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Quantum Theory of Electronic Double-Slit Diffraction *

WU Xiang-Yao(吴向尧)[1**], ZHANG Bai-Jun(张伯军)[1], LI Hai-Bo(李海波)[1], LU Jing-Bin(陆景彬)[2], LIU Xiao-Jing(刘晓静)[1], WANG Li(王丽)[1], ZHANG Chun-Li(张春丽)[1], LIU Bing(刘兵)[1], FAN Xi-Hui(范希会)[3], GUO Yi-Qing(郭义庆)[4]

[1]*Institute of Physics, Jilin Normal University, Siping 136000*
[2]*Institute of Physics, Jilin University, Changchun 130023*
[3]*Department of Physics, Qufu Normal University, Qufu 273165*
[4]*Institute of High Energy Physics, PO Box 918(3), Chinese Academy of Sciences, Beijing 100049*

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Phenomena of electron, neutron, atomic and molecular diffraction have been studied in many experiments, and these experiments have been explained by some theoretical works. We study electronic double-slit diffraction with a quantum mechanical approach and obtain the following results: (1) When the ratio of $\frac{d+a}{a}=n$ $(n=1,2,3,\ldots)$, *orders* $n, 2n, 3n, \ldots$ *are missing in diffraction pattern. (2) When the ratio of* $\frac{d+a}{a}\neq n$ $(n=1,2,3,\ldots)$, *there is not missing order in diffraction pattern. (3) The slit thickness* c *has a large affect on the electronic diffraction pattern, which is a new quantum effect. We believe that all the predictions in our work can be tested by the electronic double slit diffraction experiment.*

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The wave nature of subatomic particle elections and neutrons was postulated by de Broglie in 1923 and this idea can explain many diffraction experiments. The matter–wave diffraction has become a large field of interest over the last years, and has been extended to atoms and more massive, complex objects, like large molecules I_2, C_{60} and C_{70}, which were found in experiments.[1−5] In such experiments, the incoming atoms or molecules usually can be described by plane waves. As is well known, the classical optics with its standard wave-theoretical methods and approximations, in particular those of Huygens and Kirchhoff, has been successfully applied to classical optics, and has yielded good agreement with many experiments. This simple wave-optical approach also gives a description of matter wave diffraction.[6,7] However, matter–wave interference and diffraction are quantum phenomena, and its fully description needs quantum mechanical approach. Recently, we have studied the neutron single slit diffraction with quantum mechanical approach and obtained some important and new results.[8] In this Letter, we study the double-slit diffraction of electron with the quantum mechanical approach. In view of quantum mechanics, the electron has the nature of wave, and the wave is described by wavefunction $\psi(\boldsymbol{r},t)$, which can be calculated with the Schrödinger wave equation. The wavefunction $\psi(\boldsymbol{r},t)$ has statistical meaning, i.e., $|\psi(\boldsymbol{r},t)|^2$ can be explained as a particle's probability density at the definite position. For double slit diffraction, if we can calculate the electronic wavefunction $\psi(\boldsymbol{r},t)$ distributing on display screen, then we can obtain the diffraction intensity for a double-slit, since the diffraction intensity is directly proportional to $|\psi(\boldsymbol{r},t)|^2$. In the double-slit diffraction, the electron wavefunctions can be divided into three parts. The first is the incoming area, the electronic wave function is a plane wave. The second is the double slit area, where the electronic wavefunction can be calculated by the Schrödinger wave equation. The third is the diffraction area, where the electronic wavefunction can be obtained by Kirchhoff's law. In the following, we calculate these wavefunctions.

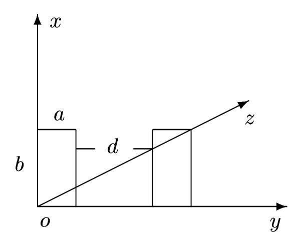

Fig. 1. Double slit geometry with a the width, b the length and d the distance between the two slits.

In an infinite plane, we consider a double-slit, its width a, length b and the slit-to-slit distance d are shown in Fig. 1. The x axis is along the slit length b and the y axis is along the slit width a. We calculate the electron wave function in the first single slit (left) with the Schrödinger equation, and the electron wavefunction of the second single-slit (right) can be obtained easily. At time t, we suppose that the incoming plane wave travels along the z axis. It is

$$\Psi_1(z,t)=Ae^{\frac{i}{\hbar}(pz-Et)}, \qquad (1)$$

where A is a constant.

