Path integral method and rapid quantum computation

Huai-yang Cui

Department of Physics, Beihang University, Beijing, 100083, China
E-mail: hycui@buaa.edu.cn

A path integral method was developed according to the usual momentum-wavefunction relation, it is different from the Feynman's path integral. In order to investigate its validity and usefulness, the path integral method was applied to hydrogen atom,the energy levels were calculated out with the same fine structure as the calculation of the Dirac wave equation, the electronic spin effect was also calculated out correctly when the hydrogen atom is put in a magnetic field. The path integral method would be useful for some physical systems when for which the Dirac equation can not be solved exactly, it was pointed out that the path integral method is a rapid quantum computation method.

PACS: 03.65.Ge, 32.10.Fn
Key words: path integral, hydrogen atom, rapid quantum computation

1 Introduction

Consider a particle of rest mass m and charge q moving in an inertial frame of reference with the relativistic 4-vector velocity u_μ, it satisfies [1]

$$u_\mu u_\mu = -c^2 \,, \tag{1}$$

where there is not distinction between covariant and contravariant components in the Cartesian coordinate system. Eq. (1) is just the relativistic energy–momentum relation when multiplying it by squared the mass and the speed of light, i.e. $E^2 = p^2c^2 + m^2c^4$. Let A_μ denote the vector potential of electromagnetic field, substituting the usual momentum-wavefunction relation

$$mu_\mu = \frac{1}{\psi}(-\mathrm{i}\hbar\partial_\mu - qA_\mu)\psi \tag{2}$$

into Eq.(1), we obtain a new quantum wave equation

$$[(-\mathrm{i}\hbar\partial_\mu - qA_\mu)\psi] \cdot [(-\mathrm{i}\hbar\partial_\mu - qA_\mu)\psi] = -m^2c^2\psi^2 \,, \tag{3}$$

where the left hand side of the above equation corresponds to the product of momentum and momentum itself, not the product of momentum operator and momentum operator. Eq. (3) is a nonlinear quantum wave equation, is not the Klein–Gordon wave equation. In the recent years, the interest in Eq. (3) is increasing, it was found that by solving Eq. (3) for hydrogen atom, the fine structure of energy can be calculated correctly, the spin effect of electron can also been revealed by Eq,(3) in a magnetic field [2, 3, 4], it was also found that the Dirac wave equation and Klein–Cordon wave equation can be derived out from Eq. (3) when we abandon the higher order terms or nonlinear terms [5].

In the present paper, a path integral method based on the momentum-wavefunction relation was developed, it differs from the Feynman's path integral. The path integral method was applied to hydrogen atom, the energy levels were calculated out with the same fine structure and spin effect as the Dirac wave equation. It was pointed out that the path integral method is a rapid quantum computation method.

2 Path integral method

Consider Eq. (2), its path integral form is given by

$$\psi = \mathrm{e}^{\mathrm{i}/\hbar \int (p_\mu + qA_\mu)\mathrm{d}x_\mu} \,, \tag{4}$$

where $p_\mu = mu_\mu$ is the momentum of the particle, in the Cartesian coordinate system $(x_1, x_2, x_3, x_4 = \mathrm{i}ct)$, from the Eq. (1), the momentum components satisfy

$$p_1^2 + p_2^2 + p_3^2 + p_4^2 = -m^2c^2 \,. \tag{5}$$

In the following sections, in order to investigate the validity and usefulness of Eq. (4), we apply the path integral to hydrogen atom. Obviousely, the path integral Eq.(4) is different from the Feynman's path integral.

3 The fine structure of hydrogen atom

In the followings, we use Gaussian units, and use m_e to denote the rest mass of electron. In a spherical polar coordinate system $(r, \theta, \varphi, \mathrm{i}ct)$, the nucleus of hydrogen atom provides a spherically symmetric potential $V(r) = \dfrac{e}{r}$ for the electron $(q = -e)$, the displacement elements and vector potential are given by

$$\begin{aligned}
\mathrm{d}x_r &= \mathrm{d}r \,, \\
\mathrm{d}x_\theta &= r\mathrm{d}\theta \,, \\
\mathrm{d}x_\varphi &= r\sin\theta \mathrm{d}\varphi \,, \\
A_r &= A_\theta = A_\varphi = 0 \,, \\
A_4 &= \mathrm{i}V = \mathrm{i}\,\frac{e}{r} \,.
\end{aligned}$$

Then, the wavefunction is given by

$$\psi = \mathrm{e}^{\mathrm{i}/\hbar \int p_r \mathrm{d}x_r}\, \mathrm{e}^{\mathrm{i}/\hbar \int p_\theta \mathrm{d}x_\theta}\, \mathrm{e}^{\mathrm{i}/\hbar \int p_\varphi \mathrm{d}x_\varphi}\, \mathrm{e}^{\mathrm{i}/\hbar \int (p_4 + qA_4/c)\,\mathrm{d}x_4} \,.$$

