Electron trajectory in the hydrogen atom

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A trajectory in the Schrödinger wave for an electron in an attractive Coulomb potential with the dynamical behavior is proposed and illustrated for a scattering and a bound state. The scattering cross section derived from the trajectories is almost exactly equal to that from the usual wave theory. The statistical nature of the result is examined. The period of one cycle in the bound state is exactly equal to that of the corresponding classical motion.

1 Introduction

Nowadays, we can move an atom to put on the arbitrary positions on metal. We can measure whether one electron adhered to the capacitor. There is no uncertainty to operate one atom. We also have ascertained that there is no indeterminacy on determining a submicron diameter by a longer wavelength laser precisely. It would be one of the urgent requisites to make a dynamical equation of motion of an atomic scale ‘particle’ without any contradiction to the wave theory.

The trajectory of the harmonic oscillator in the wave equation has been discussed. Since the system treats only the bound state, the statistical nature, one of the important characteristics, in quantum theory can not be seen clearly. In the present paper, by using the method of the mcf, a trajectory of an electron in an attractive Coulomb potential, like the hydrogen atom in a state with a positive or negative energy, is proposed. On discussing the cross section for the scattering state, the statistical but in principle determinate nature like classical mechanics will be seen as an illustration.

In section 2 the dynamical theory that would lead to a trajectory is described. The traveling waves and usual stationary wave functions are discussed. In section 3 the trajectory of an electron in the scattering state by the Coulomb potential is investigated. In sections 4 and 5 the cross section and the flux of the beam of particles are discussed. In section 6 the trajectory of an electron in the hydrogen atom in a bound state is analyzed and illustrated. Conclusion and remarks on the wave functions are given in section 7.

2 Dynamics and wave function

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

$$i\hbar \frac{\partial \Psi(r, t)}{\partial t} = \left( -\frac{\hbar^2}{2m} \nabla^2 - \frac{e^2}{r} \right) \Psi(r, t), \quad (1)$$

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

$$\Psi(r, t) = e^{-iEt/\hbar} \Phi_1(x_1, E, \alpha)\Phi_2(x_2, \alpha, \beta)\Phi_3(x_3, \beta), \quad (2)$$
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

\[
\Phi_j(x_j) = \sqrt{P_j(x_j)} \exp\{iW_j(x_j)\}, \quad j = 1, 2, 3,
\]

is sought, where functions \( P_j \)'s and \( W_j \)'s are real. This should be called a traveling wave. Let functions \( W_j \)'s satisfy the condition that in each classical region of \( x_j \) for \( j = 1, 2, 3 \)

\[
W_j(x_j) \approx W_j(x_j)_{cl},
\]

where the sum of them

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

is the Hamilton characteristic function of the Hamilton-Jacobi equation in classical mechanics. 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

\[
W(x_1, x_2, x_3, E, \alpha, \beta) = W_1(x_1, E, \alpha) + W_2(x_2, \alpha, \beta) + W_3(x_3, \beta)
\]

is named the mode characteristic function (mcf) for the system.

The equations of motion for the electron are assumed

\[
\frac{\partial W}{\partial E} = \frac{1}{\hbar}(t - t_0), \quad \frac{\partial W}{\partial \alpha} = c_{\alpha}, \quad \frac{\partial W}{\partial \beta} = c_{\beta},
\]

where \( t_0, c_{\alpha} \) and \( c_{\beta} \) are constants (independent of \( t \)) that are determined by initial conditions for the system. Variable \( t \) is considered the dynamical time for the system. The trajectory derived from Eqs. (7) should be called the mode trajectory.

The square integrable wave function is obtained as follows. Let the endpoints of the \( x_j \) coordinate be \( a_j \) and \( b_j \). The electron moves in the region \( a_j \leq x_j \leq b_j \). Let it start from a point \( x_{j0} \) to the increasing \( x_j \) direction and the mcf in the coordinate space be \( W_j(x_j) \). The traveling wave associated with the motion reversing from \( b_j \) to \( a_j \) should be assumed to be given by \( \sqrt{\rho_j(x_j)} \exp[i\{−W_j(x_j) + 2W_j(b_j)\}] \), which is also the solution of Eq. (7).

The wave observed at \( x_j (\geq x_{j0}) \) should be the superposition of the traveling waves associated with the alternating motion of the electron

\[
\Phi_j(x_j) - \Phi_j^*(x_j)e^{i2W_j(b_j)}.
\]

This is finite, zero, at \( b_j \). If the electron turns at \( a_j \) and runs to \( x_{j0} \), the mcf should be assumed to be given by \( W_j(x_j) - 2W_j(a_j) + 2W_j(b_j) \). The wave function for \( x_j (\leq x_{j0}) \) is written as

\[
-\Phi_j^*(x_j)e^{i2W_j(b_j)} + \Phi_j(x_j)e^{i(−2W_j(a_j)+2W_j(b_j))}.
\]

This is finite, zero, at \( a_j \). The wave functions (8) and (9) are finite for \( a_j \leq x_j \leq b_j \) for any ‘mode’ with real values of parameters. They are not always equal at \( x_{j0} \). As a wave function, it might be multi-valued. If and only if \( 2[W_j(b_j) - W_j(a_j)] \) is a multiple of \( 2\pi \), they are equal and constitute a stationary wave function in \( a_j \leq x_j \leq b_j \).

