第三章 量子力学导论

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§12 波粒二象性

需要掌握的知识点：

（1）了解哪些现象电磁波显示粒子性，哪些现象粒子显示波动性

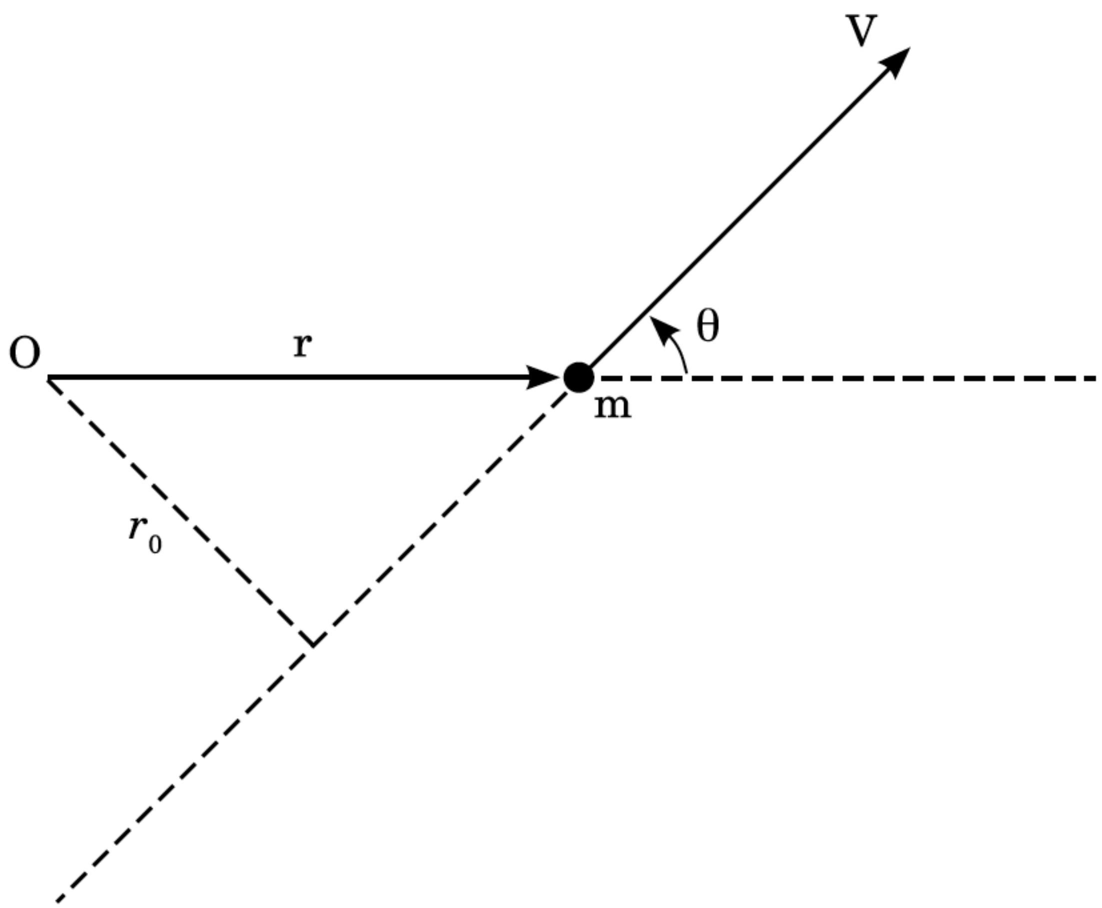
（2）理解德布罗意物质波的假设

（3）解释德布罗意假设如何给出玻尔氢原子量子理论中角动量量子化的基本原理

（4）了解戴维孙−革末实验

（5）使用德布罗意假设解释电子衍射现象

什么是粒子性?



动量：$\vec{p} = m\vec{v}$

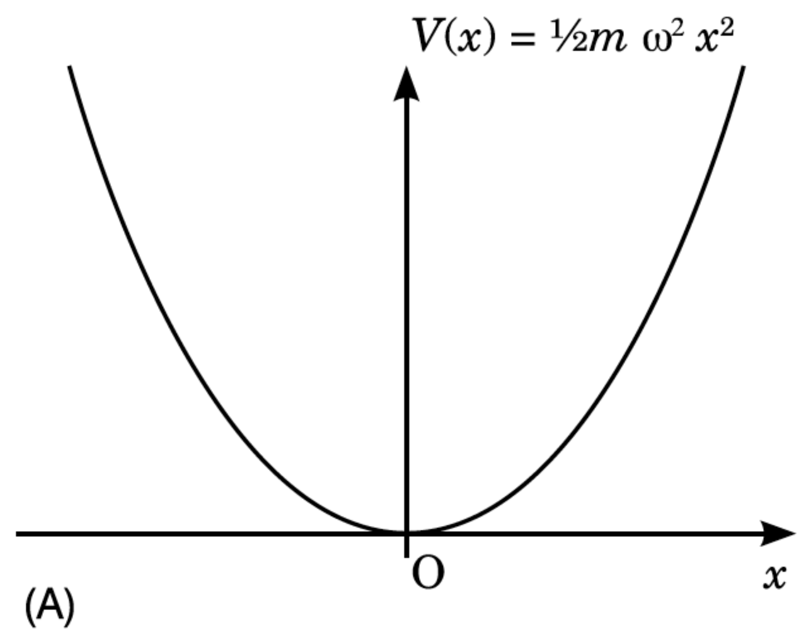
角动量：$\vec{\ell} = \vec{r} \times \vec{p}$

