Two-point characteristic function for the Kepler–Coulomb problem

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Hamilton's two-point characteristic function \( S(q_1, t_1, q_2, t_2) \) designates the extremum value of the action integral between two space–time points. It is thus a solution of the Hamilton–Jacobi equation in two sets of variables which fulfills the interchange condition \( S(q_1, t_1, q_2, t_2) = - S(q_2, t_2, q_1, t_1) \). Such functions can be used in the construction of quantum-mechanical Green's functions. For the Kepler–Coulomb problem, rotational invariance implies that the characteristic function depends on three configuration variables, say \( r_i, r_j, r_k \). The existence of an extra constant of the motion, the Runge–Lenz vector, allows a reduction to two independent variables: \( x = r_1 + r_2 + r_3 \) and \( y = r_1 - r_2 - r_3 \). A further reduction is made possible by virtue of a scale symmetry connected with Kepler's third law. The resulting equations are solved by a double Legendre transformation to yield the Kepler–Coulomb characteristic function in implicit functional form.

The periodicity of the characteristic function for elliptical orbits can be applied in a novel derivation of Lambert's theorem.

1. INTRODUCTION

Hamilton's two-point characteristic function can be defined as the action along a real trajectory connecting two space–time points:

\[
S(q_1, t_1, q_2, t_2) = \int_{t_1}^{t_2} L(q, \dot{q}, t) dt.
\]

By Hamilton's principle, the value of the integral between two fixed points represents an extremum wrt variations in path. The function \( S(q_1, t_1, q_2, t_2) \) might not exist for certain pairs of points or might be multivalued for others. The two-point characteristic function is a solution of the Hamilton–Jacobi equation in two sets of variables:

\[
\frac{\partial S}{\partial t_1} + H(q, \frac{\partial S}{\partial q_1}, t_1) = 0
\]

(2)

and

\[
\frac{\partial S}{\partial t_2} + H(q, \frac{\partial S}{\partial q_2}, t_2) = 0
\]

(3)

The second equation follows from the first by virtue of the interchange condition

\[
S(q_1, t_1, q_2, t_2) = - S(q_2, t_2, q_1, t_1)
\]

(4)

implied by the integral structure of the characteristic function. Initial and final momenta are given by relations of the form

\[
p_1 = - \frac{\partial S}{\partial q_1}, \quad p_2 = \frac{\partial S}{\partial q_2}.
\]

(5)

The two-point characteristic function finds utility in the construction of quantum-mechanical Green's functions and density matrices. An example is the kernel \( K(q_1, t_1, q_2, t_2) \) which represents a solution of the time-dependent Schrödinger equation

\[
\left\{ \frac{\partial^2}{\partial t_1^2} - H_1 \right\} K(q_1, t_1, q_2, t_2) = 0
\]

subject to the initial condition

\[
K(q_1, t_1, q_2, t_2) = \delta(q_1 - q_2).
\]

(7)

This Green's function can be structured in the form

\[
K(q_1, t_1, q_2, t_2) = F(q_1, t_1, q_2, t_2) \exp \left( \frac{i}{\hbar} S(q_1, t_1, q_2, t_2) \right)
\]

(8)

exponentially dependent on the two-point characteristic function. The exchange condition (4) is thus consistent with the Hermitian property

\[
K(q_1, t_1, q_2, t_2) = K(q_2, t_2, q_1, t_1).
\]

(9)

The preexponential function \( F \) in (8) is determined such as to fulfill Eqs. (6) and (7). For the free particle and harmonic oscillator, this is relatively straightforward.

The Coulomb Green's function \( K(r_1, t_1, r_2, t_2) \) has not yet been worked out in closed form, although the time-independent function \( G(r_2, r_1, E) \) is known. We have attempted to construct the time-dependent function via the representation (8) and have thereby been led to evaluation of the corresponding characteristic function.