In what follows, the wave equation (7) is analyzed in the polar coordinate system, \((r, \theta, \phi)\). The Hamilton characteristic function is summarized as follows:

\[
W_{cl}(r, \theta, \phi, E, l, \mu) = W_{r,cl}(r, E, l) + W_{\theta,cl}(\theta, l, \mu) + \mu \hbar,
\]
where \( W_{r,cl} \) and \( W_{\theta,cl} \) are determined from equations
\[
\frac{1}{2m} \left[ \left( \frac{\partial W_{r,cl}}{\partial r} \right)^2 + \frac{l^2 \hbar^2}{r^2} \right] - \frac{e^2}{r} = E, \quad (11)
\]
\[
\left( \frac{\partial W_{\theta,cl}}{\partial \theta} \right)^2 + \frac{\mu^2 \hbar^2}{\sin^2 \theta} = l^2 \hbar^2. \quad (12)
\]

Here, \( E \) stands for the energy and will be expressed in terms of \( \eta_s, (24) \), for the scattering state or \( \eta, (76) \), for the bound state. Parameters \( l \) and \( \mu \) are real numbers and \( l \hbar \) stands for the angular momentum and \( \mu \hbar \) is one of its components. These expressions have been introduced for convenience for comparison with the quantum theory.

### 3 Scattering state

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, \( E, \nu \) and \( \mu \) as
\[
\Psi(r,t) = \exp \left( -\frac{iEt}{\hbar} \right) \Phi(r,E), \quad (13)
\]
\[
\Phi(r,E) = R(r,E,\nu)Y(\theta,\nu,\mu) \exp(i\mu \phi). \quad (14)
\]

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 numbers as will be seen in Eqs. (15) and (21). [6]

The mcf expressed in terms of the spherical polar coordinates are obtained as follows. The function \( Y(\theta,\nu,\mu) \) satisfies the differential equation
\[
\left[ \frac{d^2}{d\theta^2} + \cot \theta \frac{d}{d\theta} + \nu(\nu + 1) - \frac{\mu^2}{\sin^2 \theta} \right] Y(\theta,\nu,\mu) = 0. \quad (15)
\]

The solution is a linear combination of linearly independent associated Legendre functions, \( P_{\nu}^{\mu}(\cos \theta) \) and \( Q_{\nu}^{\mu}(\cos \theta) \). [7] A traveling wave in the \( \theta \) coordinate space is given by
\[
Q_{\nu}^{\mu}(\cos \theta) + \frac{i\pi}{2} P_{\nu}^{\mu}(\cos \theta) = \left[ \frac{2}{\pi} \sin \theta \frac{\partial W_{\theta}}{\partial \theta} \right]^{-1/2} \exp \left[ iW_{\theta}(\theta,\nu,\mu) \right] \equiv \sqrt{P_{\theta}} e^{iW_{\theta}}. \quad (16)
\]

The mcf for the \( \theta \) component should be determined as
\[
W_{\theta}(\theta,\nu,\mu) = \arctan \left[ \frac{\pi P_{\nu}^{\mu}(\cos \theta)}{2 Q_{\nu}^{\mu}(\cos \theta)} \right], \quad (17)
\]
because of the similarity to the characteristic function \( W_{r,cl} \) in the classical region and the validity of the results derived from this as will be seen in the following.

An expression for function \( \tan(W_{\theta}) \) is written for \( 0 < \theta < \pi \) as [8]
\[
\frac{\pi P_{\nu}^{\mu}(\cos \theta)}{2 Q_{\nu}^{\mu}(\cos \theta)} = \sum_{k=0}^{\infty} \frac{(1/2 + \mu)_k (1 + \nu + \mu)_k}{k!(\nu + 3/2)_k} \sin[(2k + \nu + \mu + 1)\theta]/
\]
\[
\sum_{k=0}^{\infty} \frac{(1/2 + \mu)_k (1 + \nu + \mu)_k}{k!(\nu + 3/2)_k} \cos[(2k + \nu + \mu + 1)\theta]. \quad (18)
\]
The value of $W_\theta$ at $\theta = 0$ or $\pi$ is

$$W_\theta(0) \equiv W_\theta(0, \nu, \mu) = \pi \mu, \quad W_\theta(\pi) \equiv W_\theta(\pi, \nu, \mu) = \pi \nu. \quad (19)$$

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

$$W_\theta(\theta, \nu, \mu) \approx (\nu + \frac{1}{2}) \theta + (\frac{1}{4} + \frac{1}{2} \mu) \pi, \quad (\epsilon < \theta < \pi - \epsilon, \epsilon > 0). \quad (20)$$

Both the derivative $\partial W_\theta / \partial \nu$ and $\partial W_\theta / \partial \mu$ are monotonic as a function of $\theta$ and very similar to those of the characteristic function $W_{\theta, cl}$ in a restricted (or classical) region as found by a computer calculation.

Radial wave function satisfies the differential equation

$$\left[ \frac{d^2}{dr^2} - \frac{\nu(\nu + 1)}{r^2} + \frac{2m}{h^2} \left( \frac{e^2}{r} + E \right) \right] u(r) = 0, \quad (21)$$

where $u(r, E, \nu) = rR(r, E, \nu)$.

