Trajectory of motion of an electron in the Coulomb scattering in terms of the Schrödinger wave equation and the Hamilton Jacobi equation

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Abstract

The trajectory of motion of a scattering electron in the Coulomb potential from the wave function of the Schrödinger equation is presented in two ways, spherical polar coordinates and Temple coordinates, and is compared with each other and with the corresponding motion of classical mechanics. A good correspondence among dynamics by wave functions and the classical dynamics has been acknowledged by comparing computed examples. Detailed computing examples discriminate the optimal dynamics of the wave function that should be verified by an experiment.

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1 Introduction

We can manipulate an atom to move to where we intend these days. Quantum mechanics teaches that the motion of the atom in the region of minute scale should obey the wave equation.

To detect the exact length of e.g. 1 nm it is necessary to measure the fluctuation of the wave motion reflecting the effect of the 1 nm length. But the wave length could be far larger than 1 nm. This has been verified and realized as SNOM [scanning near field optical microscope]. We have shown that the interval of 1 nm can be detected by the visible light of wave length of 441.6nm. These indicate that the measurement of a matter of length less than the wavelength by the light wave does not obey no diffraction limit nor any indeterminacy.

Molecular dynamics in chemical physics uses trajectories of the concept of classical mechanics to interpret the bond or structure of molecules. The concept of trajectory of an atom is useful to understand the structure of aggregates of atoms.

Trials to seek the trajectory in the wave motion had been done, for example, the trajectory in the Schrödinger wave and the ray in the optical diffracted wave. The concept of trajectory relates closely to the causal interpretation of quantum mechanics.

In what follows we restrict the presentation to the algorithm of the motion of an electron in the Coulomb potential from the wave function and do not touch any interpretation about the function or its absolute value.

The hint of derivation of the concept of trajectory from the wave equation is the relation between the electromagnetic wave and the geometrical optics. The relation between the Maxwell equation and the eikonal equation of geometrical optics has been investigated in detail. It is well known that the concept of ray, trajectory, derived from the light wave plays practically and theoretically important role.

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The eikonal equation in the Schrödinger equation is the Hamilton Jacobi equation which is derived by WKBJ approximation to the wave function. The Hamilton Jacobi equation determines the Hamilton’s characteristic function that determines the motion of the particle. Thus we should make the mode characteristic function from the wave function that can determine the motion of the particle.

In the present paper a trajectory and dynamics of a scattering electron in the Coulomb potential is derived from the wave function described in the spherical polar coordinates and another dynamics from the scattering wave function used by Temple and in the text book is also derived. The dynamics for the corresponding motion of the electron in classical mechanics is presented for comparison.

These classical dynamics, dynamics by the wave functions in the spherical polar coordinates and dynamics by the Temple wave functions of a scattering electron are investigated numerically and the difference among them is noted.

In section 2 the mode trajectory and dynamics of a particle derived from the wave function in completely separated coordinates system is presented.

In section 3 dynamics of the scattering electron in the Coulomb potential by the Hamilton Jacobi equation in the spherical polar coordinates is reviewed briefly. The Hamilton’s characteristic function plays the central role to derive the orbit and the time elapse of the motion of the electron as is well known.

In section 4 by following Hamilton’s characteristic function of the preceding section we make the mode characteristic function from the wave functions in the spherical polar coordinates and derive the mode trajectory and time elapse of the motion of the electron according to section 2.

In section 5 the Hamilton’s characteristic function for the Temple coordinates known in the scattering in quantum mechanics is made to derive the classical motion of the scattering electron by introducing some technical manipulation. As a result this motion is equivalent to the motion derived in section 3.

In section 6 by using the technique in section 5 we find out the mode characteristic function from the wave functions in the Temple coordinates and get the mode trajectory and time elapse of the scattering electron. The motion of the electron is almost equal to the motion in section 5.

In section 7 dynamics of the scattering electron in the Coulomb potential obtained in previous sections 4, 5 and 6 have been numerically investigated. Detail calculation indicates that dynamics in section 4 is reasonable throughout everywhere. Dynamics in section 5 shows a defect near the origin of the potential while in the other space it is almost equal to the classical dynamics in section 5.

In section 8 conclusions are described. Dynamics in section 4 should be verified by experiment.

2 Wave function and dynamics of an electron

The stationary scattering state wave function consists of travelling waves. The WKBJ approximation of the travelling wave leads to the Hamilton’s characteristic function. We find the mode characteristic function of the travelling wave and define the dynamical equations of the particle in the wave equation.

The dynamics that leads to the mode trajectory of an electron in an attractive Coulomb potential with a charge \( Z e (>0) \) is summarized. The wave function \( \Psi \) describing the motion of an electron satisfies the Schrödinger equation

\[
\frac{i\hbar}{\partial t} \frac{\partial \Psi(r,t)}{\partial t} = \left( -\frac{\hbar^2}{2m} \Delta - \frac{Ze^2}{r} \right) \Psi(r,t),
\]

where constant \( m \) or \( -e \) is electron mass or charge, respectively.

The equation is assumed to be separable in variables \( t, x_1, x_2 \) and \( x_3 \). Let the wave function be

\[
\Psi(r,t) = e^{-iEt/\hbar} \Phi(x_1, x_2, x_3, E, \alpha, \beta) = e^{-iEt/\hbar} \Phi_1(x_1, E, \alpha) \Phi_2(x_2, \alpha, \beta) \Phi_3(x_3, \beta),
\]

where \( E, \alpha \) and \( \beta \) are constants of separation, and \( E \) is assumed to be the energy of the system. These constants should be called mode parameters. The wave function of the form

\[
\Phi_j(x_j) = |\Phi_j(x_j)| \exp\{i\Im \log \Phi_j(x_j)\} = |\Phi_j(x_j)| \exp\{iW_j(x_j)\}, \quad j = 1, 2, 3,
\]

is sought, where \( \Im \) stands for the imaginary part of, and functions \( W_j \)'s are real. This should be called a travelling wave where \( W_j \)'s satisfy the following.
Let functions $W_j$ satisfy the condition that in each classical region of $x_j$ for $j = 1, 2, 3$ where classical mechanics hold true for the motion of the particle

$$W_j(x_j) \simeq W_j(x_j)_{cl},$$

(2.4)

where the sum of them

$$W_{cl} = \sum_{j=1}^{3} W_j(x_j)_{cl}$$

(2.5)

is the Hamilton characteristic function of the Hamilton-Jacobi equation in classical mechanics. \[8\] $W_j(x_j)_{cl}$ is usually obtained as the WKBJ approximation from the wave function. The classical region stands for the domain in which the characteristic function holds true.

If $W_j$’s are found uniquely, the sum of them

$$W(x_1, x_2, x_3, E, \alpha, \beta) = W_1(x_1, E, \alpha) + W_2(x_2, \alpha, \beta) + W_3(x_3, \beta) = \Im \log \{ \Phi_1(x_1) \Phi_2(x_2) \Phi_3(x_3) \}$$

(2.6)

is named the mode characteristic function (abbreviated as mcf) for the system. \[12\]

By using a general form of the separated functions \[2.3\]

$$\Phi_j(x_j; \alpha, \beta, E) = |\Phi_j(x_j; \alpha, \beta, E)| \exp \{ i \Im \log \Phi_j(x_j; \alpha, \beta, E) \}
\equiv |\Phi_j(x_j; \alpha, \beta, E)| \exp \{ i W_j(x_j; \alpha, \beta, E) \},$$

(2.7)

the dynamics of the electron is assumed to be given by

$$\frac{\partial W_j(x_j; \alpha, \beta, E)}{\partial \alpha} = \Im \frac{\partial \Phi_j(x_j; \alpha, \beta, E)}{\Phi_j(x_j; \alpha, \beta, E)} = c_\alpha,$$

(2.8a)

$$\frac{\partial W_j(x_j; \alpha, \beta, E)}{\partial \beta} = \Im \frac{\partial \Phi_j(x_j; \alpha, \beta, E)}{\Phi_j(x_j; \alpha, \beta, E)} = c_\beta,$$

(2.8b)

$$\hbar \frac{\partial W_j(x_j; \alpha, \beta, E)}{\partial E} = \hbar \Im \frac{\partial \Phi_j(x_j; \alpha, \beta, E)}{\Phi_j(x_j; \alpha, \beta, E)} = t - t_0.$$ 

(2.8c)

Here $t_0, c_\alpha$ and $c_\beta$ are constants (independent of $t$) to be determined by initial conditions for the system. Equations (2.8a) and (2.8b) determine the mode trajectory (abbreviated as m-trajectory). Variable $t$ of Eq. (2.8c) is considered to be the dynamical time for the mode trajectory.