2. KEPLER–COULOMB PROBLEM

The Hamilton–Jacobi equation for the attractive Coulomb system reads

\[
\frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^2 - \frac{Ze^2}{r} = 0.
\]

(10)

This pertains as well to the Kepler problem under the substitution \( Ze^2 = GMM \). We are, of course, in the nonrelativistic domain and are assuming \( M \gg m \) [or else reading \( m \) in Eq. (10) as the reduced mass]. For compactness we shall employ atomic units, setting \( m = e = 1 \) in Eq. (10). Equivalently, \( r \) is to be expressed in units of \( a_0 = \hbar^2/m\epsilon^2 \), \( t \) in units of \( \hbar^2/m\epsilon^2 = \alpha a_0/c \), and \( S \) in units of \( \hbar \).

Accordingly, Eqs. (2) and (3) for the Kepler–Coulomb characteristic function take the form

\[
\frac{\partial S}{\partial t_1} + \frac{1}{2} (\nabla S)^2 - \frac{Z}{r_1} = 0,
\]

(11)

\[
\frac{\partial S}{\partial t_2} + \frac{1}{2} (\nabla S)^2 - \frac{Z}{r_2} = 0.
\]

The Hamiltonian is, of course, a constant of the motion, which implies
E = -\frac{\partial S}{\partial t} = \frac{\partial S}{\partial t_1}.

Thus \( S \) must depend on \( t_1 \) and \( t_1 \) only through their difference \( t = t_2 - t_1 \), and

\[
E = -\frac{\partial S}{\partial t}.
\]

The angular momentum is likewise a constant:

\[
L = r_1 x p_1 + r_2 x p_2 = -r_1 \times \nabla_1 S = r_2 \times \nabla_2 S.
\]

Every trajectory is thus confined to the plane normal to the angular momentum vector. One can write

\[
\nabla_1 S = u_1 \frac{\partial S}{\partial r_1} + u_{12} \frac{\partial S}{\partial r_{12}},
\]

\[
\nabla_2 S = u_2 \frac{\partial S}{\partial r_2} + u_{12} \frac{\partial S}{\partial r_{12}},
\]

in terms of the nonorthogonal unit vectors

\[
u_1 = r_1/r_1, \quad u_2 = r_2/r_2, \quad u_{12} = -u_{12} = r_{12}/r_{11},
\]

\[
L = \frac{r_1 \times r_1}{r_1} \frac{\partial S}{\partial r_1} = u_1 \times u_1 \frac{\partial S}{\partial r_1} + u_{12} \frac{\partial S}{\partial r_{12}}.
\]

Thus far, \( S(x_1, y_1, t) \) has been shown to depend on the four variables \( r_1, r_2, r_{12}, \) and \( t \). A further reduction is made possible by the existence of an additional constant of the motion for the Kepler-Coulomb problem, namely the Runge-Lenz vector.\(^2\)

\[
A = (Ze^2m)^{-1}L x p + u.
\]

We find thereby

\[
A = \frac{L}{r_1} x \frac{\partial S}{\partial r_1} + \frac{L}{r_2} x \frac{\partial S}{\partial r_2} + \frac{L}{r_{12}} x \frac{\partial S}{\partial r_{12}}.
\]

Thus, \( S(x_1, y_1, t) \) is, in fact, the same variables which appear in Lambert's theorem [cf. discussion following Eq. (64)]. The Coulomb Green's function \( G(r_1, r_2, E) \) was also found to depend on just \( x \) and \( y \). Hostler\(^7\) showed that this is likewise a consequence of the "hidden symmetry" associated with the Runge-Lenz vector.

### 3. Solution of the Hamilton-Jacobi Equation

We turn next to the Hamilton-Jacobi equations (11)

\[
E = -\frac{\partial S}{\partial t},
\]

for the characteristic function \( S(x, y, t) \). Using (15) and (22), we find, in terms of the variables \( x \) and \( y \),

\[
\frac{1}{2} (\nabla_1 S)^2 = \left( \frac{\partial S}{\partial x} \right)^2 + \left( \frac{\partial S}{\partial y} \right)^2 + u_1 \cdot u_{12} \left[ \left( \frac{\partial S}{\partial x} \right)^2 - \left( \frac{\partial S}{\partial y} \right)^2 \right],
\]

\[
\frac{1}{2} (\nabla_2 S)^2 = \left( \frac{\partial S}{\partial x} \right)^2 + \left( \frac{\partial S}{\partial y} \right)^2 + u_2 \cdot u_{12} \left[ \left( \frac{\partial S}{\partial x} \right)^2 - \left( \frac{\partial S}{\partial y} \right)^2 \right].
\]