For separating the variables so that $\psi = R(r)X(\theta)\phi(\varphi)\mathrm{e}^{-\mathrm{i}Et/\hbar}$ for energy eigenstates, we expect

$$\phi(\varphi) = \mathrm{e}^{\mathrm{i}/\hbar \int p_\varphi \mathrm{d}x_\varphi} \,, \tag{6}$$

$$X(\theta) = \mathrm{e}^{\mathrm{i}/\hbar \int p_\theta \mathrm{d}x_\theta} \,, \tag{7}$$

$$R(r) = \mathrm{e}^{\mathrm{i}/\hbar \int p_r \mathrm{d}x_r}\,, \tag{8}$$

$$\mathrm{e}^{-\mathrm{i}Et/\hbar} = \mathrm{e}^{\mathrm{i}/\hbar \int_0^t (p_4 + qA_4/c)\mathrm{d}_4}\,. \tag{9}$$

The angular momentum magnitude and its z-axis component magnitude are denoted by J and J_z respectively, we have

$$\begin{aligned} p_\varphi r \sin\theta &= J_z \qquad \text{(const.)} \\ \left(\sqrt{p_\theta^2 + p_\varphi^2}\right) r &= J \qquad \text{(const.)} \end{aligned}$$

From Eq.(9), we have

$$p_4 = \frac{-E - \mathrm{i}cqA_4/c}{\mathrm{i}c} = \frac{-E - \mathrm{e}^2/r}{\mathrm{i}c}$$

and we have

$$\begin{aligned} p_r &= \pm\sqrt{-m_e^2c^2 - p_\theta^2 - p_\varphi^2 - p_4^2} = \\ &= \pm\sqrt{-m_e^2c^2 - \frac{J^2}{r^2} + \frac{1}{c^2}\left(E + \frac{e^2}{r}\right)^2}\,. \end{aligned}$$

Thus we have

$$\begin{aligned} \phi(\varphi) &= \exp\left(\frac{\mathrm{i}}{\hbar}\int p_\varphi \mathrm{d}x_\varphi\right) = C_1 \exp\left(\frac{\mathrm{i}}{\hbar}\, J_z\varphi\right), \\ X(\theta) &= \exp\left(\frac{\mathrm{i}}{\hbar}\int p_\theta \mathrm{d}x_\theta\right) = C_2 \exp\left(\pm\frac{\mathrm{i}}{\hbar}\int_0^\theta \sqrt{J^2 - \frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta\right), \\ R(r) &= C_3 \exp\left(\pm\frac{\mathrm{i}}{\hbar}\int_0^r \sqrt{-m_e^2c^2 - \frac{J^2}{r^2} + \frac{1}{c^2}\left(E + \frac{e^2}{r}\right)^2}\,\mathrm{d}r\right), \end{aligned}$$

where C_1, C_2 and C_3 are integral constants. Since $\phi(\varphi)$ and $X(\theta)$ must be periodic functions, and the radical wavefunction $R(r)$ forms a "standing wave" in the range from $r = 0$ to $r = \infty$, these requirements demand

$$\frac{1}{\hbar}\int_0^{2\pi} J_z \mathrm{d}\varphi = 2\pi m\,, \qquad (m = 0,\, \pm1\,, \pm2,\, \ldots)\,, \tag{10}$$

$$\frac{1}{\hbar}\int_0^{2\pi} \sqrt{J^2 - \frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta = 2\pi k\,, \qquad (k = 0,\, 1,\, 2,\, \ldots)\,, \tag{11}$$

$$\frac{1}{\hbar}\int_0^{\infty} \sqrt{-m_e^2c^2 - \frac{J^2}{r^2} + \frac{1}{c^2}\left(E + \frac{e^2}{r}\right)^2}\,\mathrm{d}r = \pi s\,, \qquad (s = 0,\, 1,\, 2,\, \ldots)\,. \tag{12}$$

These definite integrals have been evaluated in the Appendix by using the residue theorem and contour integrations in complex space, to note that the last two integrands are multiple-valued functions when over their turning points, the results

are given by

$$\begin{aligned} & J_z = m\hbar\,, \\ & \frac{1}{\hbar}\int_0^{2\pi}\sqrt{J^2-\frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta = \frac{2\pi}{\hbar}\left(J-|J_z|\right), \\ & J = \big(k+|m|\big)\hbar = j\hbar\,, \\ \frac{1}{\hbar}\int_0^{\infty}\sqrt{-m_e^2c^2-\frac{J^2}{r^2}+\frac{1}{c^2}\left(E+\frac{e^2}{r}\right)^2}\,\mathrm{d}r &= \frac{\pi E\alpha}{\sqrt{m_e^2c^4-E^2}} - \pi\sqrt{j^2-\alpha^2} = \pi s\,, \end{aligned} \tag{13}$$

where $\alpha = \dfrac{e^2}{\hbar c}$ is known as the fine structure constant.

Form the last Eq.(13) , we obtain the energy levels given by

$$E = m_ec^2\left[1+\frac{\alpha^2}{(\sqrt{j^2-\alpha^2}+s)^2}\right]^{-1/2}, \tag{14}$$

where $j = k+|m|$, because of the restriction of $j \neq 0$ in Eq.(14), we find $j = 1, 2, 3, \ldots$

The result, Eq.(14), is completely the same as the calculation of the Dirac wave equation[6] for the hydrogen atom, it is just the **fine structure of hydrogen energy**.

