceleration vector of the representative point of the system, we can regard the RHS of Eq. \((10)\) as a force that drives its evolution. The potential function responsible for this force is \( \log(\nu(s)) \).

We now consider a conservative classical system composed of \( N \) particles described by a set of generalized coordinates \( \{q_i, p_i\} \) that have the same units, with velocity-independent potential \( V(q_1,..,q_N) \), kinetic energy \( T = \sum_{i=1}^{N} p_i^2 \) and Hamiltonian \( H = T + V \). Let the distance element in phase space be described by the Euclidean metric \( ds^2 = \sum_{i=1}^{N} dq_i^2 + dp_i^2 \). The speed \( \nu(s) \) along the physical path generated by the Hamiltonian flow equals \( \sqrt{\sum_{i=1}^{N} \left( \frac{\partial H}{\partial q_i} \right)^2 + \left( \frac{\partial H}{\partial p_i} \right)^2} \) \([13]\). We therefore express the
Nevertheless, we present two cases where Eq. (13) is
\[ P = \text{Eq. (12)} \]
dept any of the 2N coordinates. The explicit form of
Eq. (12) for coordinate \( x_i \) is
\[ \frac{\delta L}{\delta x} - \frac{d}{d\tau} \frac{\delta L}{\delta \dot{x}} = 0, \]
Eq. (12) for coordinate \( x_i \) is
\[ \frac{\delta L}{\delta x} - \frac{d}{d\tau} \frac{\delta L}{\delta \dot{x}} = 0, \]
where \( L = FG, \) \( F = \sqrt{\sum \frac{1}{\left( \frac{\partial H}{\partial \dot{x}_i} \right)^2} }, \) \( G = \sqrt{\sum \dot{x}_i^2} \) and \( x \)
denotes any of the 2N coordinates. The explicit form of
Eq. (12) for coordinate \( x_i \) is
\[ G^2 \frac{\partial F}{\partial x_i} - \frac{G^2}{2} \left( \dot{x}_i F + \dot{x}_i \sum_j \frac{\partial F}{\partial \dot{x}_j} \dot{x}_j \right) - \dot{x}_i F \sum_j \dot{x}_j \dot{x}_j \frac{G^2}{2} = 0. \]
This equation is not generally satisfied for an arbitrary canonical choice of the generalized coordinates \( q_i, p_i. \)
Nevertheless, we present two cases where Eq. (13) is
satisfied and Fermat’s principle is fulfilled.
1- A simple harmonic oscillator; \( H = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 q^2. \)
Fermat’s principle is valid in the phase space \( \{ p, Q \}, \)\nwhere \( Q = m \omega q_i \) or in the phase space \( \{ P, Q \}, \) where \( P = p/\sqrt{m} \) and \( Q = \omega \sqrt{m} q_i. \) In both cases, \( \nu(s) \) is an
integral of motion.
2- A system of \( N \) coupled harmonic oscillators with equal masses and coupling constants; \( H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} \frac{1}{2} m \omega^2 (q_i - q_j)^2. \) Fermat’s principle is valid in the
phase space \( \{ p_i, Q_i \}, \) where \( Q_i = m \omega \sqrt{N} q_i. \)
In these examples, we had to perform a simple scale
transformation in order to obtain a new set of general-
ized coordinates that have the same units, leading to a
metric space in which Fermat’s principle is fulfilled.
In other examples, one might need to look for more compli-
cated canonical transformations that would render \( \nu(s) \) an
integral of motion in the new phase space. For
externally driven systems whose time-dependent Hamilto-
nian is \( H(p, q, t), \) we define the new Hamiltonian, \( H' = H(q, p, \tau) + \eta, \) where \( (\tau, \eta) \) is an extra degree of freedom
that satisfies \( \dot{\tau} = \frac{\partial H}{\partial \eta} = 1 \) and \( \dot{\eta} = -\partial H/\partial \tau = -\partial H/\partial \tau. \)
The above discussion can be generalized to the extended phase space which consists of the original
phase space supplemented by the new coordinates \( (\tau, \eta). \)
We point out that the conjecture implies also that if the
state of the system is projected to a sub-manifold of the
full space \( S, \) where a metric is defined and \( \nu(s) \) of the
projected state is an integral of motion, Fermat’s principle
will hold in that space as well. A direct example of this
case is the configuration space \( \{ q_i \} \) for a system of free
particles (Fig. 1-c) or the aforementioned Riemannian
manifold having the metric \( ds' \) for a system of interact-
ing particles. The ability to find such a sub-manifold or
the canonical transformation that renders \( \nu(s) \) an inte-
gral of motion relies on our ability to find the integrals of
motion of the given dynamical system, not a trivial task
in many cases. Therefore, the generalized Fermat prin-
цип is more likely to be relevant in integrable classical
systems than in non-integrable systems.

In conclusion, we have introduced a conjecture that
generalizes Fermat’s principle in Hilbert and phase spaces of
quantum and classical systems respectively and illuminates
new aspects of Fermat’s surmise of natural economy.
The generalized Fermat principle provides a new
geometric variational principle satisfied naturally by the
Schrödinger Hamilton’s equations of motion in the
proper space that has an associated metric distance when
the speed of evolution is an integral of motion. This prin-
inciple may have implications for the protein folding
problem, one of the major challenges of biological sciences
(10). The mechanism followed by a protein to evolve from
its unfolded structure to the native structure that has a
minimum free energy is not fully understood. The puzzle
lies in the ultrashort time the protein takes to fold
with respect to the astronomical number of intermediate
conformations. Although the folding protein is an open
system, we may gain some insight into this problem by
searching for the proper space \( S \) where the generalized
Fermat principle is fulfilled.

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