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** Email: wuxy2066@163.com

The potential in the single slit is

$$V(x,y,z)=\begin{cases}0 & 0\le x\le b, 0\le y\le a, 0\le z\le c,\\ \infty & \text{otherwise},\end{cases} \tag{2}$$

where c is the thickness of the single slit. The time-dependent and time-independent Schrödinger equations are

$$i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t)=-\frac{\hbar^2}{2M}\Big(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\Big)\psi(\boldsymbol{r},t), \tag{3}$$

$$\frac{\partial^2\psi(\boldsymbol{r})}{\partial x^2}+\frac{\partial^2\psi(\boldsymbol{r})}{\partial y^2}+\frac{\partial^2\psi(\boldsymbol{r})}{\partial z^2}+\frac{2ME}{\hbar^2}\psi(\boldsymbol{r})=0, \tag{4}$$

where $M(E)$ is the mass (energy) of the electron. In Eq. (4), the wavefunction $\psi(x,y,z)$ satisfies the boundary conditions

$$\psi(0,y,z)=\psi(b,y,z)=0, \tag{5}$$

$$\psi(x,0,z)=\psi(x,a,z)=0. \tag{6}$$

The partial differential Eq. (4) can be solved by the method of separation of variable. By writing

$$\psi(x,y,z)=X(x)Y(y)Z(z). \tag{7}$$

The general solution of Eq. (3) is

$$\begin{aligned}\psi_2(x,y,z,t)&=\sum_{mn}\psi_{mn}(x,y,z,t)\\&=\sum_{mn}D_{mn}\sin\frac{n\pi x}{b}\sin\frac{m\pi y}{a}\\&\quad\cdot e^{i\sqrt{\frac{2ME}{\hbar^2}-\frac{n^2\pi^2}{b^2}-\frac{m^2\pi^2}{a^2}}z}e^{-\frac{i}{\hbar}Et}.\end{aligned} \tag{8}$$

Equation (8) is the electronic wavefunction in the first single slit. Since the wavefunctions are continuous at $z=0$, we have

$$\psi_1(x,y,z,t)\mid_{z=0}=\psi_2(x,y,z,t)\mid_{z=0}, \tag{9}$$

from Eq. (9), we obtain the coefficient $D_{m,n}$

$$\begin{aligned}D_{mn}&=\frac{4}{ab}\int_0^a\int_0^b A\sin\frac{n\pi\xi}{b}\sin\frac{m\pi\eta}{a}d\xi d\eta\\&=\begin{cases}\dfrac{16A}{mn\pi^2} & m,n,\ \text{odd},\\ 0 & \text{otherwise},\end{cases}\end{aligned} \tag{10}$$

substituting Eq. (10) into Eq. (8), we can obtain the electronic wave function in the first single slit.

$$\begin{aligned}\psi_2(x,y,z,t)&=\sum_{m,n=0}^{\infty}\frac{16A}{(2m+1)(2n+1)\pi^2}\\&\quad\cdot\sin\frac{(2n+1)\pi x}{b}\sin\frac{(2m+1)\pi y}{a}\\&\quad\cdot e^{i\sqrt{\frac{2ME}{\hbar^2}-\frac{(2n+1)^2\pi^2}{b^2}-\frac{(2m+1)^2\pi^2}{a^2}}z}e^{-\frac{i}{\hbar}Et}.\end{aligned} \tag{11}$$

The electron wavefunction in the second single slit can be obtained by making the coordinate translations $x'=x$, $y'=y-(a+d)$, $z'=z$, and we can obtain the electron wavefunction $\psi_3(x,y,z,t)$ in the second single slit

$$\begin{aligned}\psi_3(x,y,z,t)&=\sum_{m,n=0}^{\infty}\frac{16A}{(2m+1)(2n+1)\pi^2}\\&\quad\cdot\sin\frac{(2n+1)\pi x}{b}\\&\quad\cdot\sin\frac{(2m+1)\pi(y-(a+d))}{a}\\&\quad\cdot e^{i\sqrt{\frac{2ME}{\hbar^2}-\frac{(2n+1)^2\pi^2}{b^2}-\frac{(2m+1)^2\pi^2}{a^2}}z}\\&\quad\cdot e^{-\frac{i}{\hbar}Et}.\end{aligned} \tag{12}$$