4 Electronic spin

If we put the hydrogen atom into an external uniform magnetic field $\mathbf{B}$ which is along the z axis with the vector potential $(A_r, A_\theta, A_\varphi) = (0, 0, \frac{1}{2}Br\sin\theta)$, i.e. $\mathbf{B} = B\mathbf{e}_z$, where $\mathbf{e}_z$ is the unit vector along the z axis. According to Eq. (4), the energy eigenstates of the hydrogen atom is described by

$$\begin{aligned} \psi &= R(r)X(\theta)\phi(\varphi)\mathrm{e}^{-\mathrm{i}Et/\hbar}\,, \\ \phi(\varphi) &= \exp\left(\frac{\mathrm{i}}{\hbar}\int\Big(p_\varphi+\frac{qA_\varphi}{c}\Big)\mathrm{d}x_\varphi\right), \\ X(\theta) &= \exp\left(\frac{\mathrm{i}}{\hbar}\int p_\theta \mathrm{d}x_\theta\right), \\ R(r) &= \exp\left(\frac{\mathrm{i}}{\hbar}\int p_r\mathrm{d}x_r\right), \\ \mathrm{e}^{-\mathrm{i}Et/\hbar} &= \exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t\Big(p_4+\frac{qA_4}{c}\Big)\mathrm{d}x_4\right). \end{aligned}$$

The magnitude of the angular momentum is denoted by J and its component along the z-axis by J_z, then

$$\begin{aligned} p_\varphi r\sin\theta &= J_z\,, \qquad (\text{const.})\,, \\ (\sqrt{p_\theta^2+p_\varphi^2})r &= J\,, \qquad (\text{const.})\,, \end{aligned}$$

we also have the same expressions as

$$p_4 = \frac{-E - \mathrm{i}cqA_4/c}{\mathrm{i}c} = \frac{-E - \mathrm{e}^2/r}{\mathrm{i}c}\,,$$
$$p_r = \pm\sqrt{-m_e^2c^2 - p_\theta^2 - p_\varphi^2 - p_4^2} = \pm\sqrt{-m_e^2c^2 - \frac{J^2}{r^2} + \frac{1}{c^2}\left(E + \frac{e^2}{r}\right)^2}\,,$$

thus we have

$$\begin{aligned}
\phi(\varphi) &= \mathrm{e}^{\mathrm{i}/\hbar\int(p_\varphi + qA_\varphi/c)\mathrm{d}x_\varphi} = \\
&= \exp\left(\frac{\mathrm{i}}{\hbar}\int\Big(p_\varphi + \frac{q}{2c}\,r\sin\theta B\Big)r\sin\theta\,\mathrm{d}\varphi\right) = \\
&= C_1\exp\left(\frac{\mathrm{i}}{\hbar}\left(J_z - \frac{e}{2c}\,r^2\sin^2\theta B\Big)\varphi\right)\right) = C_1 e^{\mathrm{i}m\varphi}\,, \\
X(\theta) &= e^{\mathrm{i}/\hbar\int p_\theta\mathrm{d}x_\theta} = C_2\exp\left(\pm\frac{\mathrm{i}}{\hbar}\int_0^\theta\sqrt{J^2 - \frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta\right) = \\
&= C_2\exp\left(\pm\frac{\mathrm{i}}{\hbar}\int_0^\theta\sqrt{J^2 - (m\hbar + \frac{e}{2c}\,r^2\sin^2\theta B)^2\sin^{-2}\theta}\,\mathrm{d}\theta\right) \simeq \\
&\simeq C_2\exp\left(\pm\frac{\mathrm{i}}{\hbar}\int_0^\theta\sqrt{J^2 - \frac{m^2\hbar^2}{\sin^2\theta} - \frac{m\hbar er^2B}{c}}\,\mathrm{d}\theta\right), \\
R(r) &= C_3\exp\left(\pm\frac{\mathrm{i}}{\hbar}\int_0^r\sqrt{-m_e^2c^2 - \frac{J^2}{r^2} + \frac{1}{c^2}\Big(E + \frac{e^2}{r}\Big)^2}\mathrm{d}r\right),
\end{aligned}$$

where C_1, C_2 and C_3 are integral constants, we have neglected $O(B^2)$ terms. Since $\phi(\varphi)$ and $X(\theta)$ must be periodic functions, and the radical wavefunction $R(r)$ forms a "standing wave" in the range from $r = 0$ to $r = \infty$, these requirements demand

$$\begin{aligned}
\frac{1}{\hbar}\int_0^{2\pi}(J_z - \tfrac{1}{2}\,er^2\sin^2\theta B)\,\mathrm{d}\varphi = 2\pi m\,, &\qquad (m = 0,\,\pm1,\,\pm2\,\ldots), \\
\frac{1}{\hbar}\int_0^{2\pi}\sqrt{J^2 - \frac{m^2\hbar^2}{\sin^2\theta} - \frac{m\hbar er^2B}{c}}\,\mathrm{d}\theta = 2\pi k\,, &\qquad (k = 0,\,1,\,2,\,\ldots)\,, \\
\frac{1}{\hbar}\int_0^{\infty}\sqrt{-m_e^2c^2 - \frac{J^2}{r^2} + \frac{1}{c^2}\left(E + \frac{e^2}{r}\right)^2}\,\mathrm{d}r = \pi s\,, &\qquad (s = 0,\,1,\,2,\,\ldots)
\end{aligned}$$