With $E$ positive the linearly independent solutions are

$$u_M = e^{-i\rho} \rho^{\nu+1} M(\nu + 1 + i\eta_s, 2\nu + 2, i2\rho), \quad (22)$$

$$u_V = e^{-i\rho} \rho^{\nu+1} V(\nu + 1 + i\eta_s, 2\nu + 2, i2\rho), \quad (23)$$

where

$$\rho = \sqrt{\frac{2mE}{h^2}} r, \quad \eta_s = \frac{e^2}{\hbar} \sqrt{\frac{m}{2E}}. \quad (24)$$

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

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

$$= -\pi \cot \pi b \frac{\Gamma(b-a)}{\Gamma(b)\Gamma(1-a)} M(a, b, z)$$

$$+ \Gamma(b-1)z^{1-b} M(1+a-b, 2-b, z). \quad (25)$$

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

For the far region from the center of the potential, $\rho \gg 1$, by putting $a = \nu + 1 + i\eta_s$ and $b = 2\nu + 2$, it holds that

$$M(a, b, i2\rho) \simeq e^{i\rho} \Gamma(b) \left[ \frac{e^{-i(\rho - \pi a/2)}}{\Gamma(a^*)} (2\rho)^{-a} \left( 1 + \frac{ia(1 - a^*)}{2\rho} \right) + c.c. \right], \quad (26)$$

$$V(a, b, i2\rho) \simeq e^{i\rho} [-i \sin(\pi a) G(\rho, a) - \cos(\pi a) G(\rho, a)^*], \quad (27)$$

where

$$G(\rho, a) = \Gamma(a) e^{-i(\rho - \pi a/2)} (2\rho)^{-a} \left( 1 + \frac{ia(1 - a^*)}{2\rho} \right), \quad (28)$$

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 traveling wave in the far region from the origin should be written as

$$u = e^{-i\rho} \rho^{\nu+1} \left[ V(a, b, i2\rho) + iM(a, b, i2\rho) \sin(\pi a) \frac{\Gamma(a)\Gamma(b-a)}{\Gamma(b)} \right]. \quad (29)$$
By equations mentioned above, this leads to

\[ u \approx e^{-i\pi\nu}e^{\frac{1}{2}i\pi\eta_s}2^{-1-\nu} |\Gamma(a)| \exp[i(\rho + \eta_s \log(2\rho) - \arg \Gamma(a) - \frac{1}{2}\pi(1 + \nu))] \times \left(1 + i \frac{\nu(1 + \nu) + \eta_s^2}{2\rho} - \frac{\eta_s}{2\rho} + O(\rho^{-2})\right), \]

for \( \rho \) large. It would suggest that the traveling wave in the \( r \) coordinate space should be given by

\[ u = u_V + i u_M \sin(\pi a)\frac{\Gamma(a)\Gamma(b - a)}{\Gamma(b)} \equiv e^{-i\pi\nu}(u_R + i u_I) \]

\[ = e^{-i\pi\nu} \sqrt{u_R^2 + u_I^2} \exp\left(i \arctan \frac{u_I}{u_R}\right) \equiv e^{-i\pi\nu} \sqrt{P_r} e^{iW_r}, \]

and thus the mcf in the \( r \) coordinate is given by

\[ W_r(r, E, \nu) = \arctan \frac{u_I}{u_R}. \]

Here, functions \( u_R \) and \( u_I \) have been assumed to be real. The parameter \( \nu \) is a real number. The ratio \( u_R/u_I \) is written as

\[ \frac{u_I}{u_R} = \frac{\cos(\pi b) - \exp(-2\pi\eta_s)}{\sin(\pi b)} - H, \]

\[ H = 2^{2-b} \frac{\Gamma(b-1)}{\Gamma(a)|^2} \exp(-\pi\eta_s)\rho^{1-b}M(a+1-b, 2-b, i2\rho)M(a,b,i2\rho). \]

Function \( H \) is real since it holds by Kummer’s transformation that

\[ e^{-i\rho}M(a, b, i2\rho) = e^{i\rho}M(a, b, i2\rho)^*, \]

\[ e^{-i\rho}M(a + 1 - b, 2 - b, i2\rho) = e^{i\rho}M(a + 1 - b, 2 - b, i2\rho)^*. \]

Function \((14)\) with expressions \((16)\) and \((31)\) specifies a traveling wave associated with the motion of an electron in the 'mode' \((E, \nu, \mu)\) in the scattering state.

In the far region from the origin the mcf is approximated as

\[ W_r(r, E, \nu) \approx \rho + \eta_s \log 2\rho - \arg \Gamma(a) - \frac{1}{2}\pi(1 + \nu) + \frac{\nu(1 + \nu) + \eta_s^2}{2\rho} + O(\rho^{-2}). \]

This is nearly equal to the corresponding Hamilton characteristic function. It indicates the validity of the definition of the mcf \((32)\). For \( r \) small, it is obtained that

\[ W_r(0) \equiv W_r(0, E, \nu) = \frac{1}{2}\pi. \]