Noting that

\[
u_1 \cdot u_{12} - u_2 \cdot u_{12} = (u_1 + u_2) \cdot u_{12} = r_1 - r_2 \frac{x y}{r_{12}},
\]

the difference between Eqs. (11) reduces to

\[
\frac{1}{2} \left( \frac{\partial S}{\partial x} \right)^2 - \frac{Z}{x} \left( \frac{\partial S}{\partial y} \right)^2 = 0.
\]

With the help of (25), the sum of Eqs. (11) works out to

\[
\frac{\partial S}{\partial t} + \left( \frac{\partial S}{\partial x} \right)^2 - \frac{Z}{x} \left( \frac{\partial S}{\partial y} \right)^2 = 0.
\]

Equations (25) and (26) are equivalent to the symmetrical relations

\[
\left( \frac{\partial S}{\partial x} \right)^2 - \frac{Z}{x} \left( \frac{\partial S}{\partial y} \right)^2 = 0.
\]

which have precisely the form of the original Hamilton-Jacobi equations (11) for \( L = 0 \) and \( r_1, r_2 \) replaced by \( x/2, \ y/2 \).

In accordance with Eq. (4), \( S \) must fulfill the time-reversal condition

\[
S(x, y, t) = -S(x, y, t)
\]

which rules out solutions to (27) obtained simply by separation of variables.

A further symmetry property makes possible a closed-form solution of these coupled equations. This is the invariance of (25)-(27) under the scale transformation: \( x, y \to \ell^2 x, \ell^2 y; t \to \ell^2 t; S \to \ell S \). Thus

\[
S(x, y, t) = \xi S(x_1, y_1, t_1),
\]

showing that \( S \) is a linear homogeneous function of the variables \( x^{1/2}, \ y^{1/2}, \ t^{1/2} \). The condition (28) is, in fact, a special case of (29), for \( \xi = 1 \). By virtue of this homogeneity property, the characteristic function can be represented in the following form: \( t^{1/2} x \) function of \( x^{1/2}/t^{1/2} \) and \( y^{1/2}/t^{1/2} \).

Specifically, the following definition of variables is convenient:

\[
S = (32 Z^2 t^{1/2} f(u, v)), \quad u = (x^3/16 Z t^{1/2})^{1/6}, \quad v = (y^3/16 Z t^{1/2})^{1/6}
\]

for \( t > 0 \), \( 0 < u < u \). Equations (27) thereby transform to

\[
\frac{1}{2} (f - u f_x - v f_y) + v^2 (f^2 - 1) = 0,
\]

\[
\frac{1}{2} (f - u f_x - v f_y) + v^2 (f^2 - 1) = 0.
\]

These equations are most readily solved by a double Legendre transformation, whereby

\[
F = u f_x + v f_y - f, \quad U = f_x, \quad V = f_y.
\]
\[ F_y = u, \quad F_y = v. \]

We find thereby
\[ F_y = \left( \frac{3}{4} \right)^{1/2}, \quad F_y = \left( \frac{3}{4} \right)^{1/2}. \] (33)

The positive square roots are appropriate since \( u, v > 0 \). Some further inequalities are required in order to precisely characterize the solution. Equation (25) implies, since \( x > y \), that
\[ \frac{\partial S}{\partial y} > \frac{\partial S}{\partial x}. \] (34)

Since the angular momentum vector is directed parallel to \( u \times u \), Eq. (17) implies that
\[ \frac{\partial S}{\partial y} = \frac{\partial S}{\partial x} > 0. \] (35)

The last two inequalities show that \( \partial S/\partial y < 0 \). Thus, in all cases,
\[ f_x < 0. \] (36)

For \( E > 0 \), \( \partial S/\partial t < 0 \) and
\[ f_x - u f_y - v f_y \leq 0. \] (37)

Since \( f_x > 0 \),
\[ u f_x + v f_y < 0, \quad u f_x - v |f_y| \geq 0. \] (38)

Thus
\[ f_x > 0 \quad \text{for} \quad E > 0. \] (39)