These definite integrals have been evaluated in the Appendix, given by

$$J_z - \tfrac{1}{2}\,er^2\sin^2\theta B = m\hbar\,,$$
$$\frac{1}{\hbar}\int_0^{2\pi}\sqrt{J^2 - \frac{m^2\hbar^2}{\sin^2\theta} - \frac{m\hbar er^2B}{c}}\,\mathrm{d}\theta = 2\pi\left(\frac{1}{\hbar}\sqrt{J^2 - \frac{m\hbar er^2B}{c}} - |m|\right),$$

we get

$$J^2 - \frac{m\hbar e r^2 B}{c} = \big(k + |m|\big)^2 \hbar^2 = j^2 \hbar^2 \,.$$

We have

$$\begin{aligned}
&\frac{1}{\hbar}\int_0^\infty \sqrt{-m_e^2 c^2 - \frac{J^2}{r^2} + \frac{1}{c^2}\left(E + \frac{e^2}{r}\right)^2}\,\mathrm{d}r = \\
&\quad = \frac{1}{\hbar}\int_0^\infty \sqrt{-m_e^2 c^2 - \frac{1}{r^2}\left(j^2\hbar^2 + \frac{m\hbar e r^2 B}{c}\right) + \frac{1}{c^2}\left(E + \frac{e^2}{r}\right)^2}\,\mathrm{d}r = \\
&\quad\quad = \frac{\pi E \alpha}{\sqrt{m_e^2 c^4 + m\hbar e c B - E^2}} - \pi\sqrt{j^2 - \alpha^2} = \pi s
\end{aligned}$$

and we obtain the energy levels of hydrogen atom in the magnetic field given by

$$E = \sqrt{m_e^2 c^4 + mec\hbar B}\left[1 + \frac{\alpha^2}{(\sqrt{j^2 - \alpha^2} + s)^2}\right]^{-1/2} . \tag{15}$$

In the usual spectroscopic notation of quantum mechanics, four quantum numbers: n, l, m_l and m_s are used to specify the state of an electron in an atom. After the comparison, we get the relations between the usual notation and our notation.

$$\begin{aligned}
n &= j + s, \qquad s = 0,\, 1,\, \ldots\,, \quad j = 1,\, 2, \ldots \\
l &= j - 1\,, \\
\max(m_l) &= \max(m) - 1\,.
\end{aligned}$$

We find that j takes over $1,\, 2, \ldots,\, n$; for a fixed j (or l), m takes over $-(l+1)$, $-l$, $\ldots$, 0, $\ldots$, l, $l+1$. In the present work, spin quantum number is absent.

According to Eq.(15), for a fixed (n, l), equivalent to $(n, j = l + 1)$, the energy level of hydrogen atom will split into $2l+3$ energy levels in the magnetic field, given by

$$E = \left(m_e c^2 + \frac{me\hbar B}{2m_e c}\right)\left[1 + \frac{\alpha^2}{(\sqrt{j^2 - \alpha^2} + s)^2}\right]^{-1/2} + O(B^2)\,. \tag{16}$$

Considering $m = -(l+1)$, $-l$, $\ldots$, 0, $\ldots$, l, $l+1$, this effect is equivalent to the usual Zeeman splitting in the usual quantum mechanics given by

$$E = E_{nl} + \frac{(m_l \pm 1)e\hbar B}{2m_e c}\,.$$

But our work works on it without **spin** concept, the so-called spin effect has been revealed by Eq. (16) without spin concept, this result indicates that electronic spin is a kind of orbital motion. In Stern-Gerlach experiment, the angular momentum of ground state of hydrogen atom is presumed to be zero according to the usual quantum mechanics, thus ones need make use of the spin. But in the present calculation, the so-called spin has been merged with the orbital motion of the electron.

Bear in mind that simplicity is always a merit for the physics.

5 Discussion

1.rapid quantum computation

Since the path integral method for quantum mechanics needs not to evaluate quantum wave equation (2 order or nonlinear ones), in addition, the wavefunction of the path integral is single component wavfunction, the path integral method definitely is a rapid quantum computation method. This path integral method provides a great prospects for computer computation in some research fields such as $X\alpha$, ab-initio, LMTO, DV, etc.

The path integral method developed in the present paper differs essentially from the Feynman's path integral.

2. the explanation of the wavefunction

The wavefunction ψ we employed in the calculation for hydrogen atom differs from the wave function in the usual quantum mechanics, because it is found that the wavefunction ψ keeps $|\psi| = 1$ everywhere in the hydrogen atom. But this kind of wavefunction can interference with each other, for the detail discussions consult the papers[9, 7].

6 Conclusion

Using equation

$$\mu_\mu + qA_\mu)\psi = -\mathrm{i}\hbar\partial_\mu\psi$$

and its integral solution

$$\psi = \exp\left(\frac{\mathrm{i}}{\hbar}\int (p_\mu + qA_\mu)\,\mathrm{d}x_\mu\right)$$

a path integral method for calculating quantum states of particle was developed, differing from the Feynman's path integral. The path integral method is directly applied to hydrogen atom, the energy levels are calculated out with the same fine structure and spin effect as the Dirac wave equation. The approach has a important advantage : it is a rapid computation method comparing to traditional quantum mechanics.

