

- ²²H. Poincaré, *Science et Methode* (Flammarion, Paris, 1908), p. 96.
- ²³S. Themerson, Cardinal Pólátio (Gaberbochus, London, 1961), p. 92.
- ²⁴H. B. G. Casimir (private communication, 1986).
- ²⁵D. C. Mattis, *The Theory of Magnetism* (Harper & Row, New York, 1965), p. 38.
- ²⁶J. O. Hirschfelder, C. F. Curtiss, and R. Byron Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1967), p. 960.
- ²⁷B. R. A. Nijboer, *Physica A* **79**, 420 (1975).
- ²⁸L. Rosenfeld, *Theory of Electrons* (Dover, New York, 1965), p. 14.
- ²⁹P. Mazur and B. R. A. Nijboer, *Physica* **19**, 971 (1953).
- ³⁰K. Schram, *Physica* **26**, 1080 (1960).
- ³¹S. R. de Groot, in *Studies in Statistical Mechanics*, edited by E. W. Montrell and J. L. Lebowitz (North-Holland, Amsterdam, 1969).
- ³²F. N. H. Robinson, *Macroscopic Electromagnetism* (Pergamon, Oxford, 1973).
- ³³S. R. de Groot and P. Mazur, *Non-Equilibrium Thermodynamics* (North-Holland, Amsterdam, 1962), pp. 22, 83.
- ³⁴S. G. Brush, *Statistical Physics and the Atomic Theory of Matter* (Princeton U.P., Princeton, NJ, 1983).
- ³⁵*Entropy and Information in Science and Philosophy*, edited by L. Kubát and J. Zeman (Elsevier, Amsterdam, 1975).
- ³⁶E. C. G. Stueckelberg de Breidenbach and P. B. Scheurer, *Thermocinétique Phénoménologique Galiléenne* (Birkhauser, Basel, 1974).
- ³⁷C. Truesdell, *An Idiot's Fugitive Essays on Science* (Springer, New York, 1984).
- ³⁸I. Prigogine, *From Being to Becoming* (Freeman, New York, 1980).
- ³⁹I. Prigogine and I. Stengers, *Order Out of Chaos* (Bantam, New York, 1984).
- ⁴⁰I. E. Farquhar, *Ergodic Theory in Statistical Mechanics* (Wiley-Interscience, London, 1964).
- ⁴¹C. Kittel, *Introduction to Solid State Physics* (Wiley, New York, 1967), 3rd ed., p. 142.

Demonstration of single-electron buildup of an interference pattern

A. Tonomura, J. Endo, T. Matsuda, and T. Kawasaki

Advanced Research Laboratory, Hitachi, Ltd., Kokubunji, Tokyo 185, Japan

H. Ezawa

Department of Physics, Gakushuin University, Mejiro, Tokyo 171, Japan

(Received 17 December 1987; accepted for publication 22 March 1988)

The wave-particle duality of electrons was demonstrated in a kind of two-slit interference experiment using an electron microscope equipped with an electron biprism and a position-sensitive electron-counting system. Such an experiment has been regarded as a pure thought experiment that can never be realized. This article reports an experiment that successfully recorded the actual buildup process of the interference pattern with a series of incoming single electrons in the form of a movie.

I. INTRODUCTION

The two-slit interference experiment with electrons is frequently discussed in textbooks on quantum mechanics, and is referred to as "impossible, absolutely impossible to explain in any classical way, and has in it the heart of quantum mechanics."¹ In this experiment (see Fig. 1), electrons incident on a wall with two slits pass through the slits and are detected one by one on a screen behind them. Accumulation of successive single electrons detected at the screen builds up an interference pattern. According to the interpretation in quantum mechanics, a single electron can pass through both of the slits in a wave form called "probability amplitude" when the uncertainty of the electron position in the wall plane covers the two slits, and when no observation is made of the electron at either one of the slits. The electron is then detected as a particle at a point somewhere on the screen according to the probability distribution of the interference pattern. However, if the electron is caught when passing through the slits, it takes place at either one of the two slits, never both, and the probability distribution on the screen will be completely different.

Although in textbooks this experiment is talked about as

a matter of fact, "this experiment has never been done in just this way, since the apparatus would have to be made on an impossibly small scale," as Feynman points out.¹ However, this is not necessarily true. In fact, several attempts have been made up to now; Zeilinger *et al.*² confirmed the

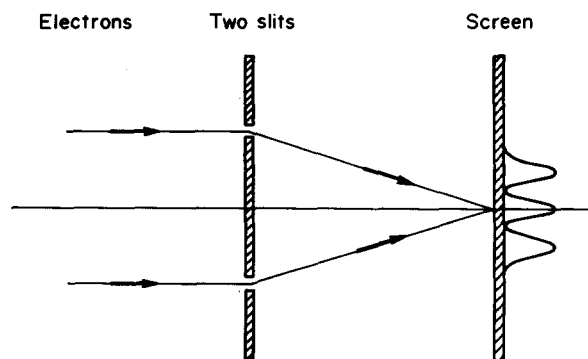


Fig. 1. Two-slit electron interference experiment.