### 3 Orbit of an electron in the Coulomb potential by Hamilton Jacobi equation in terms of spherical polar coordinates

In the spherical polar coordinates system, $(r, \theta, \phi)$, the Hamilton characteristic function can be written as follows and satisfies the Hamilton-Jacobi equation \[8\]

$$W_{cl}(r, \theta, \phi, E, l) = W_{r,cl}(r, E, l) + W_{\theta,cl}(\theta, l),$$

$$\frac{1}{2m} (\nabla W_{r,cl})^2 - \frac{Ze^2}{r} = \frac{1}{2m} \left( \frac{\partial W_{r,cl}}{\partial r} \right)^2 + \frac{1}{2m} \frac{1}{r^2} \left( \frac{\partial W_{\theta,cl}}{\partial \theta} \right)^2 - \frac{Ze^2}{r} = E.$$ 

(3.1)

$E$ stands for the energy and the charge $Ze$ is attractive for the electron if $Z > 0$. We restrict the motion of an electron to the scattering state of $E > 0$ throughout in what follows. The motion of an electron can be restricted in a plane $(r, \theta)$ as is well known. By introducing a variable of separation $L$ standing for the angular momentum, $W_{r,cl}$ and $W_{\theta,cl}$ are determined from equations

$$\frac{1}{2m} \left( \frac{\partial W_{r,cl}}{\partial r} \right)^2 + \frac{L^2}{r^2} - \frac{Ze^2}{r} = E,$$

(3.2)

$$\left( \frac{\partial W_{\theta,cl}}{\partial \theta} \right)^2 = L^2.$$ 

(3.3)
Some calculation gives the results.

\[ \frac{\partial W_{r,cl}}{\partial r} = \sqrt{2mE + \frac{Ze^2}{r}} \frac{L^2}{r^2} = \frac{\sqrt{2mE}}{r} \sqrt{(r-r_1)(r-r_2)}, \]

\[ r_{1,2} = \frac{-Ze^2}{2E} \pm \sqrt{\left( \frac{Ze^2}{2E} \right)^2 + \frac{L^2}{2mE}}, \]

\[ \frac{\partial W_{r,cl}}{\partial L} = -2 \arctan \left( \frac{r}{r_1 - 1} \right), \]

\[ \frac{\partial W_{r,cl}}{\partial E} = \frac{m}{2E} \frac{\sqrt{(r-r_1)(r-r_2)} - \frac{Ze^2}{2E} \log \left| \frac{\sqrt{r-r_1} + \sqrt{r-r_2}}{\sqrt{r-r_1} - \sqrt{r-r_2}} \right|}{\left| \frac{\sqrt{r-r_1} + \sqrt{r-r_2}}{\sqrt{r-r_1} - \sqrt{r-r_2}} \right|}. \]

The orbit equation from \( r = \infty, pr \sin \theta = L > 0(\theta \rightarrow \pi) \) to the returning point \( r = r_1, \theta(r_1) \) is

\[ - \frac{\partial W_{r,cl}}{\partial L} - \frac{\partial W_{\theta,cl}}{\partial L} = 2 \tan^{-1} \sqrt{\frac{r/r_1 - 1}{r/r_2 + 1} - \theta} = 2 \tan^{-1} \sqrt{\frac{-r_2}{r_1}} - \pi = \text{const.} \tag{3.4} \]

The returning orbit equation from \( r_1, \theta(r_1) \) to \( r \rightarrow \infty, \theta_{sc}(r = \infty) \) is

\[ - \frac{\partial W_{r,cl}}{\partial L} - \frac{\partial W_{\theta,cl}}{\partial L} = -2 \tan^{-1} \sqrt{\frac{r/r_1 - 1}{r/r_2 + 1} - \theta} = 2 \tan^{-1} \sqrt{\frac{-r_2}{r_1}} - \pi = \text{const. defined at } r = r_1. \tag{3.5} \]

It can be proved that the orbit thus obtained is equivalent to the Temple orbit by classical mechanics (5.12) and (5.13), or (5.14).

\[ \theta_{sc} = -4 \tan^{-1} \left( \sqrt{\frac{-r_2}{r_1}} + \pi \right). \tag{3.6} \]

This expression of the scattering angle is equivalent to (5.15).

The time elapse of the orbit is

\[ t_{in,sc} = \mp \frac{\partial W_{r,cl}}{\partial E} = \mp \frac{m}{2E} \frac{\sqrt{(r-r_1)(r-r_2)} - \frac{Ze^2}{2E} \log \left| \frac{\sqrt{r-r_1} + \sqrt{r-r_2}}{\sqrt{r-r_1} - \sqrt{r-r_2}} \right|}{\left| \frac{\sqrt{r-r_1} + \sqrt{r-r_2}}{\sqrt{r-r_1} - \sqrt{r-r_2}} \right|}, \]

\[ \simeq \mp \frac{m}{2E} r \text{ as } r \rightarrow \infty. \tag{3.7} \]

This is concordant with Temple time elapse (5.16) and (5.17).

### 3.1 Cross section

The differential cross section is expressed in terms of the scattering angle \( \theta_{sc} \) and the impact parameter \( s = L/\sqrt{2mE} \) by (3.93) in the textbook

\[ \sigma(\theta_{sc}) = \frac{s}{\sin \theta_{sc}} \left| \frac{ds}{d\theta_{sc}} \right|. \tag{3.8} \]

From (3.6) the impact parameter is related to the scattering angle as

\[ s = \frac{Ze^2}{2E} \cot \frac{\theta_{sc}}{2}. \tag{3.9} \]

The differential cross section is

\[ \sigma(\theta_{sc}) = \frac{1}{4} \left( \frac{Ze^2}{2E} \right)^2 \csc^4 \left( \frac{\theta_{sc}}{2} \right) = \frac{\eta^2}{4k^2} \csc^4 \left( \frac{\theta_{sc}}{2} \right). \tag{3.10} \]

This is the same as (6.19) where \( k \) and \( \eta \) is determined in (4.18).
4 Mode trajectory of an electron by the wave function in terms of spherical polar coordinates

The scattering state of an electron in the Coulomb potential is analyzed in the spherical polar coordinate system. The wave function $\Psi(r, t)$ is expressed in the spherical polar coordinates with mode parameters, constants of separation of variables, $E, \nu$ and $\mu$ as

$$\Psi(r, t) = \exp(-iEt/\hbar) \Phi(r, E),$$

$$\Phi(r, E) = R(r, E, \nu)Y(\theta, \nu, \mu) \exp(i\mu \phi).$$

Constant $E$ stands for the energy and $\hbar \nu$ for the orbital angular momentum, and $\hbar \mu$ represents the component of the angular momentum along the polar axis. When $\nu$ and $\mu$ are integral numbers, they are usual azimuthal and magnetic quantum number. \[13\]

In what follows $\mu = 0$ is assumed. $Y(\theta, \nu, 0)$ is written as $Y_\nu(\theta)$.

The mcf expressed in terms of the spherical polar coordinates are obtained as follows. The function $Y_\nu(\theta)$ satisfies the differential equation

$$\left[ \frac{d^2}{d\theta^2} + \cot \theta \frac{d}{d\theta} + \nu(\nu + 1) \right] Y_\nu(\theta) = 0.$$  

The solution is a linear combination of linearly independent associated Legendre functions, $P_\nu(x)$ and $Q_\nu(x)$. \[15\] By putting $x = \cos \theta$

$$P_\nu(x) = F\left( -\nu, \nu + 1; 1; \frac{1-x}{2} \right),$$

$$Q_\nu(x) = \frac{\pi}{2} \left\{ -\frac{\Gamma(1/2 + \nu/2)}{2 \Gamma(1 + \nu/2)} \sin(\frac{x}{2}) F\left( -\nu, \frac{1+\nu}{2}; \frac{1}{2}; x^2 \right) 
- \frac{x \Gamma(1 + \nu/2)}{\Gamma(1/2 + \nu/2)} \cos(\frac{x}{2}) F\left( -\frac{\nu}{2}, 1 + \frac{\nu}{2}; -\frac{1}{2}; x^2 \right) \right\}.$$  

$$\frac{\partial}{\partial \nu} P_\nu(x) = \left\{ -\frac{\partial}{\partial a} + \frac{\partial}{\partial b} \right\} F\left( a, b; 1; \frac{1-x}{2} \right)_{a=-\nu, b=\nu+1},$$

$$\frac{\partial}{\partial \nu} Q_\nu(x) = \frac{\pi}{2} \left\{ -\frac{\Gamma(1/2 + \nu/2)}{2 \Gamma(1 + \nu/2)} \sin(\frac{x}{2}) \left\{ \psi(1/2 + \nu/2) - \psi(1 + \nu) \right\} 
+ \pi \cot(\frac{x}{2}) - \frac{\partial}{\partial a} + \frac{\partial}{\partial b} \right\} F\left( a; b; \frac{1}{2}; x^2 \right)_{a=-\frac{1}{2}(1-\nu), b=\frac{1}{2}(1+\nu)} 
- \frac{x \Gamma(1 + \nu/2)}{\Gamma(1/2 + \nu/2)} \cos(\frac{x}{2}) \left\{ \psi(1 + \nu/2) - \psi(1/2 + \nu/2) \right\} - \pi \tan(\frac{x}{2}) - \frac{\partial}{\partial a} + \frac{\partial}{\partial b} \right\} F\left( a, b; \frac{3}{2}; x^2 \right)_{a=\frac{3}{2}(1-\nu), b=1+\nu}. \quad (4.7)$$
\[ F(a, b; c; z) \] is the hypergeometric function usually written as \( _2F_1(a, b; c; z) \).

