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The Green function treatment of one and two rectangular apertures diffraction การศึกษาปรากฏการณ์เลี้ยวเบนผ่านช่องเปิดสี่เหลี่ยมเดี่ยวและคู่โดยวิชีฟังก์ชันกรีน

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ABSTACT

In this paper, the free Green function is required for calculation of the probability amplitudes as well as probabilities to predict the diffraction patterns corresponding to one and two rectangular apertures. Also, it is verified that under the Fraunhofer regime they take the same forms as classical optical cases (without h). In addition, the asymptotic behaviors of probabilities are investigated at the point very far away from the center of detection screen. By analyzing these results, the elementary truth of quantum mechanics is implied that it is not the probabilities to be added, but the probability amplitudes instead. As is well known, the interpretation of these phenomena plays a vital role in laying the actual foundation of quantum mechanics.

บทคัดย่อ

ในงานชิ้นนี้เราอาศัยฟังก์ชันกรีนสำหรับอนุภาคอิสระเพื่อคำนวณแอมพลิจูดความน่าจะเป็นและความน่าจะ เป็นเพื่อทำนายลวดลายการเลี้ยวเบนผ่านช่องเปิดเดียวและคู่ อีกทั้งยังเป็นการพิสูจน์ว่าภายใต้เงื่อนไขแบบเฟราโฮเฟอร์ ลวดลายการเลี้ยวเบนมีรูปแบบเดียวกันกับกรณีการเลี้ยวเบนแบบคลาสสิกของแสง (ไม่มี h) นอกจากนี้ยังได้ศึกษา พฤติกรรมของความน่าจะเป็นที่ระยะไกลมากจากตำแหน่งกึ่งกลางของฉากตรวจวัด จากการวิเคราะห์ผลลัพธ์ดังกล่าว ทำให้เราทราบความจริงพื้นฐานของกลศาสตร์ควอนตัมว่าการรวมความน่าจะเป็นโดยตรงนั้นเป็นวิธีที่ผิด วิธีที่ถูกคือ การรวมแอมพลิจูดความน่าจะเป็นแทน อย่างที่เราทราบกันดีการตีความปรากฏการณ์นี้มีความสำคัญยิ่งในการสร้าง รากฐานที่มั่นคงของกลศาสตร์กวอนตัม

Keywords: Green function, Frauhofer Diffraction, Diffraction pattern คำสำคัญ: ฟังก์ชันกรีน การเลี้ยวเบนแบบเฟราโฮเฟอร์ ลวดลายการเลี้ยวเบน

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Introduction

The diffraction phenomena are extremely overemphasized; especially it is used to justify validity of the quantum theory as appeared today. Generally, the diffraction is considered as *the bending of light or particles around edges of obstacles or apertures*, we can therefore detect them outside the classical-geometrical-shadow regions of obstacles. In optics, diffractions can be classified according to the aperture-screen separation distance into two categories: Fraunhofer and Fresnel diffractions (E. Hecht, 2002). One of these, mathematically the Fraunhofer diffraction is much simpler than the other. Moreover, analytical forms of mathematical function determining diffraction through various simple shapes can be simply determined in optics and we hope this simplification will occur in quantum mechanics too. Unlike in optics, in quantum mechanics, *what we wish to calculate is the probability amplitudes or wave functions* in which all information about particles of interest is contained. By analyzing these, the fundamental truth of quantum mechanics is found that addition of probabilities does not work as it is done in classical probability theory, but what we can do is addition of probability amplitudes contributing from two slits.

Recently, many works on quantum diffractions are always developed based on *path integral formulation*, a beautiful and powerful approach, developed by one the great master of modern physics (P. Sancho, 2014; R. Sawant et al., 2014; E. R. Jones et al., 2015). It gives fine and clear descriptions about interference and diffraction. However, there is another way to do that. In physics, the Green function corresponding to Schrödinger equation is interpreted as the probability amplitude of finding a particle, which starts out at an initial position and ends up at a final one (E. B. Manoukian, 2006). In other words, it can provide the probability of particle's observations at any point on detection screen. For simplicity, we should not in this paper consider infinite screens (especially, with apertures) as *material objects* to be made up of atoms and so on, but they are objects in a geometric sense which we can represent apertures on screens by corresponding *constraints* to which possible particle's paths or trajectories adhere.