With Kirchhoff's law, we can calculate the electron wavefunction in the diffraction area. It can be calculated by the formula[9]

$$\psi_{\rm out}(\boldsymbol{r},t)=-\frac{1}{4\pi}\int_s\frac{e^{ikr}}{r}\boldsymbol{n}\cdot\Big[\nabla'\psi_{in}+\Big(ik-\frac{1}{r}\Big)\frac{\boldsymbol{r}}{r}\psi_{in}\Big]ds, \tag{13}$$

where $\psi_{\rm out}(\boldsymbol{r},t)$ is the diffraction wavefunction on display screen, $\psi_{in}(\boldsymbol{r},t)$ is the wavefunction of slit surface ($z=c$) and s is the area of the aperture or slit. The Kirchhoff formula (13) is approximate as it neglects the effect of diffraction aperture or slit on the incoming wave $\psi_{in}(\boldsymbol{r},t)$. However, when the diffraction aperture or slit is larger than the electron wave length the effect can be neglected.

For the double-slit diffraction, Eq. (13) becomes

$$\begin{aligned}\psi_{\rm out}(\boldsymbol{r},t)&=-\frac{1}{4\pi}\int_{s_1}\frac{e^{ikr}}{r}\boldsymbol{n}\cdot\Big[\nabla'\psi_2+\Big(ik-\frac{1}{r}\Big)\frac{\boldsymbol{r}}{r}\psi_2\Big]ds\\&\quad-\frac{1}{4\pi}\int_{s_2}\frac{e^{ikr}}{r}\boldsymbol{n}\cdot\Big[\nabla'\psi_3+\Big(ik-\frac{1}{r}\Big)\frac{\boldsymbol{r}}{r}\psi_3\Big]ds.\end{aligned} \tag{14}$$

In Eq. (14), the first and second terms are corresponding to the diffraction wavefunctions of the first slit and the second slit.

In the following, we firstly calculate the diffraction wavefunction of the first slit, it is

$$\psi_{{\rm out}_1}(\boldsymbol{r},t)=-\frac{1}{4\pi}\int_{s_1}\frac{e^{ikr}}{r}\boldsymbol{n}\cdot\Big[\nabla'\psi_2+\Big(ik-\frac{1}{r}\Big)\frac{\boldsymbol{r}}{r}\psi_2\Big]ds. \tag{15}$$

The diffraction area is shown in Fig. 2, where $k=\sqrt{\dfrac{2ME}{\hbar^2}}$, s_1 is the area of the first single-slit, $\boldsymbol{r}'$ is the position of a point on the surface ($z=c$), P is an arbitrary point in the diffraction area, and $\boldsymbol{n}$ is a unit vector, which is normal to the surface of the slit.

From Fig. 2, we have

$$r=R-\frac{\boldsymbol{R}}{R}\cdot\boldsymbol{r}'\approx R-\frac{\boldsymbol{r}}{r}\cdot\boldsymbol{r}'=R-\frac{\boldsymbol{k}_2}{k}\cdot\boldsymbol{r}', \tag{16}$$

then

$$\frac{e^{ikr}}{r}=\frac{e^{ik(R-\frac{\boldsymbol{r}}{r}\cdot\boldsymbol{r}')}}{R-\frac{\boldsymbol{r}}{r}\cdot\boldsymbol{r}'}=\frac{e^{ikR}e^{-i\boldsymbol{k}_2\cdot\boldsymbol{r}'}}{R-\frac{\boldsymbol{r}}{r}\cdot\boldsymbol{r}'}$$

$$\approx \frac{e^{ikR}e^{-i\boldsymbol{k}_2\cdot\boldsymbol{r}'}}{R} \quad (|\boldsymbol{r}'| \ll R), \tag{17}$$

with $\boldsymbol{K}_2 = K\frac{\boldsymbol{r}}{r}$. Substituting Eqs. (16) and (17) into Eq. (15), one can obtain