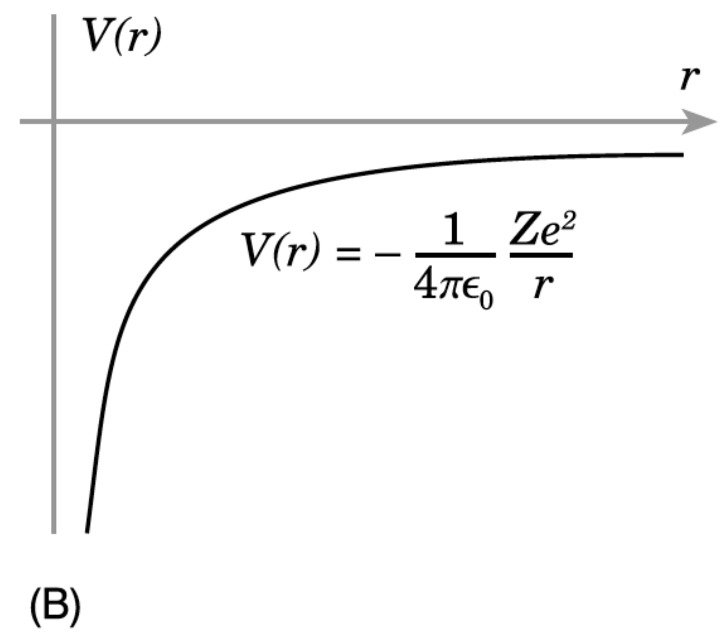
$$|\ell| = |r||p|\sin\theta$$

动能：$T = \frac{1}{2}mv^2$

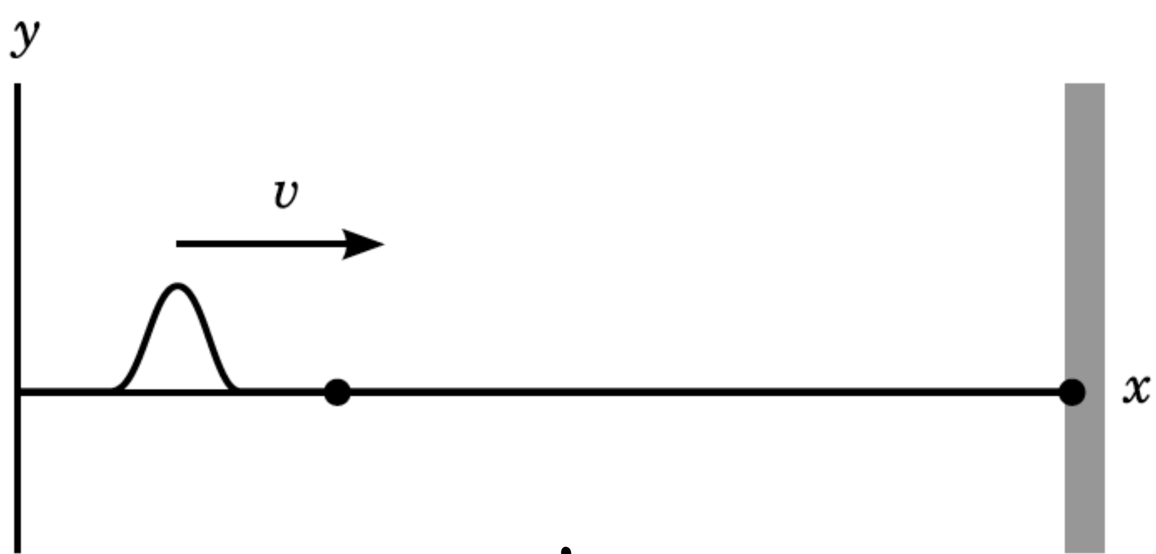
势能：

$$V_P = -\int_R^P F(x)dx$$

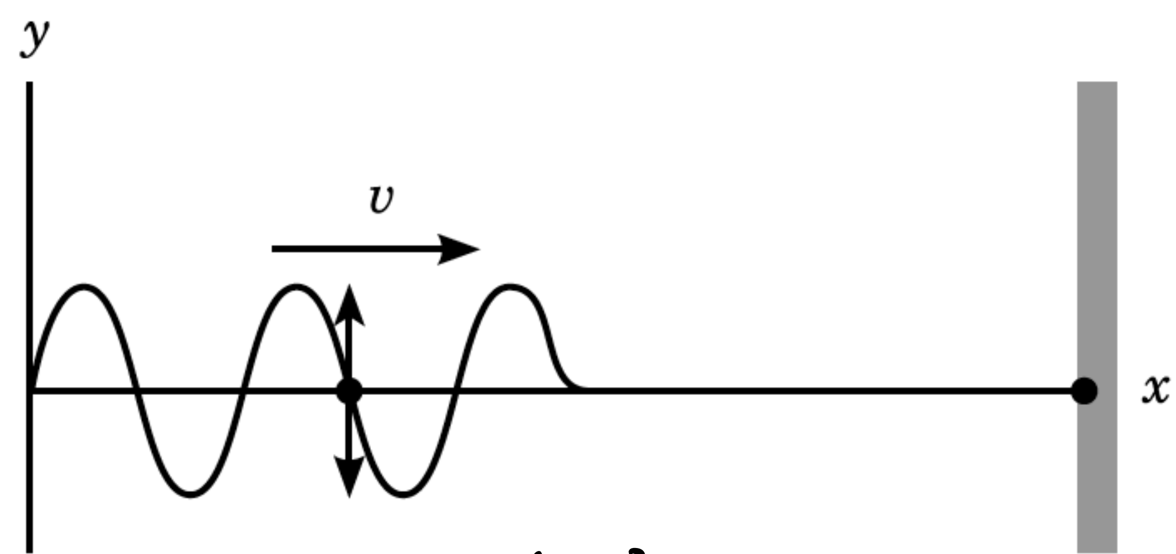




什么是波动性?