The brief outline is the following. We will, in the first stage, derive the corresponding Green function related to a free particle, which it can be done by solving the Schrödinger equation in terms of Green functions, and then apply it to explore quantum behavior of the particle diffracted by one rectangular aperture when the detection screen is very far from the aperture's plane. Namely, we simply consider the case of Fraunhofer situation. Moreover, its extension to two apertures situation is examined, it obviously provides the fundamental fact about addition of probabilities amplitudes. In the case of circular holes, the excellent explanation and detailed analysis are given in E. B. Manoukian (1989). This work insightfully and clearly examines particles' diffractions, but also their refraction off a plane. Eventually, we found that the desired expressions for diffractions take the forms of the products of two sinc functions as in classical optics and that they are quickly decreasing when the observation point is very far from a center of detection plane and eventually converge to zero at infinite limit.

Objective of the study

The primary aim of this study is to apply the Green function technique to the Diffraction of electrons passing through one and two rectangular apertures under Fraunhofer condition.



Materials and methods

Free Green function and essentials

At the onset, we begin with the simple model of electron diffraction for which is good enough to account. Since electrons move from the source, passing through either the one or two rectangular apertures, and then reach the detection screen, they are not exerted by any external force field. Thus, we can assume those electrons are **free**.

In quantum world, behavior of an electron can simply be described by the Schrodinger's equation which takes the form of differential equation as given by

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) + \frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{x},t) = 0.$$
⁽¹⁾

Notice that we model the electron is free so the potential energy in the above equation vanishes. As we saw the Schrödinger's equation is a second order partial differential equation.

In mathematics, there are many ways to find solutions or **wavefunctions**. Nevertheless, in this work we will exclusively focus on the Green function method that gives us a more benefit than others. According to the Green function technique, the above equation has to transform into that with the Green function term appearing. Then, Eq.(1) reads

$$\left[ih\frac{\partial}{\partial t} + \frac{h^2}{2m}\nabla^2\right]G(\mathbf{x},t;\mathbf{x}',t') = ih\delta^3(\mathbf{x}-\mathbf{x}')\delta(t-t') \text{ for } t-t' \ge 0,$$
(2)

where $G(\mathbf{x}, t; \mathbf{x}', t') = \langle \mathbf{x}, t | \mathbf{x}', t' \rangle$ is called the Green function corresponding to the Schrödinger equation for free particle. Generally, the Green function (more precisely the *propagator*) refers to the **probability amplitude** of a particle initially starting at one point \mathbf{x}', t' and finally ending up at another point \mathbf{x}, t . The **probability** can compute by taking the absolute square of that probability amplitude that tells us how many chances we can find the particle moving from \mathbf{x}', t' to \mathbf{x}, t .

For simplicity, we will solve Eq.(2) by using the Fourier transform. On defining the involving Fourier transform

$$G(\mathbf{x},t;\mathbf{x}',t') = \frac{1}{(2\pi\hbar)^2} \int dp G(p) e^{ip(x-x')/\hbar}$$

$$\delta^3(\mathbf{x}-\mathbf{x}')\delta(t-t') = \frac{1}{(2\pi\hbar)^2} \int dp e^{ip(x-x')/\hbar}$$
(3)

where x and p are 4-vectors. Substituting Eq.(3) into Eq.(2) and doing some algebra, we obtain

$$G(\mathbf{x},t;\mathbf{x}',t') = \frac{1}{(2\pi\hbar)^2} \int dp \frac{e^{ip(x-x')/\hbar}}{\left(p^0 - \frac{\mathbf{p}^2}{2m}\right)}$$

This integral can be evaluated by using the Gaussian integral formula together with technique of contour integral, it follows that



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$$G(\mathbf{x},t;\mathbf{x}',t') = \left(\frac{m}{2\pi i h(t-t')}\right)^{3/2} \exp\left[\frac{im|\mathbf{x}-\mathbf{x}'|^2}{2h(t-t')}\right].$$
(4)

This is the Green function describing a free particle which moves in three dimensional space.