$$\begin{aligned}\psi_{\text{out}_1}(\boldsymbol{r},t) = &-\frac{e^{ikR}}{4\pi R}e^{-\frac{i}{\hbar}Et}\int_{s_0} e^{-i\boldsymbol{k}_2\cdot\boldsymbol{r}'} \\ &\cdot \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{16A}{(2m+1)(2n+1)\pi^2} \\ &\cdot e^{i\sqrt{\frac{2ME}{\hbar^2}-(\frac{(2n+1)\pi}{b})^2-(\frac{(2m+1)\pi}{a})^2}\cdot c} \\ &\cdot \sin\frac{(2n+1)\pi}{b}x'\sin\frac{(2m+1)\pi}{a}y' \\ &\cdot \Big[i\sqrt{\frac{2ME}{\hbar^2}-\Big(\frac{(2n+1)\pi}{b}\Big)^2-\Big(\frac{(2m+1)\pi}{a}\Big)^2} \\ &+ i\boldsymbol{n}\cdot\boldsymbol{k}_2 - \frac{\boldsymbol{n}\cdot\boldsymbol{R}}{R^2}\Big]dx'dy'.\end{aligned} \tag{18}$$

Assume that the angle between $\boldsymbol{k}_2$ and x axis (y axis) is $\frac{\pi}{2}-\alpha$ $\left(\frac{\pi}{2}-\beta\right)$, and $\alpha(\beta)$ is the angle between $\boldsymbol{k}_2$ and the surface of yz (xz), then we have

$$k_{2x} = k\sin\alpha, \quad k_{2y} = k\sin\beta, \tag{19}$$

$$\boldsymbol{n}\cdot\boldsymbol{k}_2 = k\cos\theta, \tag{20}$$

where θ is the angle between $\boldsymbol{k}_2$ and z axis, and the angles θ, α, β satisfy the equation

$$\cos^2\theta + \cos^2\left(\frac{\pi}{2}-\alpha\right) + \cos^2\left(\frac{\pi}{2}-\beta\right) = 1. \tag{21}$$

Substituting Eqs. (19)–(21) into Eq. (18) yields

$$\begin{aligned}\psi_{\text{out}_1}(x,y,z,t) = &-\frac{e^{ikR}}{4\pi R}e^{-\frac{i}{\hbar}Et} \\ &\cdot \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{16A}{(2m+1)(2n+1)\pi^2} \\ &\cdot e^{i\sqrt{\frac{2ME}{\hbar^2}-(\frac{(2n+1)\pi}{b})^2-(\frac{(2m+1)\pi}{a})^2}\cdot c} \\ &\cdot \Big[i\sqrt{\frac{2ME}{\hbar^2}-\Big(\frac{(2n+1)\pi}{b}\Big)^2-\Big(\frac{(2m+1)\pi}{a}\Big)^2} \\ &+ \Big(ik-\frac{1}{R}\Big)\sqrt{\cos^2\alpha-\sin^2\beta}\Big] \\ &\cdot \int_0^b e^{-ik\sin\alpha\cdot x'}\sin\frac{(2n+1)\pi}{b}x'dx' \\ &\cdot \int_0^a e^{-ik\sin\beta\cdot y'}\sin\frac{(2m+1)\pi}{a}y'dy'.\end{aligned} \tag{22}$$

Equation (22) is the diffraction wavefunction of the first slit. Obviously, the diffraction wavefunction of the second slit is

$$\begin{aligned}\psi_{\text{out}_2}(x,y,z,t) = &-\frac{e^{ikR}}{4\pi R}e^{-\frac{i}{\hbar}Et} \\ &\cdot \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{16A}{(2m+1)(2n+1)\pi^2} \\ &\cdot e^{i\sqrt{\frac{2ME}{\hbar^2}-(\frac{(2n+1)\pi}{b})^2-(\frac{(2m+1)\pi}{a})^2}\cdot c} \\ &\cdot \Big[i\sqrt{\frac{2ME}{\hbar^2}-\Big(\frac{(2n+1)\pi}{b}\Big)^2-\Big(\frac{(2m+1)\pi}{a}\Big)^2} \\ &+ \Big(ik-\frac{1}{R}\Big)\sqrt{\cos^2\alpha-\sin^2\beta}\Big] \\ &\cdot \int_0^b e^{-ik\sin\alpha\cdot x'}\sin\frac{(2n+1)\pi}{b}x'dx' \\ &\cdot \int_{a+d}^{2a+d} e^{-ik\sin\beta\cdot y'} \\ &\cdot \sin\frac{(2m+1)\pi}{a}(y'-(a+d))dy',\end{aligned} \tag{23}$$

where d is the two slit distance. The total diffraction wavefunction for the double-slit is

$$\psi_{\text{out}}(x,y,z,t) = \psi_{\text{out}_1}(x,y,z,t) + \psi_{\text{out}_2}(x,y,z,t). \tag{24}$$