脉冲



谐波

谐波: $y = \sin \omega t$　　波长: $\lambda = vT$　　波速: $\lambda \nu = v$

$\nu = 1/T$

谐波是时间和空间的函数: $y(x,t) = A \sin[2\pi(x/\lambda - t/T)]$

波数: $k = \dfrac{2\pi}{\lambda}$　　角频率: $\omega = \dfrac{2\pi}{T} = 2\pi\nu$

$y(x,t) = A \sin[kx - \omega t)]$

驻波：波的叠加/相干

考虑同时在一个弦上传播的两个波

$$y(x,t) = y_1(x,t) + y_2(x,t)$$

其中

$$y_1(x) = A\sin(kx - \omega t)$$

从左向右

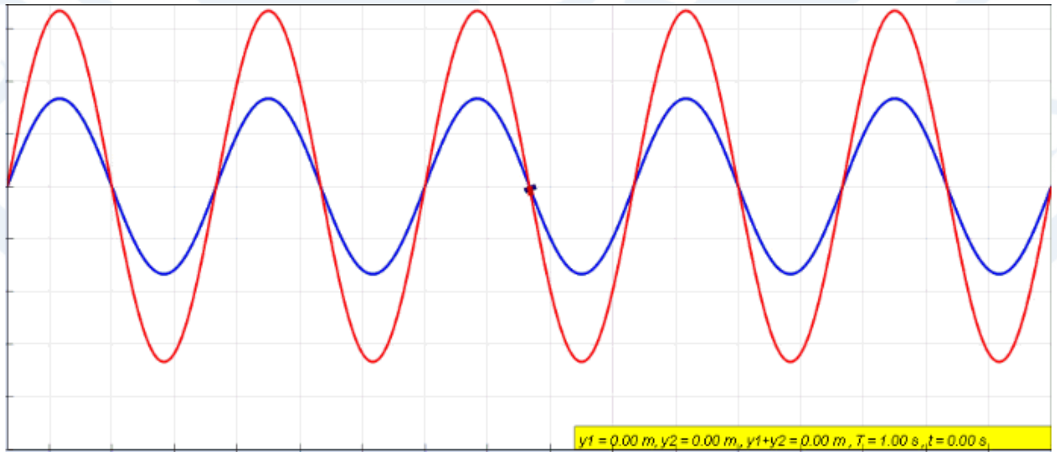
$$y_2(x) = A\sin(kx + \omega t)$$

从右向左

即

$$y(x,t) = y_1(x) + y_2(x) = A[\sin(kx - \omega t) + \sin(kx + \omega t)] = [2A\cos\omega t]\sin kx$$

上式为驻波方程



节点满足

$$x = n\frac{\lambda}{2}$$

光的波粒二象性

17世纪

牛顿：光的微粒说　　　反射，直线传播

惠更斯：光的波动说　　　折射，衍射

19世纪

菲涅尔
夫琅禾费　} 光的干涉衍射
杨氏

麦克斯韦&赫兹：光——电磁波

} 确立了光的波动说

光的波粒二象性

20世纪

光电效应
康普顿散射
} 光量子 $\begin{cases} E = h\nu = pc \\ p = \dfrac{h}{\lambda} \quad \text{或} \quad p = \hbar k \end{cases}$

波矢: $k = \dfrac{2\pi}{\lambda}$

光的波粒二象性 $\begin{cases} \text{光在传播时显示波动性} \\ \text{在能量转移时显示粒子性} \end{cases}$

德布罗意假设（1923年提出，1929年获诺奖）

从辩证思维出发,法国青年物理学家德布罗意 (de Broglie)提出,既然光具有粒子性,是否实物粒子如电子也应当具有波动性?

L.V. de Broglie
(法1892-1987)

1924.11.29 德布罗意把题为“量子理论的研究”的博士论文提交巴黎大学。

德布罗意假设（1923年提出，1929年获诺奖）

identical with the disposition of atoms suggested by Sir William Bragg for the molecule of benzene" (Challenor and Ingold, Trans. Chem. Soc., 1923, 2068), it will scarcely be maintained that Dr. Turner's suggestion of a possible stable para-linkage in diphenyl derivatives introduces any essentially novel consideration to the question of the structure of these compounds. I also referred in my letter to the remarkable behaviour of diphenyl towards ozone, mentioned by Dr. Turner, as well as to certain other noteworthy properties of the compound.

It should perhaps be pointed out that although, as Dr. Turner states, the formula considered by him contains four asymmetric carbon atoms, it would be incorrect to suppose that it therefore demands the existence of a correspondingly large number of stereoisomeric forms of 2 : 2′-derivatives of diphenyl. For the respective distributions of the groups attached to the pair of asymmetric carbon atoms in either benzene nucleus are not mutually independent, so that only one asymmetric atom in each nucleus is effective as a source of stereoisomerism.

In conclusion, I need scarcely say that experiments on the isomerism in question are being actively prosecuted in this laboratory, and are by no means limited to 2 : 2′-derivatives of diphenyl.

J. KENNER.

The Chemical Department, The University,
Sheffield, September 25.

Waves and Quanta.

THE quantum relation, energy $= h \times$ frequency, leads one to associate a periodical phenomenon with any isolated portion of matter or energy. An observer bound to the portion of matter will associate with it a frequency determined by its internal energy, namely, by its "mass at rest." An observer for whom a portion of matter is in steady motion with velocity βc, will see this frequency lower in consequence of the Lorentz-Einstein time transformation. I have been able to show (*Comptes rendus*, September 10 and 24, of the Paris Academy of Sciences) that the fixed observer will constantly see the internal periodical phenomenon in phase with a wave the frequency of which $\nu = \frac{m_0 c^2}{h\sqrt{1-\beta^2}}$ is determined by the quantum relation using the whole energy of the moving body—provided it is assumed that the wave spreads with the velocity c/β. This wave, the velocity of which is greater than c, cannot carry energy.

A radiation of frequency ν has to be considered as divided into atoms of light of very small internal mass ($< 10^{-50}$ gm.) which move with a velocity very nearly equal to c given by $\frac{m_0 c^2}{\sqrt{1-\beta^2}} = h\nu$. The atom of light slides slowly upon the non-material wave the frequency of which is ν and velocity c/β, very little higher than c.

The "phase wave" has a very great importance in determining the motion of any moving body, and I have been able to show that the stability conditions of the trajectories in Bohr's atom express that the wave is tuned with the length of the closed path.

The path of a luminous atom is no longer straight when this atom crosses a narrow opening; that is, diffraction. It is then *necessary* to give up the inertia principle, and we must suppose that any moving body follows always the ray of its "phase wave"; its path will then bend by passing through a sufficiently small aperture. Dynamics must undergo the same evolution that optics has undergone when undulations took the place of purely geometrical optics. Hypotheses based upon those of the wave theory allowed us to explain interferences and diffraction fringes. By means of these new ideas, it will probably be possible to reconcile also diffusion and dispersion with the discontinuity of light, and to solve almost all the problems brought up by quanta.