formation of the neutron interference pattern, just as quantum mechanics predicts, by counting arriving neutrons with a scanning counter. In the case of electrons, two groups, one at Tübingen University³ and the other at Bologna University,⁴ demonstrated, in the form of a movie using a highly sensitive TV camera, the observability of the electron interference pattern as it appears when the frequency of incident electrons increases; they showed the electron arrival in each frame without recording the cumulative arrivals. In the case of photons, the buildup process of the interference pattern was recorded on a movie film by Tsuchiya *et al.*⁵ with a position-sensitive counter to accumulate the arrival of single photons on the screen. We note that the typical wavelengths of photons are much larger than those of electrons. Therefore, the difficulty Feynman attributes to the two-slit experiments for electrons does not exist for photons.

The present experiment aims at realizing the two-slit thought experiment for electrons in the form of biprism interference.

II. THEORY OF THE BIPRISM INTERFERENCE PATTERN⁶

The principle of the electron biprism invented by Möllenstedt and Dücker⁷ in 1956 has been investigated from both geometric- and wave-optical aspects.⁷⁻¹⁰ Here, a brief account of the biprism interferometer is given for the reader's convenience.

The biprism consists of two parallel grounded plates with a fine filament between them, the latter having a positive potential relative to the former. If, in the coordinate system shown in Fig. 2, the electrostatic potential is given by $V(x,z)$ and the incoming electron wave by $e^{ik_z z}$, the deflected wave is given by

$$\psi(x,z) = \exp i \left(k_z z - \frac{me}{\hbar^2 k_z} \int_{-\infty}^z V(x,z') dz' \right), \quad (1)$$

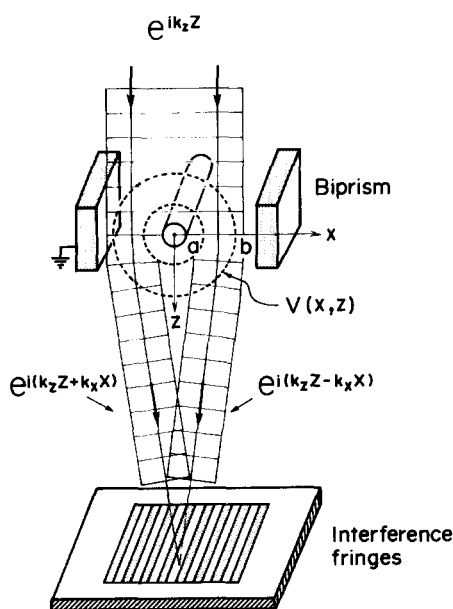


Fig. 2. Deflection of electron waves by biprism—the case of plane-wave incidence.

when $\hbar^2 k_z^2 / 2m \gg e|V(x,z)|$, as is the case in the present experiment.

The two waves having passed on each side of the filament can be approximated by

$\exp i(k_z z \pm k_x x)$ up to a constant factor, where

$$k_x = - \frac{me}{\hbar^2 k_z} \int_{-\infty}^{\infty} \left(\frac{\partial V(x,z')}{\partial x} \right)_{x=a} dz', \quad (2)$$

and the symmetry $V(x,z) = V(-x,z)$ has been taken into account. Therefore, the wave fronts of the two waves are deflected as shown in Fig. 2 and, consequently, the waves propagate toward the center, since $k_x > 0$.

This can be interpreted classically also: $-e[\partial V(x,z')/\partial x]_{x=a}$ is the x component of the force exerted on the electron. Its integral with respect to $dz/v_z = dt$, $v_z = \hbar k_z/m$ gives the impulse imparted to it, which is the same in absolute value but reversed in sign, depending on which side of the filament the electron passes.

If the two waves overlap in the observation plane to give

$$\psi(x,z) = e^{ik_z z} (e^{-ik_x x} + e^{ik_x x}), \quad (3)$$

then this leads to the interference fringes

$$|\psi(x,z)|^2 = 4 \cos^2 k_x x. \quad (4)$$

If the potential in the neighborhood of the filament is approximated by

$$V(x,z) = V_a [\ln(\sqrt{x^2 + z^2}/b) / \ln(a/b)], \quad (5)$$

then

$$k_x = \pi e V_a / \hbar v_z \ln(b/a). \quad (6)$$

For $v_z = c/2 = 1.5 \times 10^8$ m/s, $V_a = 10$ V, $a = 0.5 \mu\text{m}$, $b = 5$ mm, $k_x = (\pi/900) \text{ \AA}^{-1}$, and fringe spacing $d = 900 \text{ \AA}$. In the actual experiment, a spherical wave instead of a plane wave is incident on the biprism and, consequently, the fringe spacing becomes larger, as described in Sec. III.

III. EXPERIMENTS

Experiments were carried out using an electron microscope equipped with an electron biprism and a position-sensitive electron-counting system.