The mcf in the spherical polar coordinates is summarized as

\[ W(r, \theta, \phi, E, \nu, \mu) = \pm W_r(r, E, \nu) \pm W_\theta(\theta, \nu, \mu) \pm \mu \phi, \]

where the sign should be adopted according to the direction of the motion of the particle in each coordinate. Equations of motion \((7)\) with \( r, \theta, \phi, \nu \) or \( \mu \) in place of \( x_1, x_2, x_3, \alpha \) or \( \beta \), respectively, lead to a trajectory of the electron.
To get the trajectory, it is necessary to calculate derivatives $\partial W_r/\partial E$ and $\partial W_r/\partial \nu$. It is obtained from Eqs. (32) and (33) that

$$\frac{\partial W_r}{\partial \nu} = \frac{1}{1 + (u/I/u_R)^2} \frac{\partial}{\partial \nu} \left( \frac{u_I}{u_R} \right),$$

$$\frac{\partial}{\partial \nu} \left( \frac{u_I}{u_R} \right) = 2\pi \exp(-2\pi\eta_s) \cos \pi b - 1 - H \left[ 2(\psi(b - 1) + \psi(b) - \log 2\rho) \right.$$

$$- \psi(a) - \psi(a^*) - \frac{1}{M_2} \left( \frac{\partial M_2}{\partial a} + 2\frac{\partial M_2}{\partial b} \right)$$

$$- \frac{1}{M} \left( \frac{\partial M}{\partial a} + 2\frac{\partial M}{\partial b} \right) \right], \quad (40)$$

where $M = M(a, b, i2\rho)$, $\psi(b)$ is the psi (digamma) function and

$$M_2 = M(a + 1 - b, 2 - b, i2\rho) = M(-\nu + i\eta_s, -2\nu, i2\rho). \quad (41)$$

For example, a trajectory of an electron incident from a point distant from the origin of the potential, $(\rho_0, \theta_0, \phi_0)$, and scattered to another distant point is considered. To be specific, that $\rho_0 = \infty$ and $\theta_0 = 0$ is assumed. For the trajectory from $\rho_0$ to the origin, the mcf is written as

$$W(r, \theta, \phi, E, \nu, \mu) = -W_r + W_\theta + W_\phi, \quad (42)$$

where $W_\phi = \mu\phi$. The trajectory is given by the equations (42), or

$$\frac{\partial}{\partial \nu} (-W_r + W_\theta) = \frac{\partial}{\partial \nu} (-W_r(\infty) + W_\theta(0)) = \frac{\partial}{\partial \nu} \arctan(a) + 1/2\pi, \quad (43)$$

$$\frac{\partial}{\partial \mu} (W_\theta + W_\phi) = \frac{\partial}{\partial \mu} W_\theta(0) + \phi_0 = \pi + \phi_0. \quad (44)$$

For the path from the origin to $\rho_\pi \equiv \rho(\theta = \pi)$, the mcf is given by

$$W(r, \theta, \phi, E, \nu, \mu) = W_r + W_\theta + W_\phi - 2W_r(0). \quad (45)$$

This has been taken to be continuous to the incident mcf, (42), at the origin.

The trajectory equation is written as

$$\frac{\partial}{\partial \nu} (W_r + W_\theta - 2W_r(0))$$

$$= \frac{\partial}{\partial \nu} \arctan(a) + 1/2\pi, \quad (46)$$

and Eq. (44). Since function $\partial_r W_r$ shows monotonic decrease with respect to $\rho$ while $\partial_\theta W_\theta$ does monotonic increase with respect to $\theta$ as proved by the computer calculation, there is a point $\rho = \rho_\pi$ where $\theta$ takes $\pi$.

For the trajectory from $\rho_\pi$ to a distant scattered point, the mcf is written as

$$W(r, \theta, \phi, E, \nu, \mu) = W_r - W_\theta + W_\phi - 2W_r(0) + 2W_\theta(\pi). \quad (47)$$

The last term has been added to for the continuity of $W$ at the point $\rho = \rho_\pi$ to the expression (45).

The trajectory is given by

$$\frac{\partial}{\partial \nu} (W_r - W_\theta - 2W_r(0) + 2W_\theta(\pi)) = \frac{\partial}{\partial \nu} \arctan(a) + 1/2\pi$$

$$\phi = \frac{\partial}{\partial \mu} W_\theta + \pi + \phi_0. \quad (49)$$

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Fig. 1: A trajectory of an electron of the hydrogen atom in the scattering ‘mode’ with parameters $\eta_s = 3.3, \nu = 2.2, \mu = 1.1$, (solid line) and the classical orbit with $\eta_s = 3.3, l = 2.7, \mu = 1.1$, (circle).

The equations of the trajectory prescribed above are more easily seen if the approximate relation (20) is used. It shows that coordinate $\phi$ is constant except the point of $\rho_\pi$ where $\theta = \pi$. This indicates that the trajectory is almost on a plane like the classical orbit.

An example of a trajectory of the electron with parameters $\eta_s = 3.3, \nu = 2.2, \mu = 1.1$, projected on a plane, is shown with the corresponding classical orbit with $\eta_s = 3.3, l = 2.7, \mu = 1.1$, in Fig. 1.

The corresponding classical orbit, as is well known, is very similar to this trajectory except the neighborhood of the origin.

4 Cross section

Along the line of thought of classical mechanics, the cross section will be determined by the mode trajectory.