LOUIS DE BROGLIE.

Paris, September 12.

The "Concilium Bibliographicum."

IN the commentary added to my letter concerning the "Concilium Bibliographicum" which appeared in NATURE of June 30, p. 880, some doubts were expressed regarding the continuous appearance of its cards. May I be permitted to emphasise again that our cards are issued and delivered as heretofore to our subscribers.

Another publication of the Concilium is the "Bibliographia Zoologica," of which volumes 30 and 31 have been published and vol. 32 will be sent out shortly, indicating definitely that this zoological bibliography is not a new undertaking of the Concilium.

No doubt it is a rather complicated question to decide whether or not this zoological bibliography in book form is a duplication of the "Zoological Record." It must be recalled that apart from completeness, promptness, and accessibility, carefulness and the procedure in the arrangement of the bibliographical work play a very important rôle. Indeed, as for every application of scientific procedure, it is not only the tools but also the degree of ability to use them which governs the appreciation of those who have to work with them. One works better with one method, another is more adapted to the use of another. To all these points have to be added as important factors the influence of different education and local tradition.

In making a plea for a co-operation between the "Zoological Record" and the bibliographical service of the Concilium, a condition which unquestionably could be of real value to the zoological world, the writer wishes to suggest that these various important points of internal character be seriously considered.

When it was decided in 1921 to continue the book-form of the "Bibliographia Zoologica," the material to be published was so extensive that it was impossible to treat the whole animal kingdom in every volume. But this is certainly not a misfortune, for it is evident that a bibliography of titles has not only an immediate value, but also represents to a great extent a source for continuous reference.

J. STROHL,
Director of the "Concilium Bibliographicum."

Zurich.

Long-range Particles from Radium-active Deposit.

IN the letter which appeared in NATURE of September 15, p. 394, under this heading, by Dr. Kirsch and myself, there are two errors which obscure the sense of our communication. The maximum range of the H-particles expelled from silicon should read 12 cm., the corresponding number for beryllium being 18 cm., instead of vice versa. The last sentence should read: "Our results seem to indicate that an *expellable* H-nucleus is a more common constituent of the lighter atoms than one has hitherto been inclined to believe," the word in italics being omitted in the printing.

HANS PETTERSSON.

Göteborgs Högskola, Sweden.

[The transposition of the values 12 cm. and 18 cm. was the fault of our printers; and we much regret it. The omission of the word "expellable" was due to the authors, who did not include the word in their letter. Two separate proofs of the letter were sent to Dr. Kirsch at Vienna, but neither was returned.—EDITOR, NATURE.]

Sheffield, September 25.

Waves and Quanta.

THE quantum relation, energy $= h \times$ frequency, leads one to associate a periodical phenomenon with any isolated portion of matter or energy. An observer bound to the portion of matter will associate with it a frequency determined by its internal energy, namely, by its "mass at rest." An observer for whom a portion of matter is in steady motion with velocity βc, will see this frequency lower in consequence of the Lorentz-Einstein time transformation.

all the problems brought up by quanta.

LOUIS DE BROGLIE.

Paris, September 12.

The "Concilium Bibliographicum."

德布罗意假设（1923年提出，1929年获诺奖）

德布罗意nature文章

德布罗意假设（1923年提出，1929年获诺奖）

On the Theory of Quanta

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德布罗意假设（1923年提出，1929年获诺奖）

德布罗意博士论文

德布罗意假设（1923年提出，1929年获诺奖）

任何具有能量和动量的粒子都是频率为ν和波长为λ的德布罗意波

相对论能量

$$E = h\nu$$

$$\lambda = \frac{h}{p}$$

动量

或

$$E = \hbar\omega$$

$$\vec{p} = \hbar\vec{k}$$

$$\omega = 2\pi\nu$$

德布罗意物质波的群速率为粒子的速率u，满足

$$\lambda\nu = \frac{\omega}{k} = \frac{E/\hbar}{p/\hbar} = \frac{E}{p} = \frac{mc^2}{mu} = \frac{c^2}{u} = \frac{c}{\beta}$$

$$\beta = u/c$$

习题

计算一下物体的德布罗意物质波波长

（a）以10 m/s飞行的质量为0.65 kg的篮球；

（b）动能为1.0 eV的电子；

（c）动能为108 keV的电子

习题

(a) 篮球的动能为

$$K = m_0u^2/2 = (0.65\ \text{kg})(10\ \text{m/s})^2/2 = 32.5\ \text{J}$$

篮球静止时的质能

$$E_0 = m_0c^2 = (0.65\ \text{kg})\left(2.998\times10^8\ \text{m/s}\right)^2 = 5.84\times10^{16}\ \text{J}$$

可以发现$K/\left(K+E_0\right) \ll 1$，因此

$$p = m_0u = (0.65\ \text{kg})(10\ \text{m/s}) = 6.5\ \text{Js/m}$$

篮球的德布罗意波长为

$$\lambda = \frac{h}{p} = \frac{6.62610^{-34}\ \text{Js}}{6.5\ \text{Js/m}} = 1.0210^{-34}\ \text{m}$$

习题

TIPS:

相对论情况下的质能守恒$E^2 = p^2c^2 + E_0^2$

可以得出$p = \sqrt{\left(E^2 - E_0^2\right)/c^2} = \sqrt{K\left(K + 2E_0\right)}/c$

(b)电子静止时的质能

$$E_0 = m_0c^2 = \left(9.10910^{-31}\ \mathrm{kg}\right)\left(2.99810^8\ \mathrm{m/s}\right)^2 = 511\ \mathrm{keV}$$

尽管当$K = 1.0\ eV$, $K/\left(K + E_0\right) \ll 1$，方便起见我们仍然采用

$$\lambda = \frac{h}{p} = \frac{hc}{\sqrt{K\left(K + 2E_0\right)}} = \frac{1.241\mathrm{eV}\mu\mathrm{m}}{\sqrt{(1.0\mathrm{eV})[1.0\mathrm{eV} + 2(511\mathrm{keV})]}} = 1.23\ \mathrm{nm}$$