Now we shall develop method for dealing with the diffraction problem, this idea is very important in modern quantum theory and can easily be extended to **Feynman's path integral**. Let us take a look at the definition of Green function in inner product form

$$G(\mathbf{x},t;\mathbf{x}',t') = \left\langle \mathbf{x},t \,\middle| \,\mathbf{x}',t' \right\rangle. \tag{5}$$

We insert the completeness relation $\mathbf{1} = \int d^3 \mathbf{x}'' |\mathbf{x}'', t''\rangle \langle \mathbf{x}'', t''|$ in the last equation, Eq.(5) becomes

$$G(\mathbf{x},t;\mathbf{x}',t') = \int d^3 \mathbf{x}'' G(\mathbf{x},t;\mathbf{x}'',t'') G(\mathbf{x}'',t'';\mathbf{x}',t') .$$
⁽⁶⁾

This means that if there is any object (not physical) is placed between the initial and final points, we can divide the overall movement into two events or steps: (1) the particle starts out at an initial point \mathbf{X}' at time t' and then goes through some certain regions specified by its geometry; (2) the particle carries on motion and is observed at a final point \mathbf{X} and time t. The integration variable is related to the geometry of the inserted object or obstacle. By iteratively inserting the completeness relation, we could formulate the path integral method. In addition, we suppose that a particle goes merely through a given screen and reaches a given position at time t. Namely, if we find a particle at time t somewhere outside the region of interest, we will stop the analysis. In other words, only the possible paths or trajectories which pass through the region of interest at time t are consider, all other paths are ignored.

Since the Green function, which in view of Schrodinger's concepts is equivalent to the wavefunction that a particle leaves the point source, represents the probability amplitude that the particle is observed at a given (infinite) detection screen, it must therefore obey the **normalization condition** as given by

$$1 = \int d^3 \mathbf{x} \left| G(\mathbf{x}, t; \mathbf{x}', t') \right|^2 \,. \tag{7}$$

This means that the **sum of overall probabilities** of finding a particular particle must be unity. These tools are employed in the following section to calculate the probability amplitudes for one and two rectangular apertures diffraction.

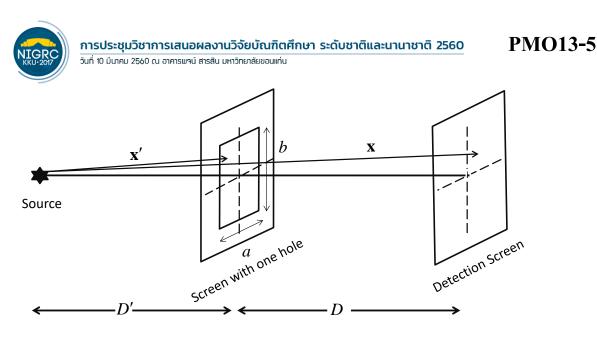


Figure 1 Schematic arrangement of one rectangular aperture

One rectangular aperture

Consider a particle which moves from a point source, placed at the origin, at the beginning of time t = 0, passes through a rectangular aperture on the infinite screen at t = t', and eventually hits on the infinite detection screen at t.

According to figure 1, we obtain

$$\left|\mathbf{x}'\right|^2 = x'^2 + y'^2 + D'^2,\tag{8}$$

$$|\mathbf{x} - \mathbf{x}'|^2 = (x - x')^2 + (y - y')^2 + D^2.$$
 (9)

In limit of Fraunhofer diffraction $D^2 \ge x^2 + y^2$ i.e., the diffracting screen is separated at very long distance from apertures. Then Eq.(9) is reduced to

$$\left|\mathbf{x} - \mathbf{x}'\right|^2 = -2xx' - 2yy' + x^2 + y^2 + D^2$$
(10)

Now our constraint is merely an area through which the particle is allowed to pass. Namely, we have to make a substitution $\int d^3 \mathbf{x}' \rightarrow \int_{\text{one aperture}} dx' dy'$. Accordingly, the Green function becomes

$$G(\mathbf{x},t;0,0) = A \int_{-a/2}^{a/2} \int_{-b/2}^{b/2} dx' dy' \exp\left[-\frac{imxx'}{h(t-t')}\right] \exp\left[\frac{imyy'}{h(t-t')}\right],$$
(11)

where A stands for the **normalization constant** in which contains any terms not involving x' and y'. On integration of the above equation, we get the resulting Green function

$$G(x,t;0,0) = abAJ_0 \left[\frac{max}{2h(t-t')}\right] J_0 \left[\frac{mby}{2h(t-t')}\right],$$

where $J_0(x) = \sin x / x$ is the Bessel function of the zero order of the first kind. We can simply determine constants including in the previous result by means of the integral formula which is in form of Gaussian integral (Gradshteyn IS, Ryzhik IM, 1985). We obtain



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$$\int_{0}^{\infty} \frac{\sin^{2} ax}{x^{2}} = \frac{a\pi}{2} \text{ for } a > 0$$
 (12)

so that the normalization constant is

$$A = \frac{m}{\sqrt{ab} 2\pi h(t - t')}.$$
(13)

Finally, the desired Green function is given by

$$G(\mathbf{x},t;0,0) = \frac{m\sqrt{ab}}{2\pi h(t-t')} J_0 \left[\frac{max}{2h(t-t')}\right] J_0 \left[\frac{mby}{2h(t-t')}\right].$$
(14)

That is what we can calculate from quantum theory employing the Green function method. Due to this result, we are lead to find the probability of finding an electron on the detection screen. To put it more precisely, the probability is equivalent to the diffraction pattern as we will see in result section. Note that this result is very analogous to the diffracted light through the rectangular screen (E. Hecht, 2002).