\[
\frac{\partial^2}{\partial x^2} P_{\nu}(x) = \left( \frac{\partial}{\partial a} + \frac{\partial}{\partial b} \right)^2 F\left( a, b; 1; \frac{1-x}{2} \right)_{a=-\nu, b=\nu+1}, \tag{4.8}
\]

\[
\frac{\partial^2}{\partial \nu^2} Q_{\nu}(x) = \frac{\sqrt{\pi}}{\Gamma(1/2 + \nu/2)} \sin(\nu \pi) \left\{ \psi'(1 + \nu/2) - \psi'(1 + \nu) - \pi^2 \sec^2(\nu \pi) \right\}
\]

\[ + \left( \psi(1 + \nu/2) - \psi(1 + \nu) + \pi \cot(\nu \pi) \right)^2 + 2 \left( \psi(1 + \nu/2) - \psi(1 + \nu) + \pi \cot(\nu \pi) \right) (-\partial_a + \partial_b) \]

\[ + (-\partial_a + \partial_b)^2 \right\} F\left( a, b; \frac{1}{2}; x^2 \right)_{a=-\nu, b=\frac{1}{2}(1+\nu)} + \frac{x \Gamma(1 + \nu/2)}{\Gamma(1/2 + \nu/2)} \cos(\nu \pi) \left\{ \psi'(1 + \nu/2) - \psi'(1 + \nu) - \pi^2 \sec^2(\nu \pi) \right\}
\]

\[ + \left( \psi(1 + \nu/2) - \psi(1 + \nu) + \pi \cot(\nu \pi) \right)^2 + 2 \left( \psi(1 + \nu/2) - \psi(1 + \nu) + \pi \cot(\nu \pi) \right) (-\partial_a + \partial_b) \]

\[ + (-\partial_a + \partial_b)^2 \right\} F\left( a, b; \frac{3}{2}; x^2 \right)_{a=-\nu, b=1+\nu}. \tag{4.9}
\]

Equations \(4.8\) and \(4.9\) will be used in \(4.33\).

A travelling wave in the \( \theta \) coordinate space is given as by using \(4.4\) and \(4.5\)

\[ Y_\nu(\cos \theta) \equiv Q_{\nu}(\cos \theta) + \frac{i \pi}{2} P_{\nu}(\cos \theta) \]

\[ = |Y_\nu(\cos \theta)| \exp(i \arg Y_\nu(\cos \theta)) \equiv |Y_\nu(\cos \theta)| \exp(i W_\theta). \tag{4.10}\]

The mcf for the \( \theta \) component should be determined as

\[ W_\theta(\theta, \nu) = \Re \log Y_\nu(\cos \theta) = \arctan \left[ \frac{\pi P_{\nu}(\cos \theta)}{2 Q_{\nu}(\cos \theta)} \right], \tag{4.11}\]

because of the similarity to the characteristic function \( W_{\theta,cl} \) in the classical region and the validity of the results derived from this as will be seen in the following.

\[ \frac{\partial}{\partial \nu} W_\theta(\theta, \nu) = \Im \frac{\partial Y_\nu(x)}{Y_\nu(x)} = \frac{\pi}{2} \frac{\partial P_{\nu}(\cos \theta) Q_{\nu}(\cos \theta) - P_{\nu}(\cos \theta) \partial \nu Q_{\nu}(\cos \theta)}{Q_{\nu}^2(\cos \theta) + \frac{1}{4} P_{\nu}^2(\cos \theta)}. \tag{4.12}\]

By the asymptotic expansion of the Legendre functions for \( \nu \gg 1 \), \(15\) it can be obtained that

\[ W_\theta(\theta, \nu) \approx (\nu + \frac{1}{2}) \theta + \frac{1}{4} \pi, \quad (\epsilon < \theta < \pi - \epsilon, \ \epsilon > 0). \tag{4.13}\]

We can recognize by numerical calculation that \( \partial_\nu W_\theta(\theta, \nu) \approx \theta \) holds true for \( \nu + \frac{1}{2} > 0 \).

The value of \( W_\theta \) at the singular points \( \theta = 0 \) or \( \pi \) are defined by the ratio of the limiting behaviour of the both Legendre functions as follows. \(15\)

\[ W_\theta(0, \nu) = 0, \quad W_\theta(\pi, \nu) = \pi \nu. \tag{4.14}\]

Behaviour of the Legendre functions near the singular points shows at \( x = -1 \) \(15\)

\[ Y_\nu(x) = Q_\nu(x) + \frac{i \pi}{2} P_\nu(x) \simeq e^{i \nu \pi} \frac{\Phi(x, \nu) + i \pi}{2}, \]

\[ \Phi(x, \nu) \equiv \log(1/2 + x/2) + \gamma + 2 \psi(\nu + 1) \simeq 2 \log(\pi/2 - \theta/2), \tag{4.15}\]

\[ \partial_\nu Y_\nu(x) \simeq i \pi Y_\nu(x) + e^{i \pi \nu} \psi'(\nu + 1), \]

\[ \partial_\nu W_\nu(x) = \Im \frac{\partial Y_\nu(x)}{Y_\nu(x)} \simeq \pi + \Im \left( \frac{2 \psi'(\nu + 1)}{\Phi(x, \nu) + i \pi} \right) \rightarrow \pi. \tag{4.16}\]
The graphical example of $\partial_\nu W_\theta(\theta, \nu)$ vs. $\theta$ for $\nu = 0.5$ and $\nu = 1.2$ with a graph of $\theta$ vs $\theta$ is shown in Fig. 1.

Radial wave function satisfies the differential equation; cf. Classic eq. (10.75) in Goldstein [8]

$$\frac{d^2 u}{dr^2} - \frac{\nu(\nu + 1)}{r^2} + \frac{2m}{\hbar^2} \left( \frac{Ze^2}{r} + E \right) u(r) = 0,$$

where $u(r) = r R(r, E, \nu)$. By putting

$$\eta_s = \frac{Ze^2}{\hbar^2} \frac{\sqrt{2mE}}{\hbar}, k \rho = \rho,$$

With $E$ positive the linearly independent solutions are

$$u_M = e^{-i\rho} \rho^{\nu+1} M(\nu + 1 + i\eta_s, 2\nu + 2, i\rho),$$

$$u_V = e^{-i\rho} \rho^{\nu+1} V(\nu + 1 + i\eta_s, 2\nu + 2, i\rho),$$

where $u_M = u_M^*$ is real [17].