习题

(b)当$K = 108\ keV$时，$K/(K+E_0) = 108/619$，相对论效应不能忽略

$$\lambda = \frac{h}{p} = \frac{hc}{\sqrt{K(K+2E_0)}} = \frac{1.241\text{eVm}}{\sqrt{108\text{keV}[108\text{keV} + 2(511\text{keV})]}} = 3.55\text{pm}$$

戴维孙—革末实验

The Scattering of low Speed Electrons by Platinum and Magnesium

C. Davisson and C. H. Kunsman
Phys. Rev. **22**, 242 – Published 1 September 1923

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戴维孙–革末实验

1926年：　了解德布罗意物质波假设；

1927年：　观察到电子衍射现象。

戴维孙—革末实验

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Published: 01 April 1927

The Scattering of Electrons by a Single Crystal of Nickel

C. Davisson & L. H. Germer

Nature **119**, 558–560 (1927) | Cite this article

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Diffraction of Electrons by a Crystal of Nickel

C. Davisson and L. H. Germer
Phys. Rev. **30**, 705 – Published 1 December 1927

Physics

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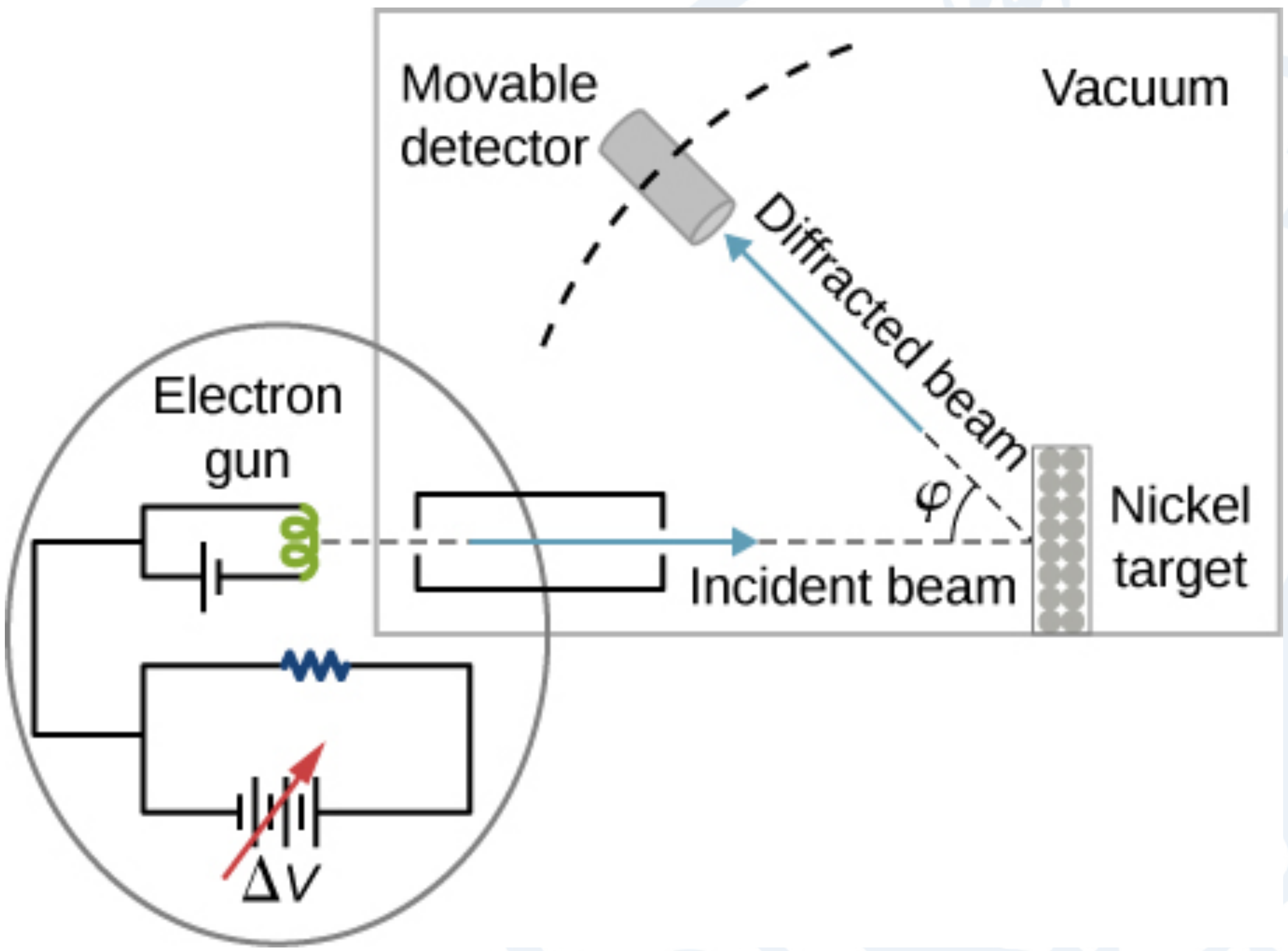
戴维孙—革末实验

历史上第一次证明电子具有波动性的实验



当镍靶具有具有许多随机取向的微观晶体结构时，散射电子束的强度在任何方向上都大致相同。

当镍靶具有规则的晶体结构时，散射电子束的强度在特定角度显示出明显的最大值，结果显示出清晰的衍射图案

$$e\Delta V = K = \frac{p^2}{2m} \Rightarrow p = \sqrt{2me\Delta V}$$

$\Delta V = 54\ eV,\ \ \varphi = 50^{\circ}$时最大

戴维孙–革末实验

Letters to the Editor.

[*The Editor does not hold himself responsible for opinions expressed by his correspondents. Neither can he undertake to return, nor to correspond with the writers of, rejected manuscripts intended for this or any other part of* Nature. *No notice is taken of anonymous communications.*]

The Scattering of Electrons by a Single Crystal of Nickel.