Two rectangular apertures

As before, due to figure 2, we can write down

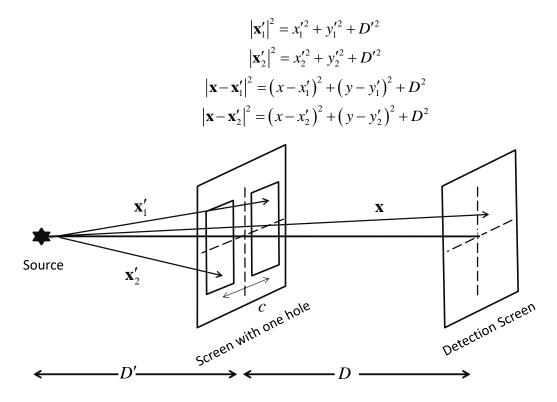


Figure 2 Arrangement for two holes aperture

In this section, we consider a particle which is released at t = 0 from a point source placed at the origin. This time, an electron has two alternatives to move through i.e., either the left or right openings (looking from the source along common axis toward the screen) at time t = t', and finally at t reaches a certain observation point on



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the last screen. We let c be The separation distance of these two apertures. Note that we propose the same electron could not emerge from two holes simultaneously, so it is forced to choose one of holes. Thus, there are two contributions to add up to the total probability amplitude or mathematically we could write down

$$G(\mathbf{x},t;0,0) = G_1(\mathbf{x},t;0,0) + G_2(\mathbf{x},t;0,0), \qquad (15)$$

where the subscript means the contribution popping up from the first and second holes, respectively. This way of summing probability amplitudes is in great detail explained by many authors (E. B. Manoukian, 2006; R. P. Feynman et al., 1965). The above equation is very important in quantum theory that tells us the correct probability calculation has to start with summing each contribution up and do the absolute square. Eq. (15) can be evaluated simply by making use of the result from one hole diffraction as follows

$$G(\mathbf{x},t;0,0) = A \left\{ \int_{-c+a/2}^{-c-a/2} \int_{-b/2}^{b/2} dx' dy' \exp\left[-\frac{imxx'}{h(t-t')}\right] \exp\left[\frac{imyy'}{h(t-t')}\right] + \int_{c+a/2}^{c-a/2} \int_{-b/2}^{b/2} dx' dy' \exp\left[-\frac{imxx'}{h(t-t')}\right] \exp\left[\frac{imyy'}{h(t-t')}\right] \right\}$$

where A related to two integrands are equal because the sizes of two apertures are the same. This means that an electron has equal chances to go through either. This integral can be calculated straightforwardly from the previous result, we obtain

$$G(\mathbf{x},t;0,0) = abAJ_0 \left[\frac{max}{2h(t-t')}\right] J_0 \left[\frac{mby}{2h(t-t')}\right] \cos\left[\frac{mcx}{2h(t-t')}\right].$$
(16)

By the same token, we can determine constants by using integral formulas (Gradshteyn IS, Ryzhik IM, 1985)

$$\int_{0}^{\infty} \frac{\sin^{2}(ax)\cos^{2}(bx)}{x^{2}} dx = \frac{1}{4}\pi \left[a + \max(0, a - b)\right],$$
(17)

where $\max(0, a-b)$ is the maximum value in range of 0 to a-b. Hence, we obtain

$$A = \frac{m}{\sqrt{2ab}\pi i h(t - t')} \tag{18}$$

Finally, we get the desired Green function as given by

$$G(\mathbf{x},t;0,0) = \frac{m\sqrt{ab}}{\sqrt{2}\pi i h(t-t')} J_0 \left[\frac{max}{2h(t-t')}\right] J_0 \left[\frac{mby}{2h(t-t')}\right] \cos\left[\frac{mcx}{2h(t-t')}\right].$$
(19)

So far, we showed how the Green function relating to the master equation in quantum physics came from and applied it to handle the problems of diffraction by one and two rectangular apertures. The solution to diffraction problem is the Green function which provides information about a particle in a sense that it tells us how many



chances we would find the particle at any point. With these results, they lead us to calculation of probability as we shall see in the next section.