Coherent electron waves from a sharp field-emission tip were, after collimation, sent to an electron biprism. The biprism interference pattern was enlarged by the electron lenses and the single-electron buildup of the interference pattern was observed in time sequence on the TV monitor of a two-dimensional position-sensitive electron-counting system, which was connected to a storage memory. Electrons could be detected one by one, since the detection efficiency was approximately 100% and the detection error was less than 1%.

The detailed experimental arrangement is shown in Fig. 3. Electrons are emitted from a field-emission tip by an applied electrostatic potential $V_1 = 3 - 5$ kV, and then accelerated to the anode of potential $V_0 = 50$ kV. The electron beam accelerated to V_0 is associated with a wave of wavelength

$$\lambda = h / \sqrt{2meV_0(1 + eV_0/2mc^2)}, \quad (7)$$

which, in the present case, is 0.054 \AA . The total emission current is intentionally limited to $\sim 1 \mu\text{A}$, only 10^{-4} of which passes through the anodes. The electrons are focused through the condenser lens into fine probe P_1 , and

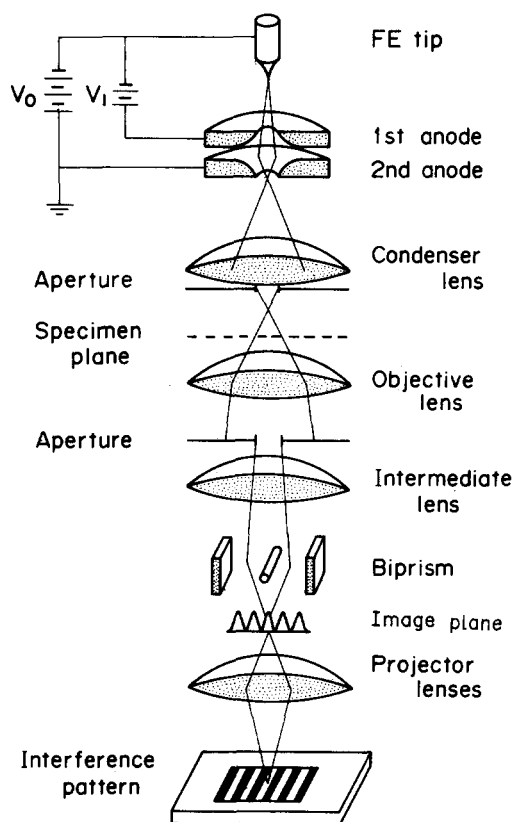


Fig. 3. Electron-optical diagram of the interference experiment.

then illuminate the specimen plane. At this stage, $\frac{1}{10}$ of the electrons pass through the condenser aperture. The electron amplitude in the specimen plane is reproduced through the objective and intermediate lenses onto the image plane of the intermediate lens. Only the central portion of the beam passes through the field-limiting aperture located just above the intermediate lens and is focused by the lens into fine probe P_2 . The total current is controlled by changing the focal length of the intermediate lens and, in a typical case, is 1.6×10^{-16} A or 10^3 electrons/s.

The beam issuing from the probe is then incident on the biprism, and the two partial beams are deflected by the angles $\pm k_x/k_z$ [see Eq. (2)] on each side of the biprism. The divergence angle 2α of the incident beam is approximately 4×10^{-8} rad. Consequently, the transverse coherence length given by $\lambda/2\alpha$ is $140 \mu\text{m}$, which is larger than the diameter of the biprism filament ($< 1 \mu\text{m}$) but smaller than the distance between the two grounded electrodes ($\sim 10 \text{ mm}$). The two beams interfere on the image plane to form interference fringes, one-half of the angle β between the interfering beams being given by

$$\beta = l/(l+l')(k_x/k_z), \quad (8)$$

and the fringe spacing by

$$d = \lambda/2\beta, \quad (9)$$

which is larger by a factor $(l+l')/l$ than the value given at the end of Sec. II.

In this experiment, $\lambda = 0.054 \text{ \AA}$, $V_a = 10 \text{ V}$, $l'/l = 6$, and $2\beta = 8 \times 10^{-6}$ rad, so that $d = 7000 \text{ \AA}$. The interference pattern is finally magnified 2000 times through two projector lenses onto the detector plane. The detector is

approximately 12 mm in diameter and the enlarged fringe spacing is 1.4 mm.

Electrons are detected by a two-dimensional position-sensitive electron-counting system, which is schematically illustrated in Fig. 4. This system is a combination of a fluorescent film and the photon-counting image acquisition system (PIAS) produced by Hamamatsu Photonics K.K. We paid special attention to suppressing both counting loss and detection noise to less than 1%. When a 50-kV electron hits the fluorescent film, approximately 500 photons are produced from the spot. The photons excite the photo cathode through the fiber plate and photo electrons are produced. They are accelerated to 3 kV through the electrostatic lens and the point image of electrons is formed at the upper surface of the multichannel plate (MCP). The number of electrons is multiplied there and the position is then measured by the position sensor. The signal of the electron arrival at each channel is transferred to the storage memory and the accumulated electron image is displayed on the TV monitor.