From the diffraction wavefunction $\psi_{\text{out}}(x,y,z,t)$, we can obtain the relative diffraction intensity I on the display screen,

$$I \propto |\psi_{\text{out}}(x,y,z,t)|^2. \tag{25}$$

Next, we present our numerical calculation of relative diffraction intensity. The main input parameters are $M = 9.11\times10^{-31}$ kg, $R = 1$ m, $A = 10^6$, $\alpha = 0.01$ rad, $E = 0.0001$ eV, Planck's constant $\hbar = 1.055\times10^{-34}$ Js and $\lambda = \frac{2\pi\hbar}{\sqrt{2ME}}$ is the electronic wavelength. We can obtain the relation between the diffraction angle β and relative diffraction intensity I. In double slit diffraction, we can obtain the results: (1) When the ratio of $\frac{d+a}{a} = n$ ($n = 1,2,3,\ldots$), orders $n, 2n, 3n, \ldots$ are missing in diffraction pattern. In Fig. 3, with $a = 20\lambda$, $d = 40\lambda$ and $\frac{d+a}{a} = 3$, the orders $3, 6, 9, \ldots$ are missing (the middle pattern is the zero order). In Fig. 5, the orders $3, 6, 9, \ldots$ are missing. In double-slit diffraction, the missing order can be said to be due to a combination of interference and diffraction. (2) When the ratio of $\frac{d+a}{a} \neq n$ ($n = 1,2,3,\ldots$), there is no missing order in the diffraction pattern. In Fig. 4, with $a = 20\lambda$, $d = 45\lambda$ and $\frac{d+a}{a} = 3.25$ (not an integer), there is no missing order in the diffraction pattern. In Fig. 6, with $\frac{d+a}{a} = 3.5$, there is no missing order in the diffraction pattern either. (3) The slit length b has an affect on the diffraction intensity. When b is larger, the diffraction intensity increases, as shown in Figs. 3 and 7. (4) The slit thickness c has a large affect on the intensity and formation of diffraction patterns. In Figs. 3 and 8–10, with $\frac{d+a}{a} = 3$, the slit thicknesses c correspond to $\lambda, 10\lambda, 100\lambda$ and 1000λ. There should be missing order at $3, 6, 9, \ldots$. However, we find that when the slit thickness c increases, the missing-order phenomenon disappears, as shown in Figs. 8–10. There are obvious missing orders when slit thickness c is small, as shown in Fig. 3. Otherwise, when the slit thickness c increases, the intensity of diffraction pattern also increases.

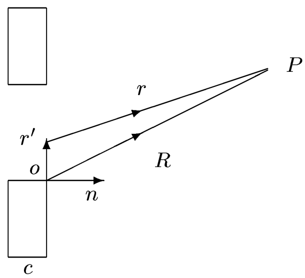

Fig. 2. Diffraction area of the single slit.

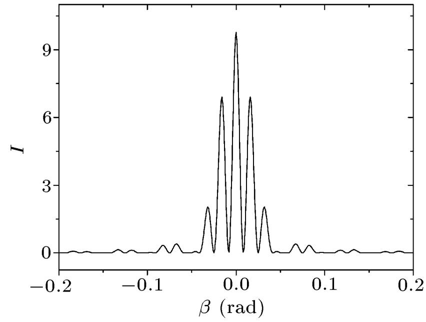

Fig. 3. Relation between β and I with $a = 20\lambda$, $b = 1000\lambda$, $c = \lambda$ and $d = 40\lambda$.

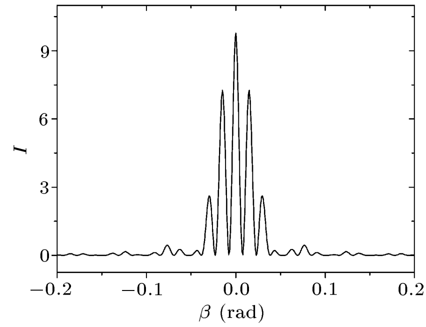

Fig. 4. Relation between β and I with $a = 20\lambda$, $b = 1000\lambda$, $c = \lambda$ and $d = 45\lambda$.