The present calculation is characterized by using the usual momentum-wavefunction relation directly, it provides an insight into the foundations of quantum mechanics.

A Appendix: The evaluations of the integrations

In this appendix we give out the evaluations of the integrations appeared in the preceding sections, i.e. Eq. (11) and Eq. (12).

A.1 Wave-attenuating boundary condition

Consider the integrand in Eq. (11), it is a multiple-valued function, may be written as

$$\sqrt{J^2-\frac{J_z^2}{\sin^2\theta}}=\sqrt{f(\theta)}\,,\qquad f(\theta)=J^2-\frac{J_z^2}{\sin^2\theta}\,.$$

The function $f(\theta)$ may be divided into the three regions: $(0,a)$, (a,b), and (b,π), where a and b are the turning points at where the function $f(\theta)$ changes its sign, as shown in Figure 1. Like $\sqrt{-5}=\pm\mathrm{i}\sqrt{5}$ or $(\pm\mathrm{i}\sqrt{5})^2=-5$, we find

$$\begin{aligned}
&\int_0^a\sqrt{f(\theta)}\,D\theta=\int_0^a\sqrt{-|f(\theta)|}=\,\mathrm{d}\theta=\pm\mathrm{i}\int_0^a\sqrt{|f(\theta)|}\,\mathrm{d}\theta=\pm\mathrm{i}A\,,\\
&\int_a^b\sqrt{f(\theta)}\,\mathrm{d}\theta=\int_a^b\sqrt{|f(\theta)|}\,\mathrm{d}\theta=B\,,\\
&\int_b^\pi\sqrt{f(\theta)}\,\mathrm{d}\theta=\int_b^\pi\sqrt{-|f(\theta)|}\,\mathrm{d}\theta=\pm\mathrm{i}A\,,
\end{aligned}$$

where A and B are two real numbers, then the integration of Eq. (11) has three possible solutions given by

$$\int_0^{2\pi}\sqrt{J^2-\frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta=\begin{cases}2(B+2\mathrm{i}A)\\2B\\2(B-2\mathrm{i}A)\end{cases}$$

The second branch of this result is reasonable, because only it can fulfil the requirement that the wavefunction is a periodic function for the varialbe θ. The multiple-valued result arises from $\sqrt{-|f(\theta)|}=\pm\mathrm{i}\sqrt{|f(\theta)|}$.

How to determine the sign of the multiple-valued function reasonably? Let us turn to our experience that we have had in the usual quantum mechanics. Consider the motion of a particle in a finitely deep potential well as shown in Figure 2, there are also two turning points a and b. If the particle moves over the turning point a or b for $E<V_0$ (bound states), its momentum will become imaginary $\pm\mathrm{i}|p|$ with uncertain sign. As we know in the usual quantum mechanics the wavefunction is given by

$$\psi(x)=\begin{cases}D\exp\left(-\mathrm{i}\dfrac{i|p|}{\hbar}\,x\right), & x<a\,,\\[2ex] G\sin\left(\dfrac{|p_0|}{\hbar}\,x+\delta\right), & a<x<b\,,\\[2ex] D\exp\left(-\mathrm{i}\,\dfrac{-\mathrm{i}|p|}{\hbar}\,x\right), & x>b\,.\end{cases}$$

In which we have taken the plus sign for the imaginary momentum in $x<a$ and minus sign in $x>b$, to satisfy the **wave-attenuating boundary condition** for the regions over the turning points.

In the followings, we use this wave-attenuating boundary condition to determine the sign of double-valued imaginary momentum: take plus sign in the region over

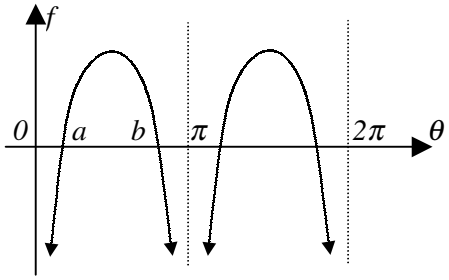

Fig. 1. The function has sign-changed points a and b.

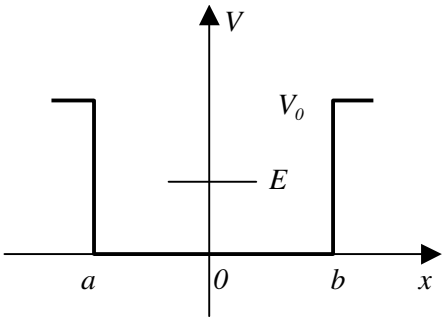

Fig. 2. A finitely deep potential well that has two turning points a and b.

the left turning point, whereas take minus sign in the region over the right turning point.