The differential cross section for the classical orbits of uniform incident beam is given by

$$\sigma(\theta)_{el} = \frac{e^4}{16E^2} \frac{1}{\sin^4(\theta/2)} = \left(\frac{\hbar^2}{me^2}\right)^2 \eta_s^2 \eta_s^2 \frac{1}{4 \sin^4(\theta/2)}.$$  (50)

where $\theta$ is the scattering angle of the electron beam and parameter $\eta_s$ (24) has been used. This is equal to that obtained in quantum mechanics not to mention. The scattering angle is expressed, in terms of the angular momentum $\hbar l$ and energy $E$, as

$$\theta = 2 \arctan \left( \sqrt{\frac{m}{2E \hbar}} \frac{e^2}{\hbar} \right).$$  (51)

The impact parameter, $s$, is related to the angular momentum as $s = \hbar \sqrt{2mE}$.  

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Equation (48) leads to the scattering (or deviated) angle of the electron trajectory, by taking \( \rho = \infty \) and using the approximate relation (20), or \( \partial W_{\eta=\infty} \approx \theta \),

\[
\theta_{sc} = \pi - \frac{\partial}{\partial \nu} W_{\theta, \rho=\infty} = 2 \frac{\partial}{\partial \nu} \arg \Gamma(a). \tag{52}
\]

In the remote region from the origin, equation (37) shows that the difference between two positions along the trajectory satisfies

\[
\frac{d\theta}{d\rho} = -\frac{\nu + \frac{1}{2}}{\rho^2}. \tag{53}
\]

Integration gives rise to \( \theta_0 = \nu + \frac{1}{2} \). It is thus obtained that the impact parameter of the trajectory is given by

\[
s = r\theta = (\nu + \frac{1}{2})\hbar / \sqrt{2mE}. \tag{54}
\]

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

![Fig. 2: Scattering angle as a function of the impact parameter of an incident beam for the classical orbit (circle) and for the trajectory (solid line) with \(\eta_s = 2\).](image)

An example of the scattering angle of an incident beam as a function of the impact parameter for the classical orbit (circle) and for the trajectory (solid line) with \(\eta_s = 2\).

The differential cross section for the trajectories of uniform incident beam of the electron is obtained in the same way as the classical one, by using (52).

\[
\sigma(\theta_{sc}) = \frac{s}{\sin \theta_{sc}} \left| \frac{ds}{d\theta_{sc}} \right| = \frac{(\nu + \frac{1}{2})\hbar^2}{2mE \sin \theta_{sc}} \left| \frac{d\nu}{d\theta_{sc}} \right| = \left( \frac{\hbar^2}{mE^2} \right) \frac{\eta_s^2 (\nu + \frac{1}{2})}{2 \sin^2 \theta_{sc}} \left| \frac{\partial^2}{\partial \nu^2} \arg \Gamma(a) \right|^{-1}. \tag{55}
\]

Parameter \(\nu\) in the right hand side should be expressed in terms of \(\theta_{sc}\) through (52).
Fig. 3: Differential cross section as a function of the scattering angle of an incident beam for the classical orbit (circle) and for the trajectory (solid line) with \( \eta_s = 2 \).

An example of the differential cross section of an electron beam for the classical orbit and that for the trajectory are shown in Fig. 3.

The figures indicate that the similarity between the cross sections of the classical orbits and the trajectories is, as it were, complete.

5 Flux

The usual wave function for the Coulomb scattering is given, by Gordon, as \[ \psi(r, \theta) = \sum_{l=0}^{\infty} (2l + 1)^{i} l^{i} \exp(-i \arg \Gamma(1 + l + i\eta_s)) L_l(r) P_l(\cos \theta) \] (56)

where \[ L_l(r) = \frac{2^{l+1} \exp(-\pi/2\eta_s)}{\rho |\Gamma(1 + l + i\eta_s)|} u_0(r). \] (57)

By using (56) and (31), it can be composed of a linear combination of the travelling waves with parameters \( \eta_s, \nu = l \) and \( \mu = 0 \)

\[
\psi(r, \theta) = \sum_{l=0}^{\infty} (2l + 1) \frac{(2l)!}{\pi \Gamma(1 + l + i\eta_s)} \left( \sqrt{P_r} e^{-iW_r} - \sqrt{P_r} e^{i(W_r - 2W_r(0))} \right) \\
\times \left( \sqrt{P_\theta} e^{iW_\theta} - \sqrt{P_\theta} e^{-i(W_\theta - 2W_\theta(\pi))} \right). 
\] (58)

For \( r \) large, it is approximately expressed as \[ \psi(r, \theta) \approx \exp(i(\rho \cos \theta - \eta_s \log \rho(1 - \cos \theta)) + \frac{\eta_s}{\rho(1 - \cos \theta)}) \]
\[ \times \exp(i[p + \eta_s \log \rho(1 - \cos \theta) + \pi - 2 \arg \Gamma(1 + i\eta_s)]). \] (59)
The flux (or current) of beam of particles is defined by

\[ j = \frac{1}{2m} \psi^* \frac{\hbar}{i} \nabla \psi + \text{c.c.} \quad (60) \]

The first term of the right-hand side of the wave function (59) gives rise to the incident flux propagating along the \( z \) axis for \( r \) large

\[ j_{\text{in}} = \frac{\hbar k}{m} \hat{z}. \quad (61) \]

The second term, on the other hand, gives rise to the outgoing flux

\[ j_{\text{out}} = \frac{\hbar k}{m} \frac{\eta_s^2}{\rho^2 (1 - \cos \theta)^2} \hat{r}. \quad (62) \]

The number of particles in the outgoing flux in a solid angle is

\[ \frac{r^2 j_{\text{out}} \cdot \hat{r}}{\hbar k/m} = \left( \frac{\hbar^2 \eta_s}{m c^2} \right)^2 \frac{\eta_s^2}{4 \sin^4 \frac{1}{2} \theta}, \quad (63) \]

which gives the differential cross section.