Inequality (38) further implies, in conjunction with (31), that
\[ |f_x| > |f_y| > 0. \] (40)

Combining with (36) and (39),
\[ 0 < f_x < \infty, \quad -\infty < f_y < \infty. \] (41)

In terms of the transformed variables (32),
\[ F > 0, \quad 0 < U < \infty, \quad -\infty < V < \infty. \] (42)

It is convenient therefore to define
\[ U = \cosh \lambda, \quad V = -\cosh \mu \quad (0 < \mu < \lambda < \infty). \] (43)

(One might also define a second branch of the function with \( 0 > \lambda > -\infty \) corresponding to points \( r_1, r_2 \) re­flected wrt the axis of the Runge–Lenz vector.) Integration of Eq. (33), with the appropriate choice of constant, now gives
\[ \frac{8}{3 \sqrt{3}} \left( \frac{3}{4} \right)^{1/2} = \sinh \lambda \cosh \lambda - \lambda - \sinh \mu \cosh \mu + \mu = \sinh \lambda \cosh \lambda + 3 \lambda - \lambda - \mu. \] (44)

Reversion to the original variables is effected by the inverse transformation:
\[ f = UF_y + VF_y - F_y, \quad u = F_y, \quad v = F_y. \] (45)

After some algebra we obtain
\[ f(u, v) = u J(\lambda) - v J(\mu) \] (46)

where
\[ J(\lambda) = \frac{\sinh \lambda \cosh \lambda + 3 \lambda}{4 \sinh \lambda} \] (47)

and
\[ \sinh^3 \lambda \mu = \frac{\sinh^3 \mu}{\nu^3} = \sinh(\lambda - \mu) \cosh(\lambda + \mu) - (\lambda - \mu). \] (48)

By virtue of (30) and (48), the characteristic function can be expressed in the form
\[ S(x, y, t) = (4Zx)^{1/2} (\lambda) - (4ZY)^{1/2} (\mu). \] (49)

Alternatively,
\[ S(\lambda, \mu, t) = F\left( \frac{2}{x} \right)^{1/2} \sinh(\lambda - \mu) \cosh(\lambda + \mu) + 3(\lambda - \mu). \] (50)

In verification that the preceding represents the solution to Eqs. (25), (26), and (27), it is shown that
\[ \frac{1}{2} S = \left( \frac{Z}{x} \right)^{1/2} \sinh \lambda = -\left( \frac{Z}{y} \right)^{1/2} \sinh \mu. \] (51)

Since \( \partial S/\partial t = -E \), it follows that \( E > 0 \) (hyperbolic orbits) is associated with real \( \lambda \) and \( \mu < 0 \) (elliptical orbits) with pure imaginary \( \lambda \) and \( \mu \). The case \( E = 0 \) (parabolic orbits) is obtained with \( \lambda = \mu = 0 \). Equation (48) becomes indeterminate but (49) reduces to
\[ S(x, y) = (4Zx)^{1/2} - (4ZY)^{1/2}. \] (53)

This solution does not, however, fulfil the time-reversal condition (28).

When \( \mu = 0 \), then \( v = 0, y = 0 \) and either \( r_1 \) or \( r_2 \) is real. The characteristic function reduces to \( S(r, 0, t) \). As \( \lambda + \mu = 0, S \to 0 \).

The asymptotic region \( u, v \to \infty \) pertains to any of the limits \( Z \to 0, x, y \to \infty, \) or \( t \to 0 \). The asymptotic form of the characteristic function is obtained in the limit \( \lambda, \mu \to \infty \), whereby
\[ S = -\left( \frac{Z}{2} \right)^{1/3} \left( \frac{e^{3a} - e^{3b}}{4} \right)^{1/3}, \quad u \to 2 \left( \frac{e^a - e^{3a}}{4} \right)^{1/3}, \quad v \to 2 \left( \frac{e^b - e^{3a}}{4} \right)^{1/3}. \] (44)

Thus
\[ S = -\left( \frac{Z}{2} \right)^{1/3} \left( a^2 - b^2 \right)^2 = \frac{(x - y)^2}{2} = \frac{y^2}{2t} \] (55)

which represents the free-particle characteristic function.