A.2 Integration 1

To apply the wave-attenuating boundary condition to the following wavefunction

$$X(\theta) = C_2 \exp\left(-\frac{\mathrm{i}}{\hbar}\int \sqrt{J^2 - \frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta\right)$$

due to the wave-attenuating for the turning points, the integrand must choose the signs as

$$\int_0^a \sqrt{J^2 - \frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta = +\mathrm{i}\int_0^a \sqrt{|f(\theta)|}\,\mathrm{d}\theta = \mathrm{i}A\,, \tag{17}$$

$$\int_a^b \sqrt{J^2 - \frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta = \int_a^b \sqrt{f(\theta)}\,\mathrm{d}\theta = B\,,$$

$$\int_b^\pi \sqrt{J^2 - \frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta = -\mathrm{i}\int_b^\pi \sqrt{|f(\theta)|}\,\mathrm{d}\theta = -\mathrm{i}A\,. \tag{18}$$

Thus the integration may have a real solution, actually it may be written as

$$\int_0^{2\pi} \sqrt{J^2 - \frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta = 2\int_a^b \sqrt{J^2 - \frac{J_z^2}{\sin^2\theta}}\mathrm{d}\theta = 2B\,. \tag{19}$$

In order to evaluate the definite integral of Eq. (19), we make use of contour integral in complex plane. Consider a contour C_δ which is a unit circle around zero, as shown in Figure 3, using $z = \mathrm{e}^{\mathrm{i}\theta}$, we have

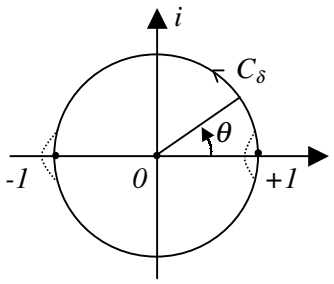

Fig. 3. Unit circle contour for evaluating integral

$$I_1 = \int_0^{2\pi} \sqrt{J^2 - \frac{J_z^2}{\sin^2\theta}}\,\mathrm{d}\theta = \int_{C_\delta} \sqrt{J^2 + \frac{4J_z^2 z^2}{(z^2-1)^2}}\,\frac{\mathrm{d}z}{\mathrm{i}z} =$$
$$= \int_{C_\delta} \frac{\sqrt{J^2(z^2-1)^2 + 4J_z^2 z^2}}{\pm(z^2-1)}\,\frac{\mathrm{d}z}{\mathrm{i}z}\,.$$

As we have known that $\sqrt{f(\theta)}|_{\theta=\pi/2 \text{ or } \theta=3\pi/2} = \sqrt{J^2 - J_z^2}$, substituting $z = \mathrm{i}$ or $z = -\mathrm{i}$ into the above integrand, we find the integrand must take the minus sign. Thus

$$I_1 = \int_{C_\delta} \frac{\sqrt{J^2(z^2-1)^2 + 4J_z^2 z^2}}{-(z^2-1)}\,\frac{\mathrm{d}z}{\mathrm{i}z}\,.$$

For scrutinizing the sign of the integrand over the turning points, we have

$$\sqrt{f(\theta)} = \frac{\sqrt{J^2(z^2-1)^2 + 4J_z^2 z^2}}{-(z^2-1)} = \frac{\sqrt{J^2(z^2-1)^2 + 4J_z^2 z^2}}{-(2\mathrm{i}z)(z^2-1)/(2\mathrm{i}z)} =$$
$$= \frac{\sqrt{J^2(z^2-1)^2 + 4J_z^2 z^2}}{-(2\mathrm{i}z)\sin\theta} = \mathrm{i}\frac{\sqrt{J^2(z^2-1)^2 + 4J_z^2 z^2}}{2z\sin\theta}\,,$$

we find that the integrand takes plus sign over the left turning point ($\theta \to 0+, z \to 1$) and minus sign over the right turning point ($\theta \to \pi-, z \to -1$), in accordance with the sign requirement of Eq. (17) and (18).

Continue our calculation, we have

$$I_1 = \int_{C_\delta} \frac{\sqrt{J^2(z^2-1)^2+4J_z^2z^2}}{-(z^2-1)}\,\frac{\mathrm{d}z}{\mathrm{i}z} = \\ = \int_{C_\delta}\left(\frac{1}{z}-\frac{1/2}{z-1}-\frac{1/2}{z+1}\right)\sqrt{J^2(z^2-1)^2+4J_z^2z^2}\,\frac{\mathrm{d}z}{\mathrm{i}}\,.$$

Now we find that the integrand has the three poles at $z=0$ and $z=\pm1$. We let the contour C_δ pass by the pole $z=+1$ through the interior of the unite circle, as indicated by the dash line in Figure 3, likewise, let the contour C_δ pass by the pole $z=-1$ through the exterior of the unite circle. The deformation made for C_δ has no influence on the integration value because the left deformation cancels the right deformation in the integration due to the opposite signs of the integrand near the left and right poles. Let C'_δ denote the deformed contour, we continue the calculation by using Laurent's series expansion and the residue theorem.

$$I_1 = \int_{C'_\delta}\left(\frac{1}{z}-\frac{1/2}{z-1}-\frac{1/2}{z+1}\right)\sqrt{J^2(z^2-1)^2+4J_z^2z^2}\,\frac{\mathrm{d}z}{\mathrm{i}} = \\ = \int_{C'_\delta}\frac{1}{z}\sqrt{J^2(z^2-1)^2+4J_z^2z^2}\,\frac{\mathrm{d}z}{i} - \int_{C'_\delta}\frac{1/2}{z-1}\sqrt{J^2(z^2-1)^2+4J_z^2z^2}\,\frac{\mathrm{d}z}{\mathrm{i}} - \\ - \int_{C'_\delta}\frac{1/2}{z+1}\sqrt{J^2(z^2-1)^2+4J_z^2z^2}\,\frac{\mathrm{d}z}{\mathrm{i}} = \\ = \int_{C'_\delta}\frac{J+O(z^2)}{z}\,\frac{\mathrm{d}z}{\mathrm{i}} - \int_{C'_\delta}\frac{|J_z|+O(z^2-1)}{z+1}\,\frac{\mathrm{d}z}{\mathrm{i}} = 2\pi\big(J-|J_z|\big)\,.$$