According to the interpretation envisaged with Gordon's work, the deviated beam should be obtained through the scattering of incident particles with various impact parameters. The outgoing flux is considered to be an assemblage of particles which, in classical mechanics sense, should be governed by a plausible causal dynamics.

In the present treatment, the associated wave with the motion of an electron with \( \eta_s, \nu \) and \( \mu = 0 \), may be expressed, for \( r \) large, as

\[ \psi(r, \theta)_\nu \simeq \sqrt{P_r P_\theta} e^{-i(W_r - W_\theta)} + \sqrt{P_r P_\theta} e^{i(W_r - W_\theta + (2\nu - 1)\pi)} \equiv \psi_{\nu, \text{in}} + \psi_{\nu, \text{out}}. \quad (64) \]

It holds approximately that

\[ P_r \simeq \rho^{-2} 2^{-2\nu + 2} e^{\pi \eta_s} |\Gamma(1 + \nu + i\eta_s)|^2, \quad P_\theta \simeq \frac{\pi}{(2\nu + 1) \sin \theta}. \quad (65) \]

The wave for a beam of particles with various impact parameters should be written as

\[ \psi(r, \theta) = \sum_\nu a_\nu \psi(r, \theta)_\nu, \quad (66) \]

where \( a_\nu \) is an arbitrary constant which will indicate the intensity and initial phase of the wave (64).

The flux is written

\[ j = \frac{1}{2m} \sum_\nu \sum_{\nu'} a_\nu^* a_{\nu'} \psi_{\nu'}^* \frac{\hbar}{i} \nabla \psi_{\nu'} + \text{c.c.} \equiv \sum_\nu \sum_{\nu'} j_{\nu, \nu'}. \quad (67) \]

For \( r \) large, the incident waves \( \psi_{\nu, \text{in}} \)'s give rise to the incident flux

\[ j_{\nu, \nu', \text{in}} \simeq \frac{\hbar k}{m} \frac{|a_\nu a_{\nu'}|}{\rho^2 \sin \theta_{\text{in}}} \pi \exp(\pi \eta_s) \frac{|\Gamma(1 + \nu + i\eta_s)\Gamma(1 + \nu' + i\eta_s)|}{\sqrt{(2\nu + 1)(2\nu' + 1)}} \times \cos \left( -\arg \Gamma(1 + \nu + i\eta_s) + \arg \Gamma(1 + \nu' + i\eta_s) \right. \\
- \left. \left( \theta + \frac{1}{2} \arctan(\nu - \nu') + \arg(a_\nu^* a_{\nu'}) \right) \right). \quad (68) \]
Similarly, the outgoing waves $\psi_{\nu,\text{out}}$'s give rise to the scattered flux

$$
\mathbf{j}_{\nu\nu',\text{out}} \simeq \frac{\hbar k}{m} \rho^2 \sin \theta_{\text{out}} \frac{\pi \exp(\pi \eta_s)}{\sqrt{(2\nu + 1)(2\nu' + 1)}} \frac{\Gamma(1 + \nu + i\eta_s)\Gamma(1 + \nu' + i\eta_s)}{2^\nu+\nu'+2} \times \cos(\arg \Gamma(1 + \nu + i\eta_s) - \arg \Gamma(1 + \nu' + i\eta_s))$$

$$+ (\theta + \frac{1}{2}\pi)(\nu - \nu') - 2\pi(\nu - \nu') + \arg(a_\nu^*a_{\nu'})).$$  

(69)

For $\nu \simeq \nu'$,

$$\arg \Gamma(1 + \nu + i\eta_s) - \arg \Gamma(1 + \nu' + i\eta_s) \simeq (\nu - \nu')\partial_\nu \arg \Gamma(1 + \nu + i\eta_s).$$

From (72),

$$\theta_{\text{out}} = \pi - (\theta_{\text{scat}} + \theta_{\text{in}}) = \pi - 2\partial_\nu \arg \Gamma(1 + \nu + i\eta_s) - \theta_{\text{in}},$$

where $\theta_{\text{in}}$ is written as $\theta_0$ in a preceding section. Thus, the argument of cosine in $\mathbf{j}_{\nu\nu',\text{out}}$ with $\theta_{\text{out}}$ equals that of cosine in $\mathbf{j}_{\nu\nu',\text{in}}$ with $\theta_{\text{in}},$

$$\arg \Gamma(1 + \nu + i\eta_s) - \arg \Gamma(1 + \nu' + i\eta_s) + (\theta + \frac{1}{2}\pi)(\nu - \nu')$$

$$- 2\pi(\nu - \nu') + \arg(a_\nu^*a_{\nu'})$$

$$\simeq (\nu - \nu')(\partial_\nu \arg \Gamma(1 + \nu + i\eta_s) + \theta_{\text{out}} + \frac{3}{2}\pi) + \arg(a_\nu^*a_{\nu'}).$$