Function $V(a, b, z)$ is defined for convenience [12]

$$V(a, b, z) = \Gamma(a) \left[ U(a, b, z) - \cos \pi a \frac{\Gamma(b - a)}{\Gamma(b)} M(a, b, z) \right]$$

$$= - \cos \pi b \frac{\Gamma(1 - b)\Gamma(b - a)}{\Gamma(1 - a)} M(a, b, z) + \Gamma(b - 1)z^{1-b}M(1 + a - b, 2 - b, z).$$

Functions $M(a, b, z)$ and $U(a, b, z)$ are the Kummer functions. [17]

For the far region from the center of the potential, $\rho \gg 1$, $b, a$ fixed where $a = \nu + 1 + i\eta_s$ and $b = 2\nu + 2$, it holds [17] [18] that

$$M(a, b, i2\rho) \simeq e^{i\rho} \Gamma(b) \left[ \frac{e^{-i(\rho - \pi a/2)}}{\Gamma(a^*)} (2\rho)^{-a} \left( 1 + i\frac{a(1 - a^*)}{2\rho} \right) + c.c. \right],$$

$$V(a, b, i2\rho) \simeq e^{i\rho} \left[ -i \sin(\pi a)G(\rho, a) - \cos(\pi a)G(\rho, a)^* \right].$$

Figure 1: $\partial_\nu W_\theta(\theta, \nu)$ vs $\theta, \nu = 0.5$ (solid line), $\nu = 1.2$ (dot line) and $\theta$ vs $\theta$ (red line).
and $G(\rho, a)^*$ is the complex conjugate (c.c.) of $G(\rho, a)$. These asymptotic forms indicate that the linear combination of functions $M$ and $V$ producing an outgoing travelling wave in the far region from the origin should be written as

$$u(r, E, \nu) = \exp(-i\rho)\rho^{\nu+1} \left[ V(a, b, i\nu) + iM(a, b, i\nu) \sin(\pi a) \frac{\Gamma(a)\Gamma(b-a)}{\Gamma(b)} \right]$$

$$= \exp(-i\rho)\rho^{\nu+1} \left[ -\exp(-i\pi b) \frac{\Gamma(1-b)\Gamma(b-a)}{\Gamma(1-a)} M(a, b, i\nu) + \Gamma(b-1)(i\nu)^{1-b} M(1+a-b, 2-b, i\nu) \right] \equiv \exp(-i\rho)\rho^{\nu+1}\bar{u}(\rho, E, \nu).$$

By equations mentioned above, this leads to the diverging spherical wave

$$u \approx \frac{1}{2}\pi\nu \cdot 2^{1-\nu} \Gamma(a^*) \exp[i\{\rho + \eta_s \log(2\rho) - \frac{1}{2}\pi(1+3\nu)\}]$$

$$\times \left( 1 + i\frac{\nu(1+\nu) + \eta_s^2}{2\rho} - \frac{\eta_s}{2\rho} + O(\rho^{-2}) \right),$$

for $\rho$ large [11, 10].

$$\partial_r u = \log(\rho) u + e^{-i\rho} \rho^{\nu+1} \left[ -e^{-i\pi b} \frac{\Gamma(1-b)\Gamma(b-a)}{\Gamma(1-a)} \left\{ -i2\pi + \psi(1-a) - 2\psi(1-b) + \psi(b-a) \right. \right.$$

$$\left. + \frac{\partial}{\partial a} + 2\frac{\partial}{\partial b} \right\} M(a, b, i\nu)$$

$$+ \Gamma(b-1)(i\nu)^{1-b} \left\{ 2\psi(b-1) - 2\log(i\nu) - \frac{\partial}{\partial A} - \frac{\partial}{\partial B} \right\} M(A, B, i\nu) \right\} u.$$
For \( \rho \) small, it is obtained from (4.26), (4.28), (4.31) that by using \( z = i2\rho \) and

\[
M(a, b, z) \approx 1, \quad \partial_r M(a, b, z) \approx 0, \quad \partial_\theta M(a, b, z) \approx 0,
\]

\[
\bar{u} \approx -e^{-i\theta_0} \frac{\Gamma(1-b)\Gamma(b-a)}{\Gamma(1-a)} + \Gamma(b-1)z^{1-b},
\]

\[
W_r(0, E, \nu) = 3\log \Gamma(b-1) - \frac{1}{2}\pi = -\frac{i}{2}\pi,
\]

\[
\partial_\nu W_r(0, E, \nu) = 0.
\]  

(4.34)  

(4.35)

For example, a trajectory of an electron incident from a starting point distant from the origin of the potential, \((\rho_{st}, \theta_{st}, \phi_{st})\), and scattered to another distant scattered point \((\rho_{sc}, \theta_{sc}, \phi_{sc})\) is considered. To be specific, that \( \rho_{st} = \infty \) and \( \theta_{st} = \pi \) is assumed for \( \nu + 1/2 > 0 \). For the m-trajectory from \( \rho_{st} \) to the origin or the returning point \( \rho_{ret} \), the mcf for descending \( \rho \) and \( \theta \) is written as, like the classical H-Jacobi characteristic function

\[
W(r, \theta, E, \nu) = -W_r(r, \nu) - W_\theta(\theta, \nu).
\]  

(4.36)

The trajectory is given by the equations (2.8a), (2.8b), (4.11) and (4.31) and by assuming \( \partial_\nu W_\theta(\theta_{st}, \nu) = \pi \) for \( \nu + 1/2 > 0 \),

\[
\frac{\partial}{\partial \nu} \{-W_r(r, \nu) - W_\theta(\theta, \nu)\} = -\partial_\nu W_r(\infty, E, \nu) - \partial_\nu W_\theta(\theta_{st}, \nu) = \Im \psi(a) - \frac{1}{2}\pi
\]

(4.37)  

\[
= -\partial_\nu W_r(\rho_{ret}, E, \nu) - \partial_\nu W_\theta(\theta_{ret}, \nu).
\]  

(4.38)

Let \( \rho_{ret} = 0 \) then \( \partial_\rho W_\rho(0) = 0 \) for \( \nu + 1/2 > 0 \), thus

\[
\partial_\nu W_\theta(\theta_{ret}) = \partial_\nu W_r(\infty) + \partial_\nu W_\theta(\theta_{st}, \nu) - \partial_\nu W_r(0) = -\Im \psi(a) + \frac{1}{2}\pi.
\]  

(4.39)

For the path from the origin or the returning point \((\rho_{ret}, \theta_{ret})\) to the scattered point \((\rho_{sc} = \infty, \theta_{sc})\), the mcf for increasing \( \rho \) and descending \( \theta \) is given by

\[
W(r, \theta, E, \nu) = W_r - W_\theta.
\]  

(4.40)

The trajectory should be taken to be continuous to the incident trajectory at the returning point \((0, \theta_{ret})\). The trajectory equation is written as

\[
\frac{\partial}{\partial \nu} (W_r - W_\theta) = \partial_\rho W_r(\rho_{ret}) - \partial_\rho W_\theta(\theta_{ret}) = \Im \psi(a) - \frac{1}{2}\pi
\]

(4.41)  

\[
= \partial_\rho W_r(\infty) - \partial_\rho W_\theta(\theta_{sc}).
\]  

(4.42)

Since function \( \partial_\rho W_r \) shows monotonic decrease with respect to \( \rho \) while \( \partial_\rho W_\theta \) does monotonic increase with respect to \( \theta \) as proved by numerical calculations, there is a point \( \rho = \rho_\pi \) where \( \theta \) takes \( \pi \). It can be \( \rho_{ret} = 0, \partial_\rho W_r(\rho = 0) = 0 \) for \( \nu + 1/2 > 0 \). The scattering angle \( \theta_{sc} \) is given by

\[
\partial_\rho W_\theta(\theta_{sc}, \nu) = -2\Im \psi(a).
\]  

(4.43)

The scattering angle \( \theta_{sc} \) of an incident beam as a function of the impact parameter \( ks \) for the classical orbit and the parameter \( \nu + 1/2 \) for the mode-trajectory is shown in Fig. 2 in §7

4.1 DYNAMICS TIME-DEPENDENCE

Eq. (2.8c) leads to the dynamics along the trajectory. Since \( \partial W_\theta/\partial E \) and \( \partial W_\theta/\partial E = \partial W_r/\partial E \) of (4.31). From (4.11), (4.26), (4.31)

\[
\frac{\partial \rho}{\partial \nu} = \frac{\rho}{2E}\frac{\partial \eta_s}{\partial \nu}, \quad \frac{\partial \eta_s}{\partial \nu} = \frac{\eta_s}{2\nu} \frac{\partial a}{\partial \nu} = -\frac{i}{2E} \partial E = \frac{\rho}{2E} \frac{\partial \eta_s}{\partial \nu},
\]

\[
\frac{t + t_0}{\hbar} = \frac{\partial W_r}{\partial E} = \frac{1}{1 + (\nu_l/\nu_R)^2} \partial E u_l u_R = \Im \left( \frac{\partial E u}{u} \right).
\]  