### 4. ELLIPTICAL ORBITS

Negative-energy solutions are most directly obtained by continuation of the variables \( \lambda \) and \( \mu \) on the imaginary axis. Defining
\[ \lambda = i \alpha / 2, \quad \mu = i \beta / 2 \] (56)

(the factors 1/2 for \( 2\pi \)-periodicity), we obtain
\[ S(\alpha, \beta, t) = (4Zx)^{1/2} F(\alpha) - (4ZY)^{1/2} F(\beta), \] (57)

\[ F(\alpha) = J(i \alpha / 2) - \frac{3 \alpha + \sin \alpha}{8 \sin \alpha / 2} \] (58)

\[ \sin^3 \alpha / 2 = \sin^3 \beta / 2 = \frac{\alpha - \beta}{2} \sin \frac{\alpha + \beta}{2} \cos \frac{\alpha + \beta}{2}. \] (59)
Also, in analogy with (50),
\[
S(\alpha, \beta, t) = \left( \frac{2^{1/2}}{[(\alpha - \beta)/2] - \sin[(\alpha - \beta)/2] \cos[(\alpha + \beta)/2]} \right)^{1/3} \times \left[ 3 \left( \frac{\alpha - \beta}{2} \right) + \sin \left( \frac{\alpha - \beta}{2} \right) \cos \left( \frac{\alpha + \beta}{2} \right) \right].
\]
(60)
The characteristic function representing an elliptical orbit should exhibit a periodic structure of the form
\[
S(\alpha + n\alpha_0, \beta + n\beta_0, t + n\tau) = S(\alpha, \beta, t) + nS(\alpha_0, \beta_0, \tau), \quad n = 0, 1, 2, \ldots,
\]
where \( \tau \) is the period of the orbit. For Eqs. (60) and (61) to be consistent, two conditions must be met:
\[
3 \left[ \left( \alpha - \beta \right) + n(\alpha_0 - \beta_0) \right] + \sin \left( \frac{\alpha - \beta}{2} + n(\alpha_0 - \beta_0) \right) \times \cos \left( \frac{\alpha + \beta}{2} + n(\alpha_0 + \beta_0) \right) \]
\[
= 3 \left( \frac{\alpha - \beta}{2} \right) + \sin \left( \frac{\alpha - \beta}{2} \right) \cos \left( \frac{\alpha + \beta}{2} \right) + n \left[ 3 \left( \frac{\alpha_0 - \beta_0}{2} \right) + \sin \left( \frac{\alpha_0 - \beta_0}{2} \right) \cos \left( \frac{\alpha_0 + \beta_0}{2} \right) \right],
\]
(62)
and
\[
\frac{t}{\pi} \left( \frac{\alpha - \beta}{2} \right) - \sin \left( \frac{\alpha - \beta}{2} \right) \cos \left( \frac{\alpha + \beta}{2} \right) \]
\[
= \frac{\tau}{2\pi} \left( \alpha - \sin \alpha \right) - (\beta - \sin \beta). \quad (64)
\]
This is, in fact, a classical result known as Lambert's theorem. In the original form of the theorem, \( \alpha \) and \( \beta \) are defined by
\[
\sin \alpha = \left( \frac{x}{2a} \right)^{1/2}, \quad \sin \beta = \left( \frac{y}{2a} \right)^{1/2},
\]
(65)
\( a \) being the semimajor axis of the ellipse. By virtue of (51), (13), (56), and the relation \( E = -Z/2a \), our definitions of \( \alpha \) and \( \beta \) are shown to coincide with (65).