(70)

It is seen thus that for $\rho \gg 1$

$$\mathbf{j}_{\nu\nu',\text{in}} \cdot (-\mathbf{r}) \rho^2 \sin \theta_{\text{in}} = \mathbf{j}_{\nu\nu',\text{out}} \cdot \mathbf{R} \rho^2 \sin \theta_{\text{out}}.$$

(71)

If it is assumed that the incident beam $\mathbf{j}_{\nu\nu'}$ with $\nu'$ clearly different from $\nu$ is incoherent, $<\cos \arg(a_\nu^*a_{\nu'})>$ (average over the initial phases) = 0, the total flux may be expressed as

$$\sum_{\nu,\nu'} \mathbf{j}_{\nu\nu'} = \sum_{\nu < \nu'} \mathbf{j}_{\nu\nu'}.$$  

(72)

The current $\mathbf{j}_{\nu\nu'}$, with $\nu' \simeq \nu$ could be discriminated from the one $\mathbf{j}_{\mu\mu'}$ with $\mu' \simeq \mu$ clearly different from $\nu$ because of the difference of the impact parameter or the angular momentum. Then, expression (71) means that the flux density of particles along the trajectory is conserved for $r$ large, or the flux density of the incident beam is equal to that of the outgoing beam. Therefore, the cross section for the incoherent incident beam can be calculated like the classical mechanical beam as (53).

6 Bound state

An electron trajectory in a hydrogen atom in a bound state is analyzed. The solution of the form of expressions (13) and (14) with energy $E$ negative is sought. The mcf in the $\theta$ coordinate space, $W_\theta$, is the same in the preceding section. (17).

The traveling wave in the radial coordinate is obtained from Eq. (14) with replacement of $i\eta_s$ or $i\rho$ by $-\eta$ or $\rho$, respectively. By writing $u(r, E, \nu) = rR(r, E, \nu)$, a traveling wave is obtained

$$u = u_V + iu_M \sin \pi a \frac{\Gamma(a)\Gamma(b - a)}{\Gamma(b)},$$

(73)

where $a = \nu + 1 - \eta$, and $b = 2\nu + 2$. Functions $u_M$ and $u_V$ are given by

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

(74)

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

(75)
The mcf in the \( r \) coordinate space, \( W_r \), for the negative energy state is thus given by

\[
W_r(r, E, \nu) = \arctan \left[ \frac{\pi \Gamma(b-a) M(a,b,2\rho)}{\Gamma(1-a)\Gamma(b) V(a,b,2\rho)} \right].
\]  

(77)

The asymptotic forms of \( W_r \) at \( r = 0 \) or \( r = \infty \) are summarized in Appendix.

The mcf for the system is given by Eq. (39) with expression (77) in place of (32). The trajectory of one round trip is found to be that obtained for the classical orbit with the same energy. This suggests that the mcf, (77) with (17), respectively. The equations of motion are, from (86),

\[
\frac{\hbar}{E} W_r - t = \frac{\hbar}{E} W_r(0) - t_0 = -t_0,
\]  

(79)

\[
\frac{\partial}{\partial \nu} (W_r + W_\theta) = \frac{\partial}{\partial \nu} (W_r(0) + W_\theta(0)) = 0,
\]  

(80)

\[
\frac{\partial}{\partial \mu} (W_\theta + W_\phi) = \frac{\partial}{\partial \mu} W_\theta(0) + \phi_0 = \pi + \phi_0,
\]  

(81)

where \( \phi_0 \) is the value of \( \phi \) at the initial time \( t_0 \). The mcf for the successive motion from \( r = \infty \) to \( r = 0 \) is

\[
W = -W_r - W_\theta + 2W_r(\infty) + 2W_\theta(\pi) + W_\phi.
\]  

(82)

The equations of motion are

\[
t = t_0 - \frac{\hbar \pi \eta}{E} - \frac{\hbar}{E} W_r, \quad \frac{\partial}{\partial \nu} (W_r + W_\theta) = 0, \quad \phi = \frac{\partial}{\partial \mu} W_\theta + \pi + \phi_0.
\]  

(83)

where use has been made of \( \partial_\nu W_r(\infty) = -\partial_\nu W_\theta(\pi) = -\pi \), by (19), and (A.8) in Appendix.

The period of one round trip is found to be \(-\hbar \pi \eta/(-E) = 2\pi \sqrt{m/(2E)} \), which is just equal to that obtained for the classical orbit with the same energy. This suggests that the mcf, (77) with (17), is the right one and the mcf could be determined uniquely for the system with the mode parameters.

A trajectory of an electron in a bound state thus determined is illustrated for the ‘mode’ with parameters \( \eta = 3, \nu = 2, \mu = 1 \), and \( \phi_0 = 0 \) at \( t = t_0 \) in Fig. 4. Both of the trajectory or the corresponding classical orbit are projected on a plane. It could be recognized that the corresponding classical orbit resembles more to the trajectory as the mode parameters \( \eta \) and \( \nu \) become larger. This shows the correspondence principle.