In a series of experiments now in progress, we are directing a narrow beam of electrons normally against a target cut from a single crystal of nickel, and are measuring the intensity of scattering (number of electrons per unit solid angle with speeds near that of the bombarding electrons) in various directions in front of the target. The experimental arrangement is such that the intensity of scattering can be measured

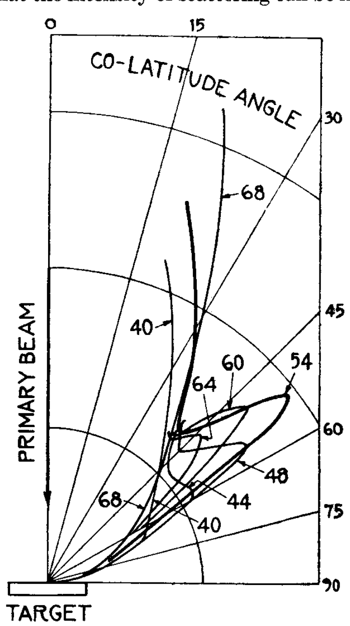


Fig. 1.—Intensity of electron scattering vs. co-latitude angle for various bombarding voltages—azimuth-{111}-330°.

in any latitude from the equator (plane of the target) to within 20° of the pole (incident beam) and in any azimuth.

The face of the target is cut parallel to a set of {111}-planes of the crystal lattice, and etching by vaporisation has been employed to develop its surface into {111}-facets. The bombardment covers an area of about 2 mm.[2] and is normal to these facets.

As viewed along the incident beam the arrangement of atoms in the crystal exhibits a threefold symmetry. Three {100}-normals equally spaced in azimuth emerge from the crystal in latitude 35°, and, midway in azimuth between these, three {111}-normals emerge in latitude 20°. It will be convenient to refer to the azimuth of any one of the {100}-normals as a {100}-azimuth, and to that of any one of the {111}-normals as a {111}-azimuth. A third set of azimuths must also be specified; this bisects the dihedral angle between adjacent {100}- and {111}-azimuths and includes a {110}-normal lying in the plane of the target. There are six such azimuths, and any one of these will be referred to as a {110}-azimuth. It follows from considerations of symmetry that if the intensity of scattering exhibits a dependence upon azimuth as we pass from a {100}-azimuth to the next adjacent {111}-azimuth (60°), the same dependence must be exhibited in the reverse order as we continue on through 60° to the next following {100}-azimuth. Dependence on azimuth must be an even function of period $2\pi/3$.

In general, if bombarding potential and azimuth are fixed and exploration is made in latitude, nothing very striking is observed. The intensity of scattering increases continuously and regularly from zero in the plane of the target to a highest value in co-latitude 20°, the limit of observations. If bombarding potential and co-latitude are fixed and exploration is made in azimuth, a variation in the intensity of scattering of the type to be expected is always observed, but in general this variation is slight, amounting in some cases to not more than a few per cent. of the average intensity. This is the nature of the scattering for bombarding potentials in the range from 15 volts to near 40 volts.

At 40 volts a slight hump appears near 60° in the co-latitude curve for azimuth-{111}. This hump develops rapidly with increasing voltage into a strong spur, at the same time moving slowly upward toward the incident beam. It attains a maximum intensity in co-latitude 50° for a bombarding potential of 54 volts, then decreases in intensity, and disappears in co-latitude 45° at about 66 volts. The growth and decay of this spur are traced in Fig. 1.

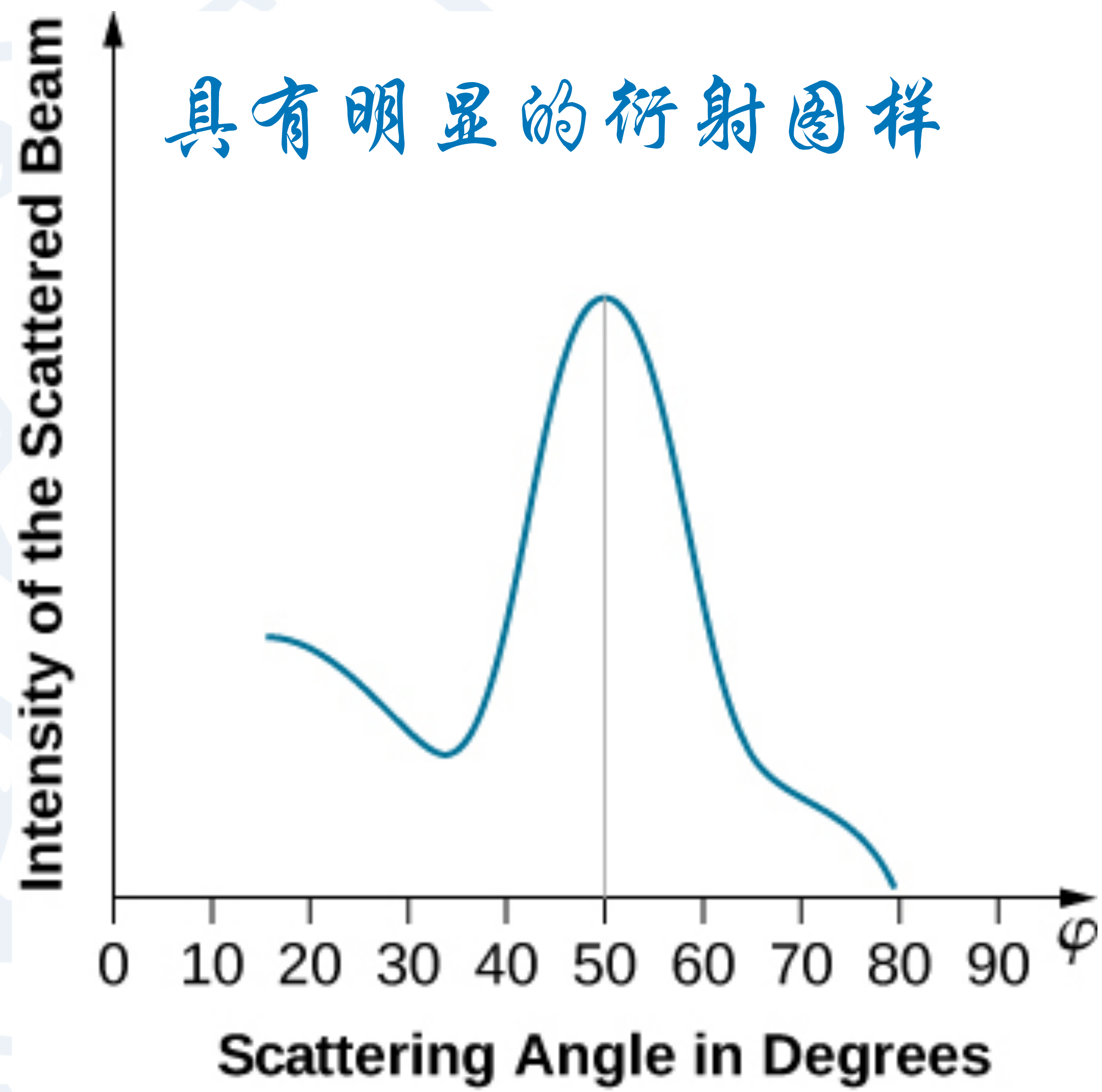
A section in azimuth through this spur at its maximum (Fig. 2—Azimuth-330°) shows that it is sharp in azimuth as well as in latitude, and that it forms one of a set of three such spurs, as was to be expected. The width of these spurs both in latitude and in azimuth is almost completely accounted for by the low resolving power of the measuring device. *The spurs are due to beams of scattered electrons which are nearly if not quite as well defined as the primary beam.* The minor peaks occurring in the {100}-azimuth are sections of a similar set of spurs that attains its maximum development in co-latitude 44° for a bombarding potential of 65 volts.