The experiment was performed at the electron arrival rate of approximately 10^3 electrons/s in the whole field of view so that the interference fringes could be formed in a reasonable time, say, 20 min. The distance from the source to the screen is 1.5 m, while the average interval of successive electrons is 150 ns. In addition, the length of the electron wave packet is as short as $\sim 1 \mu\text{m}$. Therefore, there is very little chance for two electrons to be present simultaneously between the source and the detector, and much less chance for two wave packets to overlap.

An example of the buildup process of the interference pattern is shown in Fig. 5 in the form of a time series of photographs. The photographs were taken from single frames in a TV display. Electrons were detected one by one, and the total number of accumulated electrons increases with time. At first, electrons appear to be distributed quite at random. A dim figure of the biprism fringes begins to emerge in Fig. 5(c). The fringes can finally be clearly observed in Fig. 5(e), where the total number of electrons is approximately 70 000, i.e., 14 000 electrons per fringe.

These results unambiguously demonstrate the wave-particle duality of electrons. On the one hand, a single electron passes through the two slits as a wave and forms a probability interference pattern; electron-electron interaction plays no role in this process since the subsequent elec-

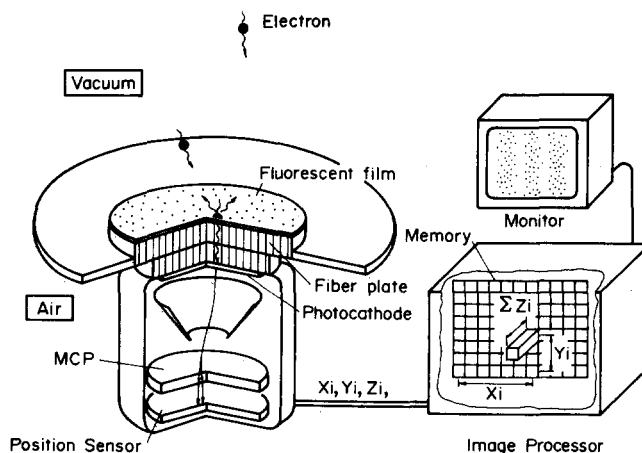


Fig. 4. Schematic diagram of position-sensitive electron-counting system.

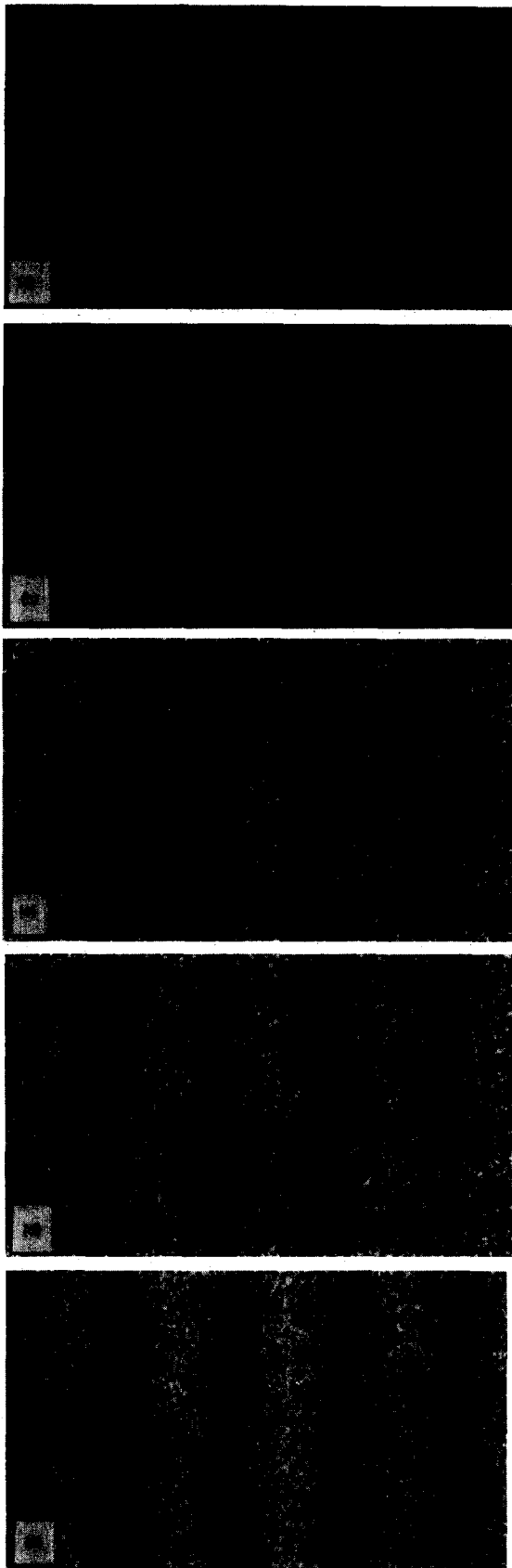


Fig. 5. Buildup of the electron interference pattern. The central field of view, $\frac{1}{3}$ width and $\frac{1}{2}$ length, of the whole field of the detector plane is shown here. The picture extends similarly to the whole field: (a) Number of electrons = 10; (b) Number of electrons = 100; (c) Number of electrons = 3000; (d) Number of electrons = 20 000; and (e) Number of electrons = 70 000.

tron is not even produced from the cathode till long after the preceding electron is detected. At the detector, on the other hand, an electron is observed as a localized particle. We must conclude that a certain position on the screen is selected, onto which the electron wavefunction collapses. The position cannot be predicted, but occurs in the probabilistic way dictated by the probability amplitude.