(4.44)
For $\rho \to \infty$ from (4.32)

$$\frac{\partial}{\partial E} W_r(r, E, \nu) \simeq \frac{\partial \rho}{\partial E} \left(1 + \frac{\eta s}{\rho}\right) + \frac{\partial \eta s}{\partial E} \log(2\rho) - 3 \left(\frac{\partial a}{\partial E} \psi(a)\right) + \frac{\partial \eta s}{\partial E} \frac{\eta s}{\rho}.$$ (4.45)

$$2E \frac{\partial u}{\partial E} = (-i\rho + \nu + 1) u + e^{-i\rho \rho^{\nu+1}} \left[-e^{-i\rho} \Gamma(1-b) \Gamma(b-a) \right] \left(i\eta s \{\psi(b-a) - \psi(1-a)\} - i\eta s \frac{\partial}{\partial a} + z \frac{\partial}{\partial z}\right) M(a, b, z)_{z=2\rho}$$

$$+ \Gamma(b-1)(2i\rho)^{1-b} \left\{1 - b - i\eta s \frac{\partial}{\partial A} + z \frac{\partial}{\partial z}\right\} M(A, 2-b, z)_{A=1+b, z=2\rho}.$$ (4.46)

$$\frac{2E}{\hbar} (t + t_0) = 2E \Im\left(\frac{\partial W_r(r, E, \nu)}{\partial E}\right).$$ (4.47)

Eq. (4.46) leads to as $\rho \to 0$,

$$2E \frac{\partial \tilde{u}}{\partial E}(\rho) \approx -\Gamma(b)(2i\rho)^{1-b},$$

$$2E \left(\frac{\partial W_r(0, E, \nu)}{\partial E}\right) = 2E \Im\left(\frac{\partial \tilde{u}(\rho = 0)}{\partial \rho (\rho = 0)}\right) = -\Im(b-1) = 0.$$ (4.48)

Incident mcf (4.37) and returning mcf (4.40) leads to the time elapse equation

$$\frac{2E}{\hbar} (t(r) + t_0)^{\text{in}} = 2E \left(-\frac{\partial W_r(r, E, \nu)}{\partial E}\right),$$

$$\frac{2E}{\hbar} (t(r = 0) + t_0)^{\text{in}} = 2E \left(-\frac{\partial W_r(0, E, \nu)}{\partial E}\right) = 0,$$

$$\frac{2E}{\hbar} (t(r) + t_0)^{\text{sc}} = 2E \left(\frac{\partial W_r(r, E, \nu)}{\partial E}\right).$$ (4.49)

Examples of the mode trajectory and time elapse of a scattering electron are drawn in Figs. 4 and 5 in §7.

4.2 Cross section

In the remote region from the origin, equation (4.33) shows that the difference between two positions along a trajectory satisfies

$$\frac{d\theta}{dp} = \frac{\partial}{\partial \rho} \frac{\partial}{\partial \nu} W_r = -\frac{\nu + \frac{1}{2}}{\rho^2}.$$ (4.50)

Integration gives rise to $\rho(\pi - \theta) = \nu + \frac{1}{2}$ for $\rho \to \infty$, $\theta \to \pi$. It is thus obtained that the impact parameter of the trajectory is given by

$$s = r \sin(\pi - \theta) = \rho \sin(\pi - \theta) = \nu + \frac{1}{2}.$$ (4.51)

This indicates that $(\nu + \frac{1}{2}) \hbar$ corresponds to $\hbar$, angular momentum in the sense of classical mechanics, and $\nu$ should be greater than $-\frac{1}{2}$. 

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More strictly speaking for the m-trajectory in the remote region $\rho \rightarrow \infty$, $\theta \rightarrow \pi$, or $x \equiv \cos \theta \rightarrow -1$, by using (4.10) and (4.33), equation (4.37) gives rise to

$$\partial_\nu W_\nu(r, E, \nu) \simeq -3\psi(a) - \frac{1}{2}\pi(1) + \frac{\nu + 1/2}{\rho}, \quad \partial_\nu W_\nu(x) \simeq \pi - \frac{2\pi\psi'(\nu + 1)}{\Phi(x, \nu)^2 + \pi^2}.$$ 

$$\nu + \frac{1}{2} \simeq \frac{\pi\psi'(\nu + 1)}{2\log^2(\pi/2 - \theta/2)}.$$  

(4.52)

Therefore $\nu + \frac{1}{2}$ does not exactly stand for $\rho \sin(\pi - \theta)$ or the (classical) impact parameter. By numerical calculation, however, Figure 2 indicates that $\nu + \frac{1}{2}$ corresponds well to the impact parameter $k s$.

That the height at the starting point $\rho \sin(\pi - \theta) \rightarrow 0$ as $\rho \rightarrow \infty$ means that m-trajectories seem to start from points of height 0 but they are discriminated by the difference of $\nu$.

The differential cross section for the trajectories of incident beam of electrons uniform per annulus $(\nu + 1/2) d\nu$ may be obtained in a similar way as the classical one (3.8) or (3.10). By using (4.43) and (4.8) and (4.10) we have

$$(d\theta_{sc} d\nu_0 + d\nu_0) \partial_\nu W_\nu(\theta_{sc}, \nu) = d\nu_0 2\pi\psi(a),$$

$$\frac{d\nu}{d\theta_{sc}} = \frac{\partial_\theta_\nu \partial_\nu W_\nu(\theta_{sc}, \nu)}{2\pi \partial_\nu W_\nu(\theta_{sc}, \nu)},$$

$$\sigma(\theta_{sc}) = \frac{s}{\sin \theta_{sc}} \left| \frac{d\nu}{d\theta_{sc}} \right|^2 = \frac{(\nu + \frac{1}{2})^2}{2mE} \frac{1}{\sin \theta_{sc}} \left| \frac{d\nu}{d\theta_{sc}} \right| = \frac{1}{k^2} \frac{\nu + \frac{1}{2}}{\sin \theta_{sc}} \frac{d\nu}{d\theta_{sc}}.$$  

(4.54)

Parameter $\nu$ in the right hand side should be expressed in terms of $\theta_{sc}$ through (4.43).

An example of the differential cross section vs the scattering angle is drawn in Fig. 3 in §7.

### 4.3 $dt/dp(\rho, E, \nu)$ for $-1/2 < \nu < 0$

Numerical analysis of the following equations indicates the existence of the point $\rho_0$ near the origin where $dt/dp(\rho_0, E, \nu) = 0$ for $-1/2 < \nu < 0$. Therefore $\nu$ should be non-negative. It leads to the limiting scattering angle of a scattered electron by $E$ by (4.43).

$$\partial_\nu W_\nu(\theta_{sc}, \nu)_{\nu=0} = -2\pi\psi(1 + i\eta_b).$$  

(4.55)

$$2E \frac{\partial}{\partial \rho} \left( \frac{\partial W_\nu(r, E, \nu)}{\partial E} \right) = 2E \frac{\partial}{\partial \rho} \left( \frac{\partial E u}{u} \right) = -1 + 4E \left( \frac{\partial E u}{u} - \frac{\partial \tilde{u}}{u} \right).$$

(4.56)

$$2E \partial_\nu \partial_\tilde{u} E = -e^{-ib} \frac{\Gamma(1 - b)}{\Gamma(1 - a)} \left[ i\eta_b \{ \psi(b - a) - \psi(1 - a) \} + 1 + z - b \right] M(a + 1, b + 1, z)$$

$$+ a M(a, b, z) - \frac{i\eta_b}{b} \left( 1 + a \frac{\partial}{\partial a} \right) M(a + 1, b + 1, z) = i2\rho$$

$$- \Gamma(b) z^{-b} \left[ 1 - b - i\eta_b \frac{\partial}{\partial A} + z \frac{\partial}{\partial z} \right] M(A, 2 - b, z) = \frac{1}{2} - b \left[ \frac{\partial}{\partial z} M(A, 2 - b, z) = i2\rho \right]$$

$$+ \Gamma(b - 1) z^{1-b} \left[ 1 - a - b \right] M(A, 2 - b, z) = i2\rho + AM(A, 2 - b, z) = i2\rho$$

$$- \frac{i\eta_b}{2 - b} \left( 1 + A \frac{\partial}{\partial A} \right) M(A + 1, 3 - b, z) = i2\rho.$$  

(4.57)
5 Temple orbit by Hamilton Jacobi equation

As to the Coulomb scattering the Temple wave form is known in quantum mechanics \[10\]. In classical mechanics the corresponding orbit has not been shown to our knowledge. To compare the classical orbit and the wave trajectory described in the next section the Temple form solution of the Hamilton Jacobi equation of the Coulomb scattering will be investigated.