Thirteen sets of beams similar to the one just described have been discovered in an exploration in the principal azimuths covering a voltage range from 15 volts to 200 volts. The data for these are set down on the left in Table I. (columns 1-4). Small corrections have been applied to the observed co-latitude angles to allow for the variation with angle of the 'background scattering,' and for a small angular displacement of the normal to the facets from the incident beam.

If the incident electron beam were replaced by a beam of monochromatic X-rays of adjustable wave-length, very similar phenomena would, of course, be observed. At particular values of wave-length, sets of three or of six diffraction beams would emerge from the incident side of the target. On the right in Table I. (columns 5, 6 and 7) are set down data for the ten sets of X-ray beams of longest wave-length which would occur within the angular range of our observations. Each of these first ten occurs in one of our three principal azimuths.

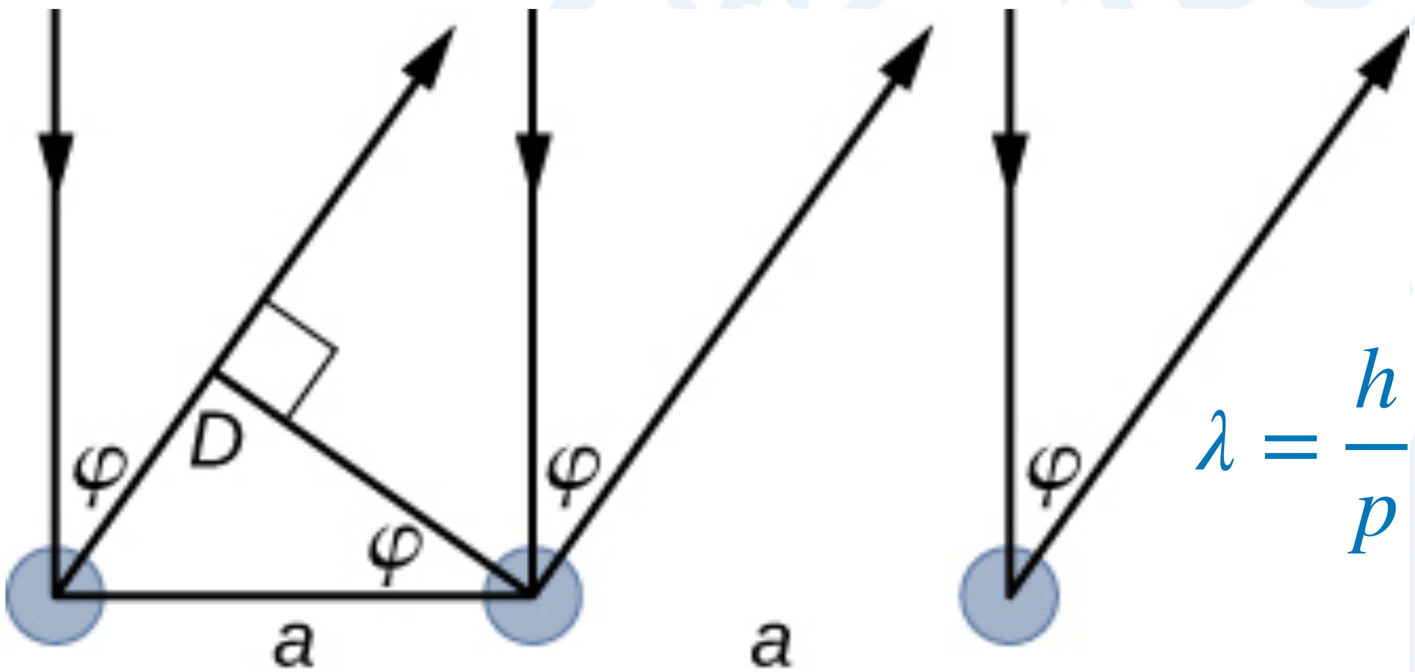
Several points of correlation will be noted between the two sets of data. Two points of difference will also be noted; the co-latitude angles of the electron beams are not those of the X-ray beams, and the three electron beams listed at the end of the Table appear to have no X-ray analogues.