A.3 Integration 2

To apply the wave-attenuating boundary condition to the following wavefunction

$$R(r) = C_3\exp\left(-\frac{\mathrm{i}}{\hbar c}\int\sqrt{\left(E+\frac{e^2}{r}\right)^2-m_e^2c^4-\frac{J^2\hbar^2c^2}{r^2}}\,\mathrm{d}r\right),$$

where it has also two turning points r_1 and r_2 from $r=0$ to $r=\infty$ when $E^2<m_e^2c^4$ (bound states), as shown in Figure 4, where

$$g(r) = \left(E+\frac{e^2}{r}\right)^2-m_e^2c^4-\frac{j^2\hbar^2c^2}{r^2}\,,$$

we take the following signs for its asymptotic behavior, i.e.

$$\sqrt{g(r)}|_{r\to0} = \frac{\sqrt{e^4-j^2\hbar^2c^2}}{r} = \mathrm{i}\,\frac{\sqrt{j^2\hbar^2c^2-e^4}}{r}\,,$$
$$\sqrt{g(r)}|_{r\to\infty} = \sqrt{E^2-m_e^2c^4} = -\mathrm{i}\sqrt{m_e^2c^4-E^2}\,.$$

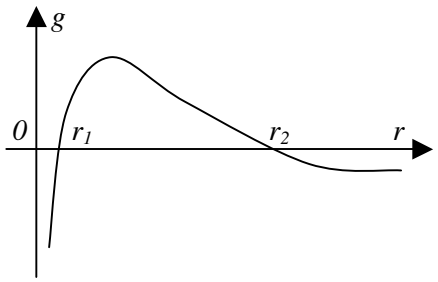

Fig. 4. The function has two sign-changed points r_1 and r_2.

In order to evaluate the definite integral of Eq.(12), consider a contour C consisting of C_γ, L_-, C_δ and L around zero in the plane as shown in Figure 5, the radius of circle C_γ is large enough and the radius of circle C_δ is small enough. The integrand of the following equation has no pole inside the contour C, so that we have

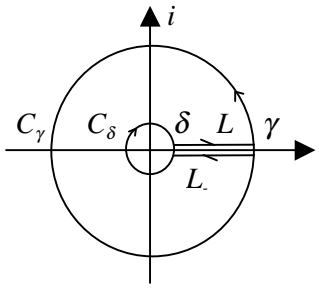

Fig. 5. Unit circle contour for evaluating integral

$$\int_C \sqrt{\left(E+\frac{e^2}{z}\right)^2 - m_e^2c^4 - \frac{j^2\hbar^2c^2}{z^2}}\mathrm{d}z = \int_{C_\gamma} + \int_{L_-} + \int_{C_\delta} + \int_L = 0\,.$$

Now we evaluate the integration on each contour with our sign choice for the double-valued function, using Laurent's series expansion and the residue theorem.

$$\begin{aligned}\int_{C_\gamma} &= \int_{C_\gamma} \sqrt{\left(E+\frac{e^2}{z}\right)^2 - m_e^2c^4 - \frac{j^2\hbar^2c^2}{z^2}}\mathrm{d}z = \\ &= -\int_{C_\gamma} \mathrm{i}\sqrt{m_e^2c^4 + \frac{j^2\hbar^2c^2}{z^2} - \left(E+\frac{e^2}{z}\right)^2}\mathrm{d}z = \end{aligned}$$

$$
\begin{aligned}
&= -\mathrm{i}\int_{C_\gamma}\left[\sqrt{m_e^2c^4-E^2}-\frac{Ee^2}{\sqrt{m_e^2c^4-E^2}}\frac{1}{z}+O\left(\frac{1}{z^2}\right)\right]\mathrm{d}z = \\
&= \mathrm{i}\frac{2\pi\mathrm{i}Ee^2}{\sqrt{m_e^2c^4-E^2}} = -\frac{2\pi Ee^2}{\sqrt{m_e^2c^4-E^2}}\,, \\
\int_{C_\delta} &= \int_{C_\delta}\mathrm{i}\sqrt{m_e^2c^4+\frac{j^2\hbar^2c^2}{z^2}-\left(E+\frac{e^2}{z}\right)^2}\,\mathrm{d}z = \\
&= \mathrm{i}\int_{C_\delta}\frac{\sqrt{m_e^2c^4z^2+j^2\hbar^2c^2-\left(Ez+e^2\right)^2}}{z}\,\mathrm{d}z = \\
&= \mathrm{i}\int_{C_\delta}\frac{\sqrt{j^2\hbar^2c^2-e^4}+O(z)}{z}\,\mathrm{d}z = \\
&= \mathrm{i}(-2\pi\mathrm{i})\sqrt{j^2\hbar^2c^2-e^4} = 2\pi\sqrt{j^2\hbar^2c^2-e^4}\,.
\end{aligned}
$$