The Hamilton Jacobi equation is the same (3.1) but rewritten as
\[
\frac{1}{2m} (\nabla W_{cl})^2 - \frac{Ze^2}{r} = E. \tag{5.1}
\]

The Temple solution may be given by putting the characteristic function as
\[
W_{cl}(x, y, z) = W_{x, cl}(x) + W_{z, cl}(\zeta), \quad \zeta = r - x.
\]

Some calculation like
\[
\frac{\partial}{\partial x} \zeta = \frac{x}{r} - 1 = -\frac{\zeta}{r}, \quad \frac{\partial}{\partial y} \zeta = \frac{y}{r}, \quad \frac{\partial}{\partial z} \zeta = \frac{z}{r}
\]
will lead to
\[
(\nabla W_{cl})^2 = (\partial_x W_{cl})^2 + (\partial_y W_{cl})^2 + (\partial_z W_{cl})^2
\]
\[
= \left(\frac{y^2 + z^2}{r^2} + \frac{\zeta^2}{r^2}\right) (\partial_x W_{cl})^2 - 2\frac{\zeta}{r} \partial_x W_{cl} \partial_\zeta W_{cl} + (\partial_\zeta W_{cl})^2
\]
\[
= 2\frac{\zeta}{r} (\partial_\zeta W_{cl})^2 - 2\frac{\zeta}{r} \partial_\zeta W_{cl} \partial_x W_{cl} + (\partial_x W_{cl})^2.
\]

This suggests that the Hamilton-Jacobi equation (5.1) is separated
\[
W_{x, cl}(x) = px, \quad p^2 = 2mE, \tag{5.2}
\]
\[
\left(\frac{dW_{z, cl}(\zeta)}{d\zeta}\right)^2 - 2 \frac{Ze^2}{r} \left(\frac{\zeta}{2E}\right) - \frac{mZe^2}{\zeta} \equal 0. \tag{5.3}
\]

Some more calculation and integration gives rise to
\[
W_{cl, \zeta}(\zeta) = \pm \frac{p}{2} \zeta \pm \frac{p}{2} \sqrt{\zeta \left(\zeta + \frac{2Ze^2}{E}\right)} \pm \frac{Ze^2}{2E} \log \left|\frac{\sqrt{\zeta + \frac{2Ze^2}{E}} - \sqrt{\zeta}}{\sqrt{\zeta + \frac{2Ze^2}{E}} + \sqrt{\zeta}}\right|.
\]

(5.2) and (5.3) leads to for \( \zeta = r - x \to \infty \)
\[
\frac{\partial W_{cl, \zeta}(\zeta)}{\partial E} + \frac{\partial W_{x, cl}(x)}{\partial E} \to \sqrt{\frac{m}{2E}} \left(\frac{r^2}{2E} + \frac{2E\zeta}{Ze^2}\right) \tag{5.5}
\]

This corresponds to the time elapse of the particle in the Coulomb field \(3.7\). Equations (5.2) and (5.3) could not, however, lead to the orbit.

To derive the orbit and dynamics in one way or another let us rotate the coordinates \((x, y)\) to \((x', y')\) with an arbitrary angle \(\varphi\)
\[
\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}.
\]

Since \((\partial_x W_{cl})^2 + (\partial_y W_{cl})^2 = (\partial_x' W_{cl})^2 + (\partial_y' W_{cl})^2\) and \(r' \equiv \sqrt{x'^2 + y'^2 + z'^2} = r\), Hamilton Jacobi equation is written as
\[
\frac{1}{2m} \left\{ (\partial_x' W_{cl})^2 + (\partial_y' W_{cl})^2 + (\partial_z W_{cl})^2 \right\} - \frac{Ze^2}{r} = E.
\]
Therefore we have the characteristic function dependent on \( \zeta' = r - x', x' \), with \( p = \sqrt{2mE} \),

\[
W_{cl}(x, y, z; \varphi, E) = W_{cl,x'}(x'; E) + W_{cl,\zeta'}(\zeta'; E),
\]

\[
W_{cl,x'}(x'; E) = \sqrt{2mE}x',
\]

\[
W_{cl,\zeta'}(\zeta'; E) = \{ W_{cl,\zeta'}^+(\zeta'; E), W_{cl,\zeta'}^-(\zeta'; E) \},
\]

\[
W_{cl,\zeta'}^\pm(\zeta') = W_{cl,\zeta'}^{\pm}(r - (\cos \varphi x - \sin \varphi y); E)
\]

\[
= \sqrt{mE} \zeta' \pm \sqrt{\frac{mE}{2} \left( \zeta' + 2Ze^2 \frac{E}{\zeta'} \right) + Ze^2 \sqrt{\frac{mE}{2E} \log \sqrt{\zeta' + \frac{2Ze^2}{E} - \sqrt{\zeta'}}}}.
\]

The orbit and the dynamics should be given by

\[
\partial_x W_{cl}(x, y, z; \varphi, E) = \partial_\varphi \left( W_{cl}^-(\zeta'); E \right)^\pm + W_{x'}(x'; E)) = y' \left( \frac{d}{d\zeta'} W_{cl}^-(\zeta'); E \right)^\pm - \frac{d}{d\zeta'} W_{x'}(x'; E)
\]

\[
= y' \left( -\sqrt{\frac{mE}{2}} \pm \sqrt{\frac{mE}{2} + \frac{mZe^2}{\zeta'}} \right) = y_0 \text{(constant)},
\]

\[
\partial_E W_{cl}(x, y, z; \varphi, E) = \partial_E \left( W_{cl}^-(\zeta'); E \right)^\pm + W_{x'}(x'; E)) = t + t_0 \text{(constant)}.
\]

Here use has been made of

\[
\partial_\varphi \zeta' = -\partial_\varphi x' = \sin \varphi x + \cos \varphi y = y'.
\]

Let \( x = r \cos \theta, y = r \sin \theta \). For the scattering state that the incident electron from \( x = \infty, py = ps = L \text{(constant)} \) is scattered by the Coulomb potential the incident characteristic function is \( W_{cl}^-(\zeta') + W_{x'}(x') \) and the scattered one is \( W_{cl}^+(\zeta') + W_{x'}(x') \) with \( \varphi \to 0 \).

\[
\partial_\varphi (W_{cl}^-(\zeta') + W_{x'}(x'))_{\varphi=0} = y \left( \partial_\varphi W_{cl}^-(\zeta') - \partial_\varphi W_{x'}(x') \right)
\]

\[
= y \left( -\sqrt{\frac{mE}{2}} - \sqrt{\frac{mE}{2} + \frac{mZe^2}{\zeta'}} \right) = -L,
\]

\[
\partial_\varphi (W_{cl}^+(\zeta') + W_{x'}(x'))_{\varphi=0} = y \left( \sqrt{\frac{mE}{2}} + \sqrt{\frac{mE}{2} + \frac{mZe^2}{\zeta'}} \right) = -L.
\]

For \( r \to \infty, \theta \to \pi, \zeta = r - x \to \infty \)

\[
\partial_\varphi (W_{cl}^-(\zeta') + W_{x'}(x'))_{\varphi=0} \to -\sqrt{2mE}y = -ps = -L.
\]

Here, \( p \) is the momentum, \( L \) is the angular momentum, and \( s \) is the impact parameter. From

\[
\partial_\varphi (W_{cl}^-(\zeta') + W_{x'}(x'))_{\varphi=0} = -ps
\]

for \( r \to \infty, \theta \to \theta_{sc} \) cf. (4.13)

\[
\sqrt{\frac{mE}{2}} \frac{Ze^2}{\zeta} = \frac{pZe^2}{E} \frac{\sin \theta_{sc}}{1 - \cos \theta_{sc}} = -ps, \text{ or } \tan \frac{\theta_{sc}}{2} = -\frac{Ze^2}{2Es} = -\frac{Zme^2}{2E} \frac{s}{L} = \frac{m}{\ell}.
\]

In what follows \( p = k\hbar \) and \( L = \ell \hbar \) are used. From (5.12) for \( px/\hbar = kx \to -\infty, \; py = ps = \ell \hbar \) is attained and the orbit equation is explicitly written from (5.12) and (5.13) as

\[
\frac{s}{r} = \frac{Ze^2}{2Es}(1 + \cos \theta) + \sin \theta, \text{ or } \frac{\ell}{kr} = \frac{m}{\ell}(1 + \cos \theta) + \sin \theta.
\]

This is a typical hyperbolic curve of orbit in the Coulomb potential.
That the orbit obtained from (5.13) should accord with this equation leads to \( y_0 = -L = -k\hbar \). By taking \( kr \to \infty \) in (5.13), the scattering angle \( \theta_{sc} \) is obtained:

\[
\theta_{sc} = 2 \arctan \left( \frac{Zme^2}{-pL} \right) = -2 \arctan \left( \frac{\eta_s}{k\hbar s} \right). \tag{5.15}
\]

This is equivalent to (3.6). The returning point where the incident orbit (5.12) transfers to the scattering orbit (5.13) is \( y = 0, \theta_{ret} = 0 \) for \( Z > 0 \). For \( Z < 0 \) it is given by the conditions \( E\zeta + 2Ze^2 = 0 \) and \( py = 2ps \), and thus \( \theta_{ret} = 2 \arctan \left( -\frac{Ze^2/(Es)}{r_{ret}} \right) \), \( r_{ret} = 2s/\sin \theta_{ret} \).