Results

As quantum mechanics tells us that if we have got the probability amplitude we can simply calculate the related probability by doing the absolute square of that amplitude. Carrying on the absolute square here means multiplying the Green function by its *complex conjugate* since the Green function is complex, not real. Then the probability of finding the electron on the detection screen is given by

$$P(\mathbf{x},t;0,0) = |G(\mathbf{x},t;0,0)|^2 = G(\mathbf{x},t;0,0)^* G(\mathbf{x},t;0,0)$$
(20)

In the first case, an electron is fired at the one rectangular aperture, we have

$$P(\mathbf{x},t;0,0) = \frac{m^2 ab}{4\pi^2 h^2 (t-t')^2} J_0^2 \left[\frac{max}{2h(t-t')}\right] J_0^2 \left[\frac{mby}{2h(t-t')}\right].$$
(21)

Someone could recognize this equation is very similar to diffraction pattern in case of light. This implies that an electron and light has some common property we will discuss this issue later on. But this time, we concentrate on Eq.(21) and plot the probability against coordinates on the detection screen. The plot roughly shows the diffraction pattern through one aperture as in figure 3.

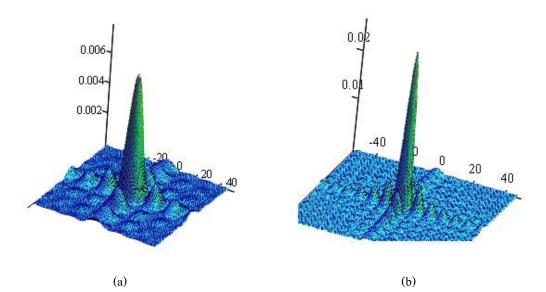


Figure 3 These plots represent diffraction patterns by the electron passing through the one rectangular aperture: (a) with 1×1 a.u.² (a.u. standing for atomic units) aperture size and 200 a.u. aperture-screen distance, (b) with 1×1 a.u.² aperture size and 100 a.u. aperture-screen distance. In both, we set up the electron's velocity is 80/137 in a.u.

As illustrated in figure 3, actually the probability is equivalent to the diffraction pattern. The higher the probability gets, more the chances of finding the particle. Moreover, we can see from Eq. (14) that at a point which is very far



from the center of a detection screen the probability is rapidly decreasing. We can express in mathematical function at asymptotic limit as follows. The Bessel function of the zero order of first kind at asymptotic limit is written by

$$\left|J_{0}(x)\right| \leq \sqrt{\frac{2}{\pi x}} \left\{ 1 + \frac{0.125}{x} + \frac{0.07}{x^{2}} + \frac{0.0732}{x^{3}} \right\} \approx \sqrt{\frac{2}{\pi x}} \left\{ 1 + O(\frac{1}{x}) \right\}.$$
 (22)

So we can rewrite Eq.(14) as

$$G(\mathbf{x},t;0,0) \le \frac{2}{\pi^2 \sqrt{xy}} \left\{ 1 + O(\frac{1}{x}) \right\} \left\{ 1 + O(\frac{1}{y}) \right\}.$$
(23)

Obviously, the probability amplitude or Green function is decreasing as the distance from center is increasing. Eventually, it approaches zero as the distance tends to infinity.

For the two rectangular apertures, we can do it in the same way i.e., we multiply Eq.(19) by its complex conjugate. It follows that

$$P(\mathbf{x},t;0,0) = \frac{m^2 ab}{2\pi^2 h^2 (t-t')^2} J_0^2 \left[\frac{max}{2h(t-t')}\right] J_0^2 \left[\frac{mby}{2h(t-t')}\right] \cos^2 \left[\frac{mcx}{2h(t-t')}\right].$$
(24)

The different thing we can obviously see is the cosine term appearing in Eq.(24). Indeed, the cosine term represents interference effect due to the second aperture we added. If we look at the diffraction pattern, we will see clearly that interference fringes inserts in a bigger diffraction pattern. Moreover, we can simply transition from two apertures to one aperture by taking the limit of Eq.(21) approaching zero. When we plot the probability versus points on the screen we get diffraction patterns as in figure 4.