A series of similar experiments was carried out for different electron intensities ranging from 5000 to 200 electrons/s. The contrast of the fringes obtained remains the same within experimental error of 10%. At the smaller intensity, the error often became large due to the long exposure time, since the error originates mainly from the drift of the biprism filament.

IV. CONCLUSION

We realized a two-slit interference experiment, once regarded as a pure thought experiment with no hope of precise execution, with a combination of both electron-counting and magnifying techniques. The resultant buildup of the interference pattern is exactly as predicted by quantum mechanics.

ACKNOWLEDGMENTS

We should like to thank Dr. Yoshiji Suzuki, Dr. Yutaka Tsuchiya, and Nobuyuki Hirai of Hamamatsu Photonics K.K. for their cooperation in developing the electron detector. Thanks are also due to Dr. Hideo Todokoro of Central Research Laboratory and Shuji Hasegawa of Advanced Research Laboratory, Hitachi, Ltd., for their helpful discussions and assistance in the experiment.

¹R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics* (Addison-Wesley, Menlo Park, CA, 1965), Vol. III, pp. 1-1-1-5.

²A. Zeilinger, R. Gaehler, C. G. Shull, and W. Treimer, in *Proceedings of the Conference on Neutron Scattering, Argonne, 1981*, edited by J. Faber, Jr. (AIP, New York, 1982), p. 93.

³The movie was shown in the International Symposium on Foundations of Quantum Mechanics held at Tokyo in 1983, by H. Lichte, Institute of Applied Physics, University of Tübingen, 74 Tübingen, West Germany; see also H. Lichte, in *New Techniques and Ideas in Quantum Measurement Theory*, edited by D. M. Greenberger (New York Academy of Sciences, New York, 1988), p. 175.

⁴The movie was produced by G. Pozzi and G. F. Missiroli, Department of Physics, University of Bologna, 40126 Bologna, Italy.

⁵Y. Tsuchiya, E. Inuzuka, T. Kurono, and M. Hosoda, in *Advances in Electronics and Electron Physics*, edited by P. Hawkes (Academic, New York, 1982), Vol. 64A, p. 21.

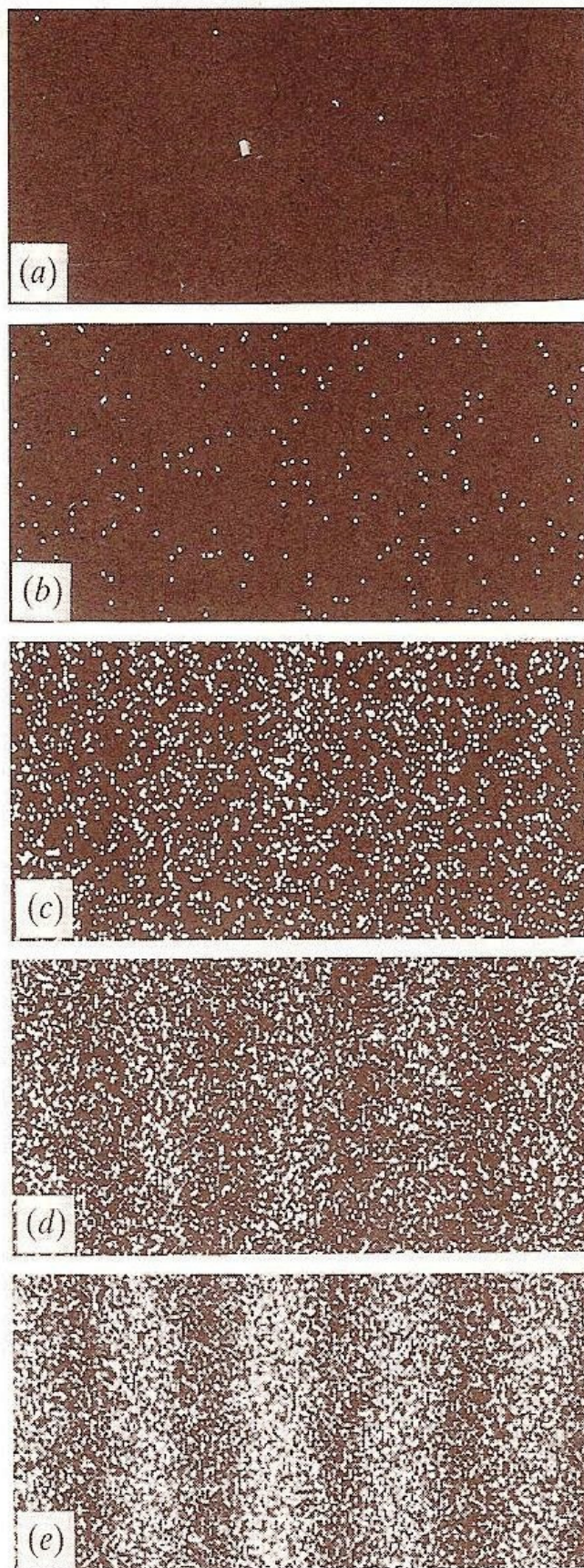
⁶H. Ezawa (in preparation).