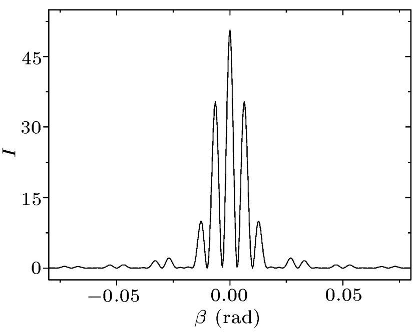

Fig. 5. Relation between β and I with $a = 50\lambda$, $b = 1000\lambda$, $c = \lambda$ and $d = 100\lambda$.

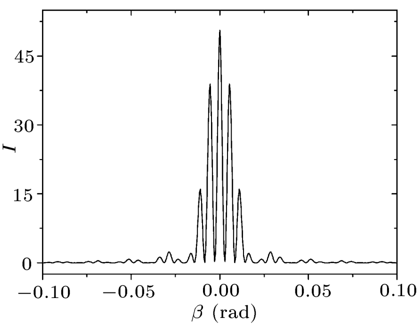

Fig. 6. Relation between β and I with $a = 50\lambda$, $b = 1000\lambda$, $c = \lambda$ and $d = 125\lambda$.

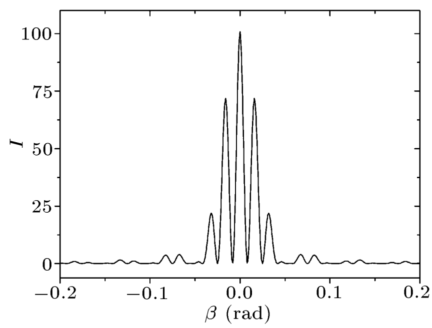

Fig. 7. Relation between β and I with $a = 20\lambda$, $b = 5000\lambda$, $c = \lambda$ and $d = 40\lambda$.

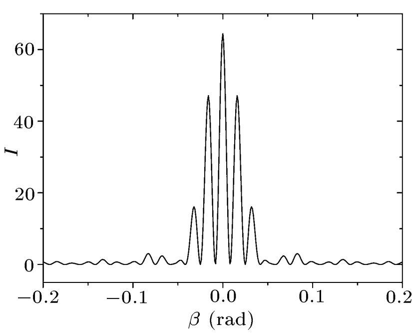

Fig. 8. Relation between β and I with $a = 20\lambda$, $b = 1000\lambda$, $c = 10\lambda$ and $d = 40\lambda$.

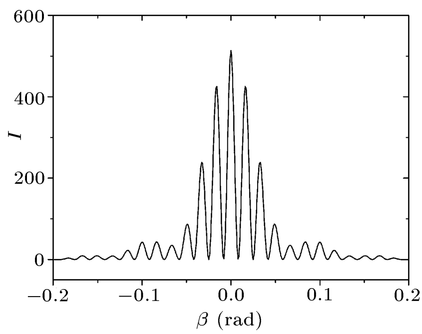

Fig. 9. Relation between β and I with $a = 20\lambda$, $b = 1000\lambda$, $c = 100\lambda$ and $d = 40\lambda$.

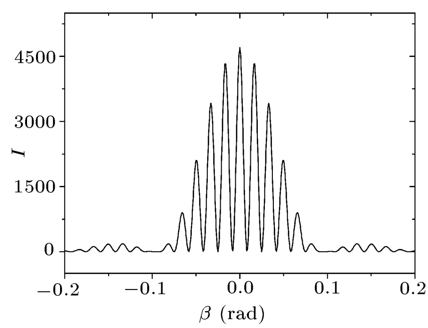

Fig. 10. Relation between β and I with $a = 20\lambda$, $b = 1000\lambda$, $c = 1000\lambda$ and $d = 40\lambda$.

In conclusion, we have studied the double-slit diffraction phenomenon of electron with quantum mechanical approach. The relation between diffraction angle and the relative diffraction intensity is presented. It is found that: (1) When the ratio of $\frac{d+a}{a} = n$ $(n = 1, 2, 3, \ldots)$, orders $2n, 3n, 4n, \ldots$ are missing in diffraction pattern. (2) When the ratio of $\frac{d+a}{a} \neq n$ $(n = 1, 2, 3, \ldots)$, there is not missing order in diffraction pattern. (3) A new quantum effect appears, i.e. the slit thickness c has a large affect on the electronic diffraction patterns. We think that all the predictions in our work can be tested by the electronic double slit diffraction experiment.

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