Because the integrand is a multiple-valued function, when the integral takes over the path L_- we have $z=\mathrm{e}^{2\pi\mathrm{i}}r\mathrm{e}^{0\mathrm{i}}$, thus

$$\int_{L-}=\int_\gamma^\delta\sqrt{\mathrm{e}^{-2\pi\mathrm{i}}(\ldots)}=-\int_\gamma^\delta=\int_\delta^\gamma=\int_L\,.$$

For a further manifestation, to define $z-H=w=\rho\mathrm{e}^{\mathrm{i}\beta}$, where

$$H=\frac{m_e^2c^4r^2+j^2\hbar^2c^2-E^2r^2-e^4}{2Ee^2}\,,$$

we have

$$
\begin{aligned}
\int_{L-} &= \int_{L-}\frac{\sqrt{2Ee^2}\sqrt{z-H}}{z}\,\mathrm{d}z=\int_{L-}\frac{\sqrt{2Ee^2}\sqrt{w}}{z}\mathrm{d}z = \\
&= \int_{L-}\frac{\sqrt{2Ee^2\rho}\,\mathrm{e}^{\mathrm{i}\beta/2}}{z}\mathrm{d}z=\int_{L(\gamma\to\delta)}\frac{\sqrt{2Ee^2\rho}\,\mathrm{e}^{\mathrm{i}(\beta+2\pi)/2}}{z\mathrm{e}^{2\pi\mathrm{i}}}\,\mathrm{d}\left(z\mathrm{e}^{2\pi\mathrm{i}}\right) = \\
&= -\int_{L(\gamma\to\delta)}\frac{\sqrt{2Ee^2\rho}\,\mathrm{e}^{\mathrm{i}\beta/2}}{z}\mathrm{d}z=\int_{L(\delta\to\gamma)}\frac{\sqrt{2Ee^2\rho}\,\mathrm{e}^{\mathrm{i}\beta/2}}{z}\,\mathrm{d}z=\int_L\,,
\end{aligned}
$$

where we have use the relation of z and w in the fourth step of the above equation, as shown in Figure 6, to note that w rotates around zero with z. Thus we have

$$\int_L=\frac{1}{2}\left(\int_L+\int_{L-}\right)=-\frac{1}{2}\left(\int_{C_\gamma}+\int_{C_\delta}\right)=\frac{\pi Ee^2}{\sqrt{m_e^2c^4-E^2}}-\pi\sqrt{j^2\hbar^2c^2-e^4}\,.$$

Thus Eq. (12) becomes

$$\frac{1}{\hbar c}\int_0^\infty\sqrt{\left(E+\frac{e^2}{r}\right)^2-m_e^2c^4-\frac{j^2\hbar^2c^2}{r^2}}\,\mathrm{d}r=\frac{\pi E\alpha}{\sqrt{m_e^2c^4-E^2}}-\pi\sqrt{j^2-\alpha^2}\,,$$

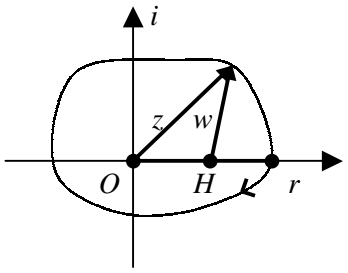

Fig. 6. contour for evaluating integral

where $\alpha = \dfrac{e^2}{\hbar c}$ is known as the fine structure constant.

A.4 Discussion: the motion over turning points

Following the sign change for imaginary momentum over turning points, discussed in the preceding sections, we find that the periodic condition or standing wave condition in hydrogen atom may written as

$$2\int_a^b \sqrt{J^2 - \frac{m^2}{\sin^2\theta}}\,\mathrm{d}\theta = 2\pi k$$
$$\frac{1}{\hbar c}\int_{r_1}^{r_2} \sqrt{\left(E + \frac{e^2}{r}\right)^2 - m_e^2c^4 - \frac{J^2\hbar^2c^2}{r^2}}\,\mathrm{d}r = \pi s\,,$$

because the contributions of the integrands in the regions over the turning points are eliminated automatically. What are their physical meanings ? A direct explanation is that it is not necessary for the electron to enter the regions over the turning points, in compliance with classical physics.

In addition, the residue theorem we used in the paper gives out accurate results for our integrations, not approximate ones.

References

[1] E.G. Harris: *Introduction to Modern Theoretical Physics*, Vol.1&2, p.263, Eq.(10–40), John Wiley & Sons, USA, 1975.

[2] H.Y. Cui: `arXiv:physics/0408025`, Aug, 2004.

[3] H.Y. Cui: in the *Proceedings of annual meeting of Chinese Physical Socity*, China Beijing, Aug, 2002.

[4] H.Y. Cui: `arXiv:physics/0212059`, Dec, 2002.

[5] H.Y. Cui: `arXiv:quant-ph/0102114`, Feb, 2001.

[6] L.I. Schiff: *Quantum Mechanics*, third ed., p.486, Eq.(53.26), McGrall-Hill, USA, 1968.

[7] H.Y. Cui: `arXiv:hep-th/0110128`, Oct, 2001.

[8] H.Y. Cui: `arXiv:physics/0102073`, Feb, 2001.

[9] H.Y. Cui: `arXiv:quant-ph/0108072`, Aug, 2001.