⁷G. Möllenstedt and H. Dücker, *Z. Phys.* **145**, 375 (1956).

⁸J. Faget and C. Fert, *Cah. Phys.* **83**, 285 (1957).

⁹T. Hibi and S. Takahashi, *J. Electron Microsc.* **12**, 129 (1963).

¹⁰J. Komrska, V. Drahos, and A. Delong, *Opt. Acta* **14**, 147 (1967).



Frontispiece. The cumulative pattern generated by the ‘self-interference’ of electrons sent one by one through a two-slit interferometer. Number of electrons: (a) 10, (b) 100, (c) 3000, (d) 20 000, (e) 70 000 (from Tonomura *et al.* (1989)).

§ DINÂMICA QUÂNTICA

Evolução temporal e Equação de Schrödinger

Tempo t_0 : $|\alpha\rangle$

Tempo $t > t_0$: $|\alpha, t_0; t\rangle$

Requerimento de continuidade:

$$\lim_{t \rightarrow t_0} |\alpha, t_0; t\rangle = |\alpha\rangle,$$

ou $|\alpha, t_0; t_0\rangle = |\alpha, t_0\rangle \equiv |\alpha\rangle$

Queremos determinar a evolução com o tempo:

$$|\alpha, t_0\rangle = |\alpha\rangle \longrightarrow |\alpha, t_0; t\rangle$$

Pergunta: Como o estado muda por uma translação temporal $t_0 \longrightarrow t$?

Como no caso das translações espaciais, ambos kets estão ligados por um operador, que aqui chamamos de Operador de evolução temporal $U(t, t_0)$:

$$|\alpha, t_0; t\rangle = U(t, t_0) |\alpha, t_0\rangle.$$

Devemos requerer que o operador seja unitário,

dada a interpretação probabilística dos kets. Supondo que os estados podem ser expandidos na base completa $\{|a'\rangle\}$ de algum observável A , temos

$$|\alpha, t_0\rangle = \sum_{a'} c_{a'}(t_0) |a'\rangle$$

$$|\alpha, t_0; t\rangle = \sum_{a'} c_{a'}(t) |a'\rangle,$$

e em geral

$$|c_{a'}(t)| \neq |c_{a'}(t_0)|.$$

Mas a condição de unitariedade se expressa por

$$\begin{aligned} \langle \alpha, t_0 | \alpha, t_0 \rangle &= \sum_{a'} |c_{a'}(t_0)|^2 = \langle \alpha, t_0; t | \alpha, t_0; t \rangle \\ &= \sum_{a'} |c_{a'}(t)|^2, \end{aligned}$$

e se os estados estão normalizados:

$$1 = \sum_{a'} |c_{a'}(t_0)|^2 = \sum_{a'} |c_{a'}(t)|^2$$

Em termos do operador \mathcal{U} temos:

$$\mathcal{U}^\dagger(t, t_0) \mathcal{U}(t, t_0) = 1$$

Requeremos também a propriedade de composição ou

de grupo:

$$U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0), \quad t_2 > t_1 > t_0$$

Em particular temos a identidade:

$$\lim_{t_2 \rightarrow t_0} U(t_2, t_0) = U(t_0, t_0) = 1$$

Construimos primeiro a transformação infinitesimal:

$$|\alpha, t_0; t_0 + dt\rangle = U(t_0 + dt, t_0)|\alpha, t_0\rangle$$

Ela deve estar "perto" da identidade, de maneira que em 1ª ordem escrevemos:

$$U(t_0 + dt, t_0) = 1 - i\Omega dt$$

com Ω um operador hermiteano: $\Omega^\dagger = \Omega$

$$\begin{aligned} U^\dagger(t_0 + dt, t_0) U(t_0 + dt, t_0) &= \\ &= (1 + i\Omega dt)(1 - i\Omega dt) = 1 + o(dt^2) \end{aligned}$$