The requirement that the associated wave (44) with the round trip motion of an electron should be unique everywhere leads to that each component of the mcf \( W_r, W_\theta \) or \( W_\phi \) must be unique at any
point except multiples of $2\pi$ and parameters $\eta$, $\nu$ and $\mu$ be integral numbers. It gives rise to the usual eigenvalues of the energy for the eigenstates. The wave functions associated with the motion in the $r$ and $\theta$ coordinates with $\eta$, $\nu$ and $\mu$ integral are composed of going and returning waves, Eqs. (8) and (9) with both $-2W_r(0) + 2W_r(\infty)$ and $-2W_\theta(0) + 2W_\theta(\pi)$ being a multiple of $2\pi$, or $[12, 13]

$$\sqrt{P_r}e^{iW_r} - \sqrt{P_r}e^{-iW_r}, \text{ and } \sqrt{P_\theta}e^{iW_\theta} - \sqrt{P_\theta}e^{-iW_\theta}. \quad (84)$$

These are regular for $0 \leq r < \infty$ and $0 \leq \theta \leq \pi$, respectively, and equivalent to the usual stationary state wave functions except numerical factors.

7 Conclusion

A trajectory of the electron in an attractive Coulomb potential has been shown. The trajectory resembles well the orbit of the corresponding state in classical mechanics. It runs also through a tunneling region. The trajectory has been derived from the mode characteristic function (mcf) which is an extension of the Hamilton characteristic function. The period of the round trip motion of the electron in the bound state is the same as that of the corresponding classical motion with the same mode parameters. The accordance of the characteristics between classical and quantum mechanics suggests the validity of the mcf and the dynamics defined.

It is to be noted that all solutions of the wave equation including waves diverging at singular points of the wave equation are necessary to derive the mcf. This suggests the role of all the solutions of the wave equation. It has been found that if the wave equation is decomposed into a set of single-variables $r$, $\theta$ and $\phi$, the resulting differential equations of 2nd order have each mcf uniquely, which should lead to a mode trajectory of an electron with some dynamical assumptions.
The wave function finite everywhere for any scattering or bound state is made by superposing the traveling waves associated with the electron motion. It is not always continuous for any bound state. The requirement that the wave function be continuous or uniquely determined at any point of the coordinate is equivalent to that the difference between the mcf’s at endpoints be a multiple of $\pi$. It leads to that the mode parameters are integral numbers and the eigenvalues of the physical quantities become discrete.

The discussion on the cross section and the flux suggests that the statistical nature of the wave theory stems from the fact that the wave consists of waves associated with the particle motion with each mode parameter which is causally determined. Not all the characteristics of statistical nature of the wave mechanics have been examined but this may be one of the most important characteristics.

These results indicate the consistent existence of the trajectory in wave mechanics and suggest a significance about the relation between a particle motion and a traveling wave function as an extension of the de Broglie postulate.

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A  Asymptotic form of $W_r(a, b, \rho)$

Asymptotic forms of $W_r(a, b, \rho)$ for negative energy states and its derivatives with respect to $E$ and $\nu$ are summarized. It holds from expression (77) that, by putting $F_r = \tan W_r$,

$$
\frac{\partial W_r}{\partial E} = -\frac{F_r}{2E(1 + F_r^2)} \left[ \eta \{ \psi(b - a) - \psi(1 - a) \} 
- \frac{1}{M} \left( \frac{\eta \partial M}{\partial a} + \frac{\eta \partial M}{\partial \rho} \right) + \frac{1}{V} \left( \frac{\eta \partial V}{\partial a} + \frac{\eta \partial V}{\partial \rho} \right) \right], \quad (A.1)
$$

$$
\frac{\partial W_r}{\partial \nu} = \frac{F_r}{1 + F_r^2} \left[ \psi(b - a) + \psi(1 - a) - 2\psi(b) 
+ \frac{1}{M} \left( \frac{\partial M}{\partial a} + 2 \frac{\partial M}{\partial b} \right) - \frac{1}{V} \left( \frac{\partial V}{\partial a} + 2 \frac{\partial V}{\partial b} \right) \right]. \quad (A.2)
$$

As $r$ tends to 0, it can be written for $b \geq 1$

$$
M(a, b, 2\rho) \approx 1 + \frac{2a}{b} \rho, \quad (A.3)
V(a, b, 2\rho) \approx \Gamma(b - 1) \left[ (2\rho)^{2 - b} - 1 \right]. \quad (A.4)
$$

By these approximations, it can be obtained that for $b \geq 1$

$$
W_r(0) = 0, \quad \frac{\partial W_r}{\partial E}(0) = 0, \quad \frac{\partial W_r}{\partial \nu}(0) = 0. \quad (A.5)
$$

Asymptotic forms for $r$ large with $a$ and $b$ fixed are

$$
M(a, b, 2\rho) \approx e^{2\rho(2\rho)^{a - b} \Gamma(b)} \Gamma(a), \quad (A.6)
V(a, b, 2\rho) \approx -e^{2\rho(2\rho)^{a - b} \Gamma(b - a)} \cos \pi a. \quad (A.7)
$$
These give rise to

\[ W_r(\infty) = -\pi a, \quad \frac{\partial W_r}{\partial E}(\infty) = \frac{\pi \eta}{2E}, \quad \frac{\partial W_r}{\partial \nu}(\infty) = -\pi. \]  

(A.8)

It is found that the variation of \( \partial W_r/\partial E \) between \( r = 0 \) and \( \infty \) is \( \pi \eta/(-2E) \).

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