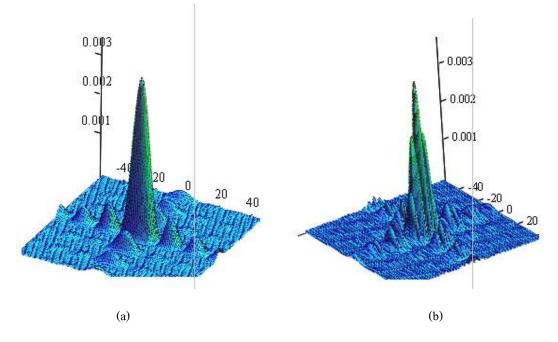


Figure 4 The plots represent diffraction patterns through two apertures. In both the aperture sizes are the same as the previous one with (a) c = 1 in a.u. and (b) c = 20 in a.u.



As we see from figure 4, when the separation between two apertures is bigger, it turns out that the center peak contains many sub-peaks within. This shows the effect of interference that result from addition of second aperture. Similarly, the probability or diffraction pattern is decreasing by deducing from the fact that the probability amplitude takes the form of Bessel function as descried in one aperture case.

Discussion

Because of the Green functions we calculate in early stage, they represent the probability amplitude of finding an electron diffracted by the aperture. In addition, the probability amplitude leads us to the probability by taking the absolute square or more correctly by multiplying with its complex conjugate. When we plot the probability against points on screen, we see that the graph is equivalent to diffraction pattern in the case of light. However, light diffracted by any obstacle will create a diffraction pattern that is indicated by bright and dark bands. Still, particle and light diffraction have something similar i.e., dark band will show a region which light cannot be observed and bright band will show a region which light can be observed. This implies that an electron can be diffracted by aperture as the same as light can do. This strange property will occur for any small particles like an electron or a neutron. In principle, we can describe this by making use of de Broglie's matter wave stating that all matter can behave like wave and wave-like behavior is determined by its wavelength. This means that electrons can do interference and diffraction but these depend on their wavelength and how to observe them.

In analyzing diffraction patterns, we need the constraints as follows. The aperture to screen distance is 200 in a.u., electron velocity is 80/137 in a.u. and 1×1 a.u.². In both cases, we need to set the size of aperture to be very small comparable to aperture distance in order that the Fraunhofer condition is required. By doing that way, the complication in form of Green function is removed and the Green function in closed form corresponding to this problem takes the form of Bessel function as Eq.(14) and Eq.(19).

In the one aperture case, we have the closed form of the probability amplitude as in Eq.(14). Therefore, we plot the probability against points on screen, as shown in Fig.3. We see that when the aperture to screen distance is smaller, the distribution of probability is smaller too. That is, we have a more chances to find an electron at center than elsewhere. Of course, the more the aperture to screen distance is bigger, the more the distribution of probability is. Note that if we sum up all probability, we will get unity. This is what we have already known from theory of probability and it occurs in quantum mechanics as well. Moreover, the probability is decreasing as the observation point is far away from the center. This makes some senses because when we fire electron through any hole we are likely to find the electron at the center and have less chances to find at far distance.

In the two apertures situation, we only add another aperture and separate them and we find that the contributions from two apertures have to sum up. Contribution in this case means the probability amplitude. The correct way to calculate the corresponding probability is to sum probability amplitude from each aperture and do the absolute square to get the probability as Eq.(15). By the same token, we get the probability describing diffraction pattern through two apertures as given by Eq.(24). We see that Eq.(24) has something different from Eq.(21) i.e. it



contains cosine term which represents interference effect. From Fig. 4, interference effect will be dominant when the separation spacing between two apertures is bigger as you clearly see many sub-peaks in main peaks such as a center peak.

Conclusions

In this work, we used the Green function method to solve the diffraction problem. We started with calculation of the Green function corresponding to a free electron. In studying diffraction, overall motion of the electron can be divided into two steps: (1) the electron moved from a source to aperture and (2) the electron continued to move from aperture to the screen. Each step was explained by its Green function. We related Green functions together by doing the product of two Green functions and integrating over the area through which the electron passed. In this case, we integrated over rectangular area. We found that the Green function is interpreted as the probability amplitude of finding the electron on the screen and this leads us to probability by taking the absolute square. The probability will tell us how many chances we have to detect the electron on the screen. By comparison with light, the probability is comparable to diffraction pattern which contains bright and dark regions. In the two apertures case, the other aperture was simply added and we found the right way to calculate contribution from each aperture is to sum all probability amplitudes. The probability was calculated by doing the absolute square of total probability amplitude. Moreover, we found that the probability includes cosine term which results from interference effect. This effect will be more obvious if we made the distance between two apertures bigger.

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