O operador Ω tem dimensão de frequência ou

inverso do tempo. Lembramos que na velha teoria quântica, o postulado de Planck-Einstein para o efeito fotoelétrico assumia a relação

$$E = \hbar\omega \quad \text{ou} \quad \omega = E/\hbar$$

Outra vez, lembramos da mecânica clássica que a função Hamiltoniana (ou Hamiltoniano) é o gerador infinitesimal da evolução temporal. Então é natural postular a relação:

$$\Omega = \frac{1}{\hbar} \mathcal{H}$$

Em MC, a evolução temporal pode ser entendida como uma transformação canônica

$$(p, q) \xrightarrow{TC} (P, Q).$$

Para o caso infinitesimal:

$$\begin{cases} Q_i = q_i + \delta q_i \\ P_i = p_i + \delta p_i \end{cases}$$

Construímos a TC infinitesimal como uma função de tipo

$$F_2 = F_2(q, P)$$

$$F_2 = \sum_i q_i P_i + \epsilon G(p, P),$$

e as equações de transformação são:

$$p_i = \frac{\partial F_2}{\partial q_i} = P_i + \epsilon \frac{\partial G}{\partial q_i}$$

ou

$$\delta p_i = P_i - p_i = -\epsilon \frac{\partial G}{\partial q_i}$$

$$Q_i = \frac{\partial F_2}{\partial P_i} = q_i + \epsilon \frac{\partial G}{\partial P_i} ,$$

ou

$$\delta q_i = Q_i - q_i = \epsilon \frac{\partial G}{\partial P_i} \approx \epsilon \frac{\partial G}{\partial p_i} .$$

Uma aplicação interessante é quando $G = H$, o Hamiltoniano, e $\epsilon = dt$, um deslocamento infinitesimal no tempo. Em virtude das equações de Hamilton da mecânica, temos

$$\delta q_i = dt \frac{\partial H}{\partial p_i} = \dot{q}_i dt = dq_i ,$$

$$\delta p_i = -dt \frac{\partial H}{\partial q_i} = -\dot{p}_i dt = dp_i ,$$

de maneira que a evolução temporal pode ser pensada como uma transformação canônica onde o Hamiltoniano é o gerador infinitesimal. Lembramos que a função geratriz

$$\sum_i q_i P_i$$

representa a identidade. Assim comparamos o caso clássico com o quântico:

$$\boxed{\sum_i q_i p_i + dt \mathcal{H}} \longleftrightarrow \boxed{1 - i\Omega dt}$$

A função geratriz clássica tem dimensão de ação (\hbar ?), de maneira que é "natural" postular

$$\hbar\Omega = \mathcal{H}$$

O operador infinitesimal da evolução temporal se escreve então como:

$$\boxed{U(t_0 + dt, t_0) = 1 - \frac{i}{\hbar} \mathcal{H} dt},$$

com $\mathcal{H}^\dagger = \mathcal{H}$, hermitiano. Por extensão, chamamos este operador de Hamiltoniano.

Equações de Schrödinger

Explicamos agora a relação fundamental de composição do operador de evolução temporal:

$$\begin{aligned} U(t+dt, t_0) &= U(t+dt, t) U(t, t_0) \\ &= \left(1 - \frac{i}{\hbar} \mathcal{H} dt\right) U(t, t_0) \end{aligned}$$

de onde

$$U(t+dt, t_0) - U(t, t_0) = -\frac{i}{\hbar} H dt U(t, t_0),$$

e tomando o limite $dt \rightarrow 0$, a relação acima pode ser escrita em forma diferencial

$$i\hbar \frac{\partial U(t, t_0)}{\partial t} = H U(t, t_0)$$

Esta é chamada de Equações de Schrödinger do operador de evolução temporal. Projetamos esta equação sobre o ket $|\alpha, t_0\rangle$:

$$i\hbar \frac{\partial U(t, t_0) |\alpha, t_0\rangle}{\partial t} = H U(t, t_0) |\alpha, t_0\rangle$$

e obtemos a equação de Schrödinger para o estado $|\alpha, t_0; t\rangle$:

$$i\hbar \frac{\partial |\alpha, t_0; t\rangle}{\partial t} = H |\alpha, t_0; t\rangle$$

Tudo o que precisamos conhecer então é o operador de evolução temporal U , e depois aplicar sobre o ket $|\alpha, t_0\rangle$. Podemos integrar a eq. de Schrödinger formalmente em alguns casos:

i) O Hamiltoniano é um operador independente do tempo. Para $t_0 \rightarrow t$, H não muda. Podemos integrar a equação de movimento:

$$\frac{\partial U(t, t_0)}{\partial t} = -\frac{i}{\hbar} H U(t, t_0)$$

A solução é uma função exponencial:

$$U(t, t_0) = A \exp\left[-\frac{i}{\hbar} H (t - t_0)\right]$$

Unitariedade implica:

$$1 = U^\dagger(t, t_0) U(t, t_0) = A^* A = |A|^2,$$

de maneira que A é uma fase constante. Escolhemos $A \equiv 1$, porque

$$\lim_{t \rightarrow t_0} U(t, t_0) = 1 \quad (\text{condição inicial})$$

Uma maneira alternativa de obter o mesmo resultado é compor sucessivas transformações infinitesimais. Seja

$$\Delta t \equiv \frac{t - t_0}{N}, \quad \text{com } N \text{ suficientemente grande}$$