The time elapse of the motion for the incident orbit (5.12) and the scattering orbit (5.13) are

\[
(t + t_0)^{inc} = \partial_E (W_r(x') + W_s(x'))_{\varphi=0} = \sqrt{\frac{m}{8E}} \left\{ \zeta - \left( \sqrt{\zeta + \left( \frac{2Ze^2}{E} \right)} - \frac{Ze^2}{E} \log \frac{\sqrt{\zeta + \sqrt{\zeta + \frac{2Ze^2}{E}}}}{\sqrt{\zeta - \sqrt{\zeta + \frac{2Ze^2}{E}}}} \right) \right\} + \sqrt{\frac{m}{2E}}x, \tag{5.16}
\]

\[
(t + t_0)^{sc} = \partial_E (W_r(x') + W_s(x'))_{\varphi=0} = \sqrt{\frac{m}{8E}} \left\{ \zeta + \left( \sqrt{\zeta + \left( \frac{2Ze^2}{E} \right)} - \frac{Ze^2}{E} \log \frac{\sqrt{\zeta + \sqrt{\zeta + \frac{2Ze^2}{E}}}}{\sqrt{\zeta - \sqrt{\zeta + \frac{2Ze^2}{E}}}} \right) \right\} + \sqrt{\frac{m}{2E}}x. \tag{5.17}
\]

From (5.10) for \( kr \to \infty, \theta \to \pi \),

\[
(t + t_0)^{inc} \approx \sqrt{\frac{m}{2E}}x + \sqrt{\frac{m}{8E}} \frac{Ze^2}{E} \log \frac{2E\zeta}{Ze^2} \approx \frac{mx}{p} + \sqrt{\frac{m}{8E}} \frac{Ze^2}{E} \log \frac{4E|x|}{Ze^2}. \tag{5.18}
\]

From (5.17) for \( kr \to \infty, \theta \to \theta_{sc} \),

\[
(t + t_0)^{sc} \approx \sqrt{\frac{m}{2E}}r - \sqrt{\frac{m}{8E}} \frac{Ze^2}{E} \log \frac{2Er(1 - \cos \theta_{sc})}{Ze^2}. \tag{5.19}
\]

These are comparable to equations (4.49) for the m-trajectory and the following eqs. (6.17) and (6.18) for the Temple m-trajectory.

The dynamics of (5.12), (5.13), (5.10) and (5.17) obtained by Hamilton-Jacobi equation in Temple coordinates are equivalent to the dynamics of (5.4), (5.5) and (5.7) obtained by Hamilton-Jacobi equation in the spherical polar coordinates, both in the Cartesian coordinates system.

Examples of the orbit and time elapse of a scattering electron for \( E = 20\text{eV} \) are shown in Fig. 4 and Fig. 5.

### 6 Temple mode trajectory from the wave function

A solution of the Schrödinger equation has been given by Temple [9] and rewritten in Mott & Massey [10]

\[
\nabla^2\psi(x, y, z) + \frac{2m}{\hbar^2} \left( E + \frac{Ze^2}{r} \right) \psi(x, y, z) = k^2 \left( \frac{1}{k^2} \nabla^2 + 1 + \frac{2\eta_s}{kr} \right) \psi(x, y, z) = 0. \tag{6.1}
\]

\[
k \equiv \sqrt{2mE}/\hbar, \quad \eta_s = \frac{Zme^2}{k^2\hbar}, \quad \text{cf. (4.18)}
\]

Temple form solution is obtained by setting

\[
\psi(x, y, z) = e^{ikr} F(\zeta), \quad \zeta = r - x,
\]

\[
\left( ik\zeta \frac{d^2}{d(ik\zeta)^2} + (1 - ik\zeta) \frac{d}{d(ik\zeta)} - i\eta_s \right) F(\zeta) = 0. \tag{6.2}
\]
The linearly independent solutions are the Kummer functions \[ \text{(14)} \].

\[ F(\zeta) = \{M(i\eta_1, 1, ik\zeta), U(i\eta_1, 1, ik\zeta)\} \].

\[ M(a, 1, z) = \sum_{n=0}^{\infty} \frac{(a)n z^n}{n!}, \quad U(a, 1, z) = -\frac{1}{\Gamma(a)} [M(a, 1, z) \log z + \psi(a) - 2\psi(1)], \]

where \( a = i\eta \) or \( 1 - i\eta \), and \( z = ik\zeta \) or \( -ik\zeta \).

For \( |z| \) large, \( a, b \) fixed asymptotic expressions for \( U(a, b, z) \), \[ M(a, 1, z) \to \frac{1}{\Gamma(a)} - \frac{1}{\Gamma(a)} \frac{\log z}{z} + \frac{1}{\Gamma(a)} \frac{\psi(a)}{z} - \frac{1}{\Gamma(a)} \frac{2\psi(1)}{z}, \]

\[ \log z < \text{arg}(z) < \frac{3\pi}{2} \].

The wave functions having the similar phase to characteristic functions of Temple form of classical mechanics should be sought. Define the incident and scattering functions from (6.2) and (6.3)

\[ \psi_{in}(x, y, z) \equiv e^{-\pi n/2} e^{ikx} U(\eta_1, 1, ik\zeta) \simeq e^{i(kx-\eta_1 \log(k\zeta))}, \]

\[ \psi_{sc}(x, y, z) \equiv e^{\pi n/2} \Gamma(1-i\eta_1) e^{ikx} M(i\eta_1, 1, ik\zeta) - \psi_{in}(x, y, z) = -\frac{e^{-\pi n/2} \Gamma(1-i\eta_1)}{\Gamma(i\eta_1)} e^{ikr} U(1-i\eta, 1, -ik\zeta) \simeq -\frac{-i\Gamma(1-i\eta_1)}{\Gamma(i\eta_1)} e^{ikr+\eta_1 \log(k\zeta)}. \]

Each wave function in the remote region \( kr \to \infty \) is shown in the following of the signature \( \simeq \). Thus \( \psi_{in}(x, y, z) \) shows the unit incident plane-like wave in the Coulomb field. \( \psi_{sc}(x, y, z) \) represents the diverging scattered wave. These functions have a singular point \( kr = 0 \). But the sum function \( \psi_{in}(x, y, z) + \psi_{sc}(x, y, z) \) is regular everywhere.

These functions cannot give rise to the trajectory like classical mechanics of the preceding section. To derive the trajectory let rotate coordinate \((x, y)\) to \((x', y')\) according to (6.4). We consider the wave in the coordinates \((x', y')\) rotated by an arbitrary angle \( \varphi \) from the coordinates \((x, y)\). The Schrödinger equation is rewritten as

\[ \nabla^2 \psi(x', y', z) + \frac{2m}{h^2} \left( E + \frac{Z e^2}{r} \right) \psi(x', y', z) = k^2 \left( \frac{1}{k^2} \nabla^2 + 1 + \frac{2\eta_1}{kr} \right) \psi(x', y', z) = 0. \]

\[ \nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2 \]

We get the expected functions

\[ \psi_{in}(x', y', z) = e^{-\pi n/2} e^{ikx'} U(\eta_1, 1, ik\zeta'), \]

\[ \psi_{sc}(x', y', z) = -\frac{e^{-\pi n/2} \Gamma(1-i\eta_1)}{\Gamma(i\eta_1)} e^{ikr} U(2 - i\eta_1, 2, -ik\zeta'). \]

Here, \( \zeta' = r - x' \). By using the relations

\[ \frac{\partial}{\partial \varphi} \psi_{in}(x', y', z) = -iky' \psi_{in}(x', y', z) + i\eta_1 e^{-\pi n/2} e^{ikx'} U(\eta_1 + 1, 2, ik\zeta'), \]

\[ \frac{\partial}{\partial \varphi} \psi_{sc}(x', y', z) = -\frac{e^{-\pi n/2} \Gamma(2 - i\eta_1)}{\Gamma(i\eta_1)} e^{ikr} U(2 - i\eta_1, 2, -ik\zeta'), \]

the mode trajectory equations (named as Temple m-trajectory) are given by

\[ C_1 = \Im \left( \frac{\partial \varphi \psi_{in}(x', y', z)}{\psi_{in}(x', y', z)} \right) \varphi = 0 = -ky + k\eta_1 \Im \left( \frac{U(\eta_1 + 1, 2, ik\zeta)}{U(i\eta_1, 1, ik\zeta)} \right) \simeq -ky, \]

\[ C_2 = \Im \left( \frac{\partial \varphi \psi_{sc}(x', y', z)}{\psi_{sc}(x', y', z)} \right) \varphi = 0 = ky \Re \left( \frac{(1 - i\eta_1) U(2 - i\eta_1, 2, -ik\zeta)}{U(1 - i\eta_1, 1, -ik\zeta)} \right) \simeq \eta_1 \cot \frac{\theta}{2}. \]

Here use has been made of (6.5). The function following \( \simeq \) shows the approximate one for \( kr \to \infty \). Corresponding characteristic functions indicate that \( C_1 = -ks = -\ell \) and \( C_2 = -ks = -\ell \) where \( s = y \) at
$r \to \infty$ is the impact parameter. The scattering angle is given by $\theta_{sc} = -2 \arctan(\eta_s/k_s) = -2 \arctan(\eta_s/\ell)$ which is equal to that of classical mechanics (5.15).