Very similar in form to (64) is Kepler's equation
\[
l = \frac{\tau}{2\pi} \left[ \left( \theta_1 - \theta_0 \right) - \left( \theta_1 - \theta_0 \right) \right] = \frac{\tau}{\pi} \left[ \left( \theta_1 - \theta_0 \right) - \left( \theta_1 - \theta_0 \right) \right] \cos \left( \frac{\theta_0 + \theta_1}{2} \right)
\]
(66)
in which \( e \) is the eccentricity and \( \theta_1, \theta_0 \) the eccentric anomalies at \( r_1 \) and \( r_2 \), respectively. Comparing (66) with (64) we can identify
\[
\alpha - \beta = \theta_2 - \theta_1, \quad \cos \left( \frac{\alpha + \beta}{2} \right) = e \cos \left( \frac{\theta_2 + \theta_1}{2} \right).
\]
(67)
Setting \( \alpha - \beta = 2\pi \), \( l = n\pi \) in Eq. (60), we obtain the characteristic function for \( n \) complete cycles
\[
S = \frac{3}{8n} \left( 2\pi n \right)^{1/2} e^{-1/3}.
\]
(68)
This is related to \( W \), the corresponding solution of the time-independent Hamilton-Jacobi equation, by
\[
S = W - E \tau.
\]
(69)
Since for elliptical orbits
\[
\tau = 2nZ (-2E)^{-3/2},
\]
we find
\[
W = nJ, \quad J = (2\pi Z)^{3/2} e^{-1/3},
\]
(70)
in agreement with the value of the canonical action
\[
J = \frac{p_r}{m} - \left( p_\theta \right) \cos \theta + p_\phi \sin \theta.
\]
(72)
This is equivalent to the more familiar result that
\[
E = -2\pi Z^2 / J^2 = -2mZ^2 e^4 / J^3
\]
(73)
which for \( J = nh \) \((n = 1, 2, 3, \ldots)\) gives the Bohr energy levels.

5. Repulsive Coulomb Potential

For a repulsive Coulomb potential, an analogous calculation leads to the characteristic function
\[
S(x, y, t) = (4\pi Z)^{1/2} \left( \lambda - (4\pi Z)^{1/2} \right) \left( \mu \right),
\]
(74)
\[
\frac{\sin \lambda \cos \lambda}{4 \cosh \lambda} = \frac{\sinh \lambda \cos \lambda}{4 \cosh \lambda},
\]
(75)
\[
\frac{\sinh \lambda \mu}{\cosh \lambda} = \frac{\sinh \lambda - \mu \cosh \lambda + (\mu - \lambda)}{(0 < \mu < \lambda < \infty)}.
\]
(76)


L. Hostler, J. Math. Phys. 5, 581 (1964). The two Green's functions are related by Fourier transformation as follows:
\[
K(Q_1, r_1, t) = \lim_{\epsilon \to 0} \int dE \left[ \left( \frac{d}{dE} \right) \left( \frac{d}{dE} \right) \right] e^{i(\epsilon + \epsilon)} dE.
\]
(77)


The properties of the Runge-Lenz vector can be developed as follows. Start with Newton's second law for a particle in a Coulomb field:

\[ K(Q_1, r_1, t) = \lim_{\epsilon \to 0} \int dE \left[ \left( \frac{d}{dE} \right) \left( \frac{d}{dE} \right) \right] e^{i(\epsilon + \epsilon)} dE. \]
\( \frac{d}{dt} \left( \frac{Ze^2}{r^3} \right) = - \frac{Ze^2}{r^3} \).

Then

\[ L \times \frac{d}{dt} \left( \frac{Ze^2}{r^3} \right) = - \frac{Ze^2}{r^3} \left( \frac{r \times dr}{dt} \right) \times r. \]

This works out to

\[ \frac{d}{dt} \left( L \times p + Ze^2 \mu r \right) = 0, \]

showing that \( A \) is a constant of the motion. The equation of the orbit is obtained from

\[ A \cdot r = Ar \cos \theta = (Ze^2 \mu)^{-1} L^2 + r, \]

\[ r = (Ze^2 \mu)^{-1} L^2 / (1 - A \cos \theta), \]

which represents a conic section. The vector \( A \) is directed towards the aphelion of the orbit; its magnitude equals the eccentricity.


8This also applies w.r.t. the original position variables:

\[ S(\xi^2 r_1, \xi^2 r_2, \xi^2 \theta) = \xi S(r_1, r_2, \theta). \]

Newton's second law for a Coulomb force is likewise invariant under the substitution \( r \rightarrow \xi^2 r, \ t \rightarrow \xi^2 t \). This implies Kepler's third law of planetary motion, that the period of an orbit is proportional to the three-halves power of its linear dimension.