Tomamos:

$$\left(1 - \frac{i}{\hbar} H \Delta t\right)^N$$

e finalmente o limite :

$$\lim_{N \rightarrow \infty} \left[1 - \frac{i}{\hbar} \mathcal{H} \frac{(t-t_0)}{N} \right]^N = \exp \left[-\frac{i}{\hbar} \mathcal{H} (t-t_0) \right]$$

ii) O Hamiltoniano é um operador dependente do tempo, mas Hamiltonianos para tempos diferentes comutam :

$$[\mathcal{H}(t_1), \mathcal{H}(t_2)] = 0$$

A solução formal neste caso é :

$$U(t, t_0) = \exp \left[\frac{i}{\hbar} \int_{t_0}^t dt' \mathcal{H}(t') \right],$$

que é obtida de maneira análoga ao caso anterior

iii) caso $[\mathcal{H}(t_1), \mathcal{H}(t_2)] \neq 0$

$$U(t, t_0) = 1 + \sum_{n=1}^{\infty} \left(\frac{-i}{\hbar} \right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n \mathcal{H}(t_1) \dots \mathcal{H}(t_n)$$

Série formal de Dyson, será demonstrada mais tarde no estudo de Teoria de Perturbações dependentes do tempo.

§ Autoestados da Energia

Seja A um particular observável com uma base completa $\{|a'\rangle\}$. Assumamos também que o Hamiltoniano é um operador compatível:

$$[A, \mathcal{H}] = 0.$$

Neste caso, os autoestados de A são também autoestados de \mathcal{H} , chamados neste caso de autoestados da energia, com autovalores $E_{a'}$:

$$\mathcal{H}|a'\rangle = E_{a'}|a'\rangle.$$

Expandimos agora o operador \mathcal{U} nesta base. Para simplificar, tomamos $t_0 = 0$:

$$\begin{aligned} \mathcal{U}(t, 0) &= \exp\left(-\frac{i}{\hbar}\mathcal{H}t\right) = \sum_{a'} \sum_{a''} |a''\rangle \langle a''| \exp\left(-\frac{i}{\hbar}\mathcal{H}t\right) |a'\rangle \langle a'| \\ &= \sum_{a'} |a'\rangle \langle a'| \exp\left(-\frac{i}{\hbar}E_{a'}t\right) \end{aligned}$$

(descomposição espectral do operador \mathcal{U}).

Estamos agora em condições de resolver o problema de valores iniciais para o ket $|\alpha, t_0; t\rangle$ em termos da base $\{|a'\rangle\}$.

Escrevemos $|\alpha, t_0=0\rangle = |\alpha\rangle$

$$|\alpha, t_0=0\rangle = \sum_{a'} |a'\rangle \langle a'|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle$$

Aplicamos agora o operador de evolução temporal:

$$\begin{aligned} |\alpha, t_0=0; t\rangle &= \mathcal{U}(t, 0) |\alpha\rangle = \sum_{a'} c_{a'} \mathcal{U}(t, 0) |a'\rangle \\ &= \sum_{a'} c_{a'} \exp\left(-\frac{i}{\hbar} E_{a'} t\right) |a'\rangle = \sum_{a'} c_{a'}(t) |a'\rangle, \end{aligned}$$

de maneira que os coeficientes lineares mudam com o tempo na forma

$$c_{a'}(t) = c_{a'}(0) \exp\left(-\frac{i}{\hbar} E_{a'} t\right)$$

Neste caso sim temos que

$$|c_{a'}(t)| = |c_{a'}(0)|,$$

quando $[A, \mathcal{H}] = 0$

► Caso particular importante: $|\alpha, t_0=0\rangle = |a'\rangle$

A evolução temporal fornece neste caso

$$|\alpha, t_0=0; t\rangle = |a'\rangle \exp\left(-\frac{i}{\hbar} E_{a'} t\right)$$

Significa que se o estado inicial do sistema é um ket $|a\rangle$, autoestado simultâneo de A e H , ele permanece como tal para todo tempo. Neste sentido se fala que um observável compatível com o Hamiltoniano H do sistema, é uma constante do movimento.

O análogo clássico é

$$\begin{aligned} \frac{dA(p,q)}{dt} &= \frac{\partial A}{\partial t} + \sum_i \left(\frac{\partial A}{\partial q_i} \dot{q}_i + \frac{\partial A}{\partial p_i} \dot{p}_i \right) \\ &= \frac{\partial A}{\partial t} + \sum_i \left(\frac{\partial A}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial H}{\partial q_i} \right) \\ &= \frac{\partial A}{\partial t} + [A, H]_{\text{Clássico}} \end{aligned}$$

$A(p,q)$ é uma constante do movimento quando $\frac{\partial A}{\partial t} = 0$, e $\frac{dA}{dt} = 0$. Assim obtemos:

$$[A, H]_{\text{Clássico}} = 0.$$

Voltando para o caso quântico, nossas considerações podem ser generalizadas para vários observáveis que comutam entre si e com o Hamiltoniano:

$$[A, B] = [A, C] = [B, C] = \dots = 0$$

$$[A, H] = [B, H] = [C, H] = \dots = 0$$