The time dependence of the mode trajectory is given by the relations

$$k \cdot \left( \frac{\partial \psi_{m}(x',y',z)}{\psi_{m}(x',y',z)} \right)_{\varphi=0} = kx + \Im \left\{ -i\eta \left( \frac{\partial \psi_{m}(a,1,ik\zeta)}{\psi_{m}(a,1,ik\zeta)} \right)_{a=\eta_s} + \eta \zeta \left( \frac{U(\eta_s + 1,2,ik\zeta)}{U(\eta_s,1,ik\zeta)} \right) \right\},$$

$$(t + t_{0})_{m} = \frac{h}{2E} \cdot \Im \left( \frac{\partial \psi_{m}(x',y',z)}{\psi_{m}(x',y',z)} \right)_{\varphi=0},$$

where $x,y$ are correlated by (6.13).

$$k \cdot \left( \frac{\partial \psi_{sc}(x',y',z)}{\psi_{sc}(x',y',z)} \right)_{\varphi=0} = kx + \eta \Re \left\{ \psi(1-i\eta) + \psi(i\eta) + \frac{\partial \psi_{sc}(a,1,-ik\zeta)}{\psi_{sc}(a,1,-ik\zeta)} \right\}$$

$$+ \zeta \Re \left\{ \frac{U(2-i\eta,1,-ik\zeta)}{\psi_{sc}(a,1,-ik\zeta)} \right\},$$

$$(t + t_{0})_{sc} = \frac{h}{2E} \cdot \Re \left( \frac{\partial \psi_{sc}(x',y',z)}{\psi_{sc}(x',y',z)} \right)_{\varphi=0},$$

where $x,y$ are correlated by (6.14).

For $r \to \infty, \theta \to \pi, x \to -\infty$

$$(t + t_{0})_{m} \simeq \frac{h}{2E} \cdot \Im \left\{ ikx + i\eta \log(ik\zeta) + \eta \zeta \log(ik\zeta) \right\} = \frac{h}{2E} \left\{ kx + \eta \log(k\zeta) - \eta \right\}. \quad (6.17)$$

For $r \to \infty, \theta \to \theta_{sc}$

$$(t + t_{0})_{sc} \simeq \frac{h}{2E} \cdot \Re \left\{ ikx + i\eta \log(ik\zeta) + \eta \zeta \log(ik\zeta) \right\}$$

$$= \frac{h}{2E} \left\{ kx - \eta \log(k\zeta) + \eta \Re \left\{ \psi(1-i\eta) + \psi(i\eta) \right\} + \eta^2 \zeta \right\}. \quad (6.18)$$

These asymptotic times for the remote point from the origin of the potential correspond well to the values in the classical mechanics (5.18) and (5.19).

Examples of Temple mode trajectory and dynamics are shown in Fig. 4 and Fig. 5.

### 6.1 Cross section

In the Temple coordinate system $x, \zeta, z$ the impact parameter $s$, or angular momentum $ps = hks = h\ell$ and the energy $E = (h\ell)^2/(2m)$ determine the dynamics of the scattering electron. The scattering angle $\theta_{sc} = -2 \arctan(Zme^2/(2Es))$ is correlated in the same way in both classical mechanics (5.19) and wave mechanics (6.14). Therefore the dependence of the cross section on the scattering angle is the same as (6.10)

$$\sigma(\theta_{sc}) = \frac{s}{\sin \theta_{sc}} \frac{ds}{d\theta_{sc}} = \frac{\eta^2}{4k^2} \csc^2 \left( \frac{\theta_{sc}}{2} \right). \quad (6.19)$$

### 7 Numerical results and discussions

In the remote region from the origin the m-trajectory in the spherical polar or Temple coordinates is very similar to the corresponding classical orbit but in the region near the neighbourhood of the center of the potential the trajectory function is too complex to see the characteristics of the motion. It is necessary to analyse numerically the trajectory near the origin in detail to judge the validity of the m-trajectory.

Scattering angle $\theta_{sc}$ as a function of the impact parameter $s$ of an incident electron with energy 20eV for $Z = 1$ for the classical orbit (red circle) (5.15), or Temple m-trajectory (6.14) and for the m-trajectory.
in the spherical polar coordinates (black dot) is shown in Fig. 2. Figure 2 indicates that \( \nu + 1/2 \) in the m-trajectory in the spherical polar coordinates has the same role as \( ks = \ell \) in classical mechanics. Thus the differential cross section for the m-trajectory should be given by (4.54).

![Figure 2: Scattering angle of an incident electron with \( E = 20eV, Z = 1 \) as a function of \( ks \) for the classical orbit or Temple trajectory (red circle) and as that of \( \nu + 1/2 \) for the m-trajectory in the spherical polar coordinates (black dot).](image)

An example of the differential cross section of an electron beam of incident energy 2000eV by nuclear charge \( Z = 6 \) for the classical orbit and that for the m-trajectory are shown in Fig. 3. The figures indicate that the similarity between the cross sections of the classical orbits and the m-trajectories seems complete for any values of charge \( Z \) and energy \( E \). The difference between them is the existence of the limit of the scattering angle given by (4.55) in the mode trajectory while \( \theta_{sc} \to -\pi \) for \( ks \to 0 \) in the classical orbit.

Examples of the m-trajectory in the spherical polar and Temple coordinates for some parameters of \( \nu, L = hks = hl, E = 20eV, Z = 1 \) and scattering angle \( \theta_{sc} \) with the corresponding orbit of classical mechanics are shown in Figs. 4 and 5. In the remote region from the origin of the potential the m-trajectory and classical orbit correspond well and thus the behavior in the neighbourhood of the origin are to be investigated in detail.

Figures 4 and 5 by a detailed numerical calculation indicate a lack of the Temple m-trajectory and an irregular time elapse in a small region near the origin, although in the region outside of the small region the trajectory is almost equal to the corresponding orbit of classical mechanics.

The m-trajectory in the polar coordinate system is sound. But for the m-trajectory with \(-1/2 < \nu < 0\) which might be considered to exist the time elapse in the neighbourhood of the origin has a peculiar character. It has been clarified by numerical calculation. It suggests that \( \nu \) should be non-negative.
Figure 3: Differential cross section as a function of the scattering angle of an incident beam with $E=2000\text{eV}$, $Z=6$ for the classical orbits or Temple trajectories (red box) and for the $m$-trajectories (black dot).

Figure 4: Dynamics of a scattering electron near the center of the hydrogen with Energy=20eV, $\nu = 0.629$, $m$-trajectory (black); Temple $m$-trajectory (blue) and the classical orbit (green line) with $k s = 1.2, s = 52.4\text{pm}$. Parameters $\nu$ and $ks$ have been set so that the scattering angle is all the same $\theta_{sc} = -69^\circ$. 
Figure 5: Another example of dynamics of a scattering electron with $E = 20\text{eV}$, $\nu = 1.2$, $ks = 1.79$, $\theta_{sc} = -49.5^\circ$. Other specifications are the same as Fig. 4.

8 Conclusion

The Schrödinger wave equation can describe the mode trajectory and dynamics of an electron of the Coulomb scattering in the space-time if the wave function is well manipulated to treat the motion of the particle. It is similar to the classical motion especially in the remote region from the origin of the potential as it should be.

The mode trajectory in Temple coordinates is not complete specifically in the near region around the origin of the potential.

The mode trajectory and dynamics in the spherical polar coordinates for $\nu \geq 0$ and $E > 0$ is sound. It may be proved by an experiment to show the existence of the limiting scattering angle.

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