The first of these differences is systematic and may



戴维孙—革末实验

特别注意是电子散射与X射线散射不同，X射线可以穿透物体表面，但是（低能）电子只能与物体表面发生作用



$$D = a\sin\varphi$$
$$D = n\lambda \quad n = 1, 2, 3, \ldots$$
$$n\lambda = a\sin\varphi$$

$$p = \sqrt{2me\Delta V} = 2.478\times 10^{-5}\ eVs/m$$

$$\lambda = \frac{h}{p} = \frac{4.136\times 10^{-15}\mathrm{eV\cdot s}}{2.478\times 10^{-5}\mathrm{eV\cdot s/m}} = 1.67\mathrm{\AA}$$

$$a = 2.15\mathrm{\AA}$$

$$\sin\varphi = 0.776n$$

$$\varphi \approx 50^\circ$$

汤姆逊衍射实验

同年，英国的汤姆逊用多晶体做电子衍射实验,也得到了电子衍射照片。

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Published: 18 June 1927

Diffraction of Cathode Rays by a Thin Film

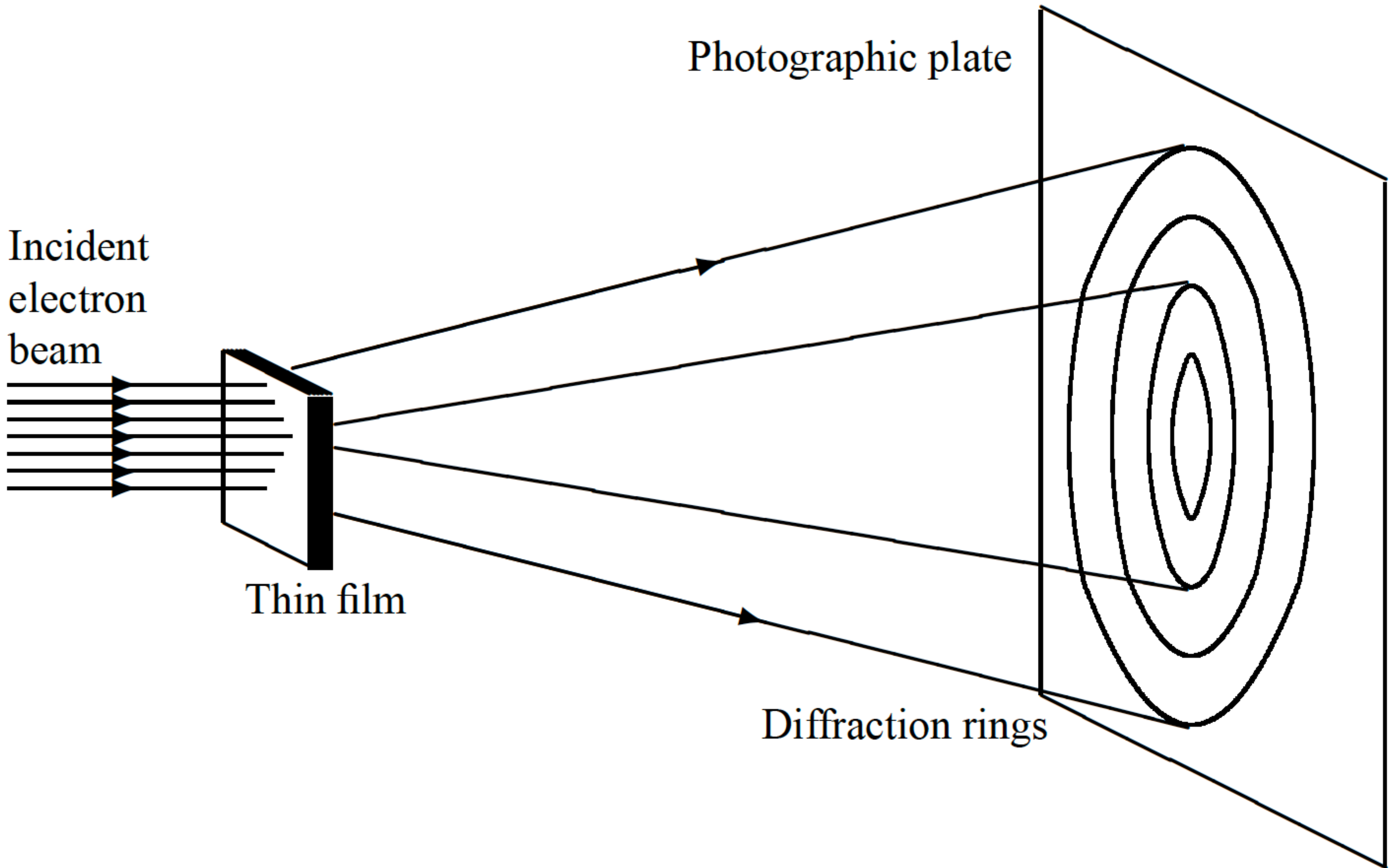
G. P. THOMSON & A. REID

Nature **119**, 890 (1927) | Cite this article

5761 Accesses | **163** Citations | **47** Altmetric | Metrics

汤姆逊衍射实验

同年，英国的汤姆逊用多晶体做电子衍射实验,也得到了电子衍射照片。



十年后，戴维逊、汤姆逊因电子衍射实验的成果共获1937年度诺贝尔物理奖。

德布罗意波长$\lambda = 1\mathring{A}$时各粒子动能

光子	电子	中子	氦原子
12.4 keV	150 eV	81 meV	20 meV

单原子气体（monatomic gas）在室温下的动能为
https://en.wikipedia.org/wiki/Monatomic_gas

$$K_T = \frac{3}{2}k_B T = \frac{3}{2}\left(8.6210^{-5}\text{eV/K}\right)(300\ \text{K}) = 38.8\ \text{meV}$$

德布罗意波和量子态

定态 ⟷ 驻波

(a) (b)

$$l = n\lambda/2$$

电子绕一周之后相位不变

圆周长是波长的整数倍

$$2\pi r_n = n\lambda = n\frac{h}{p} \rightarrow L_n = pr_n = n\frac{h}{2\pi} = n\hbar$$

玻尔量子化条件

波粒二象性（电子散射实验）

1961年，Claus Jönsson在德国进行了第一个电子束双缝实验，证明电子束确实形成了干涉图案，这意味着电子集体表现为波。

Springer Link

Home › Zeitschrift für Physik › Article

Published: August 1961

Elektroneninterferenzen an mehreren künstlich hergestellten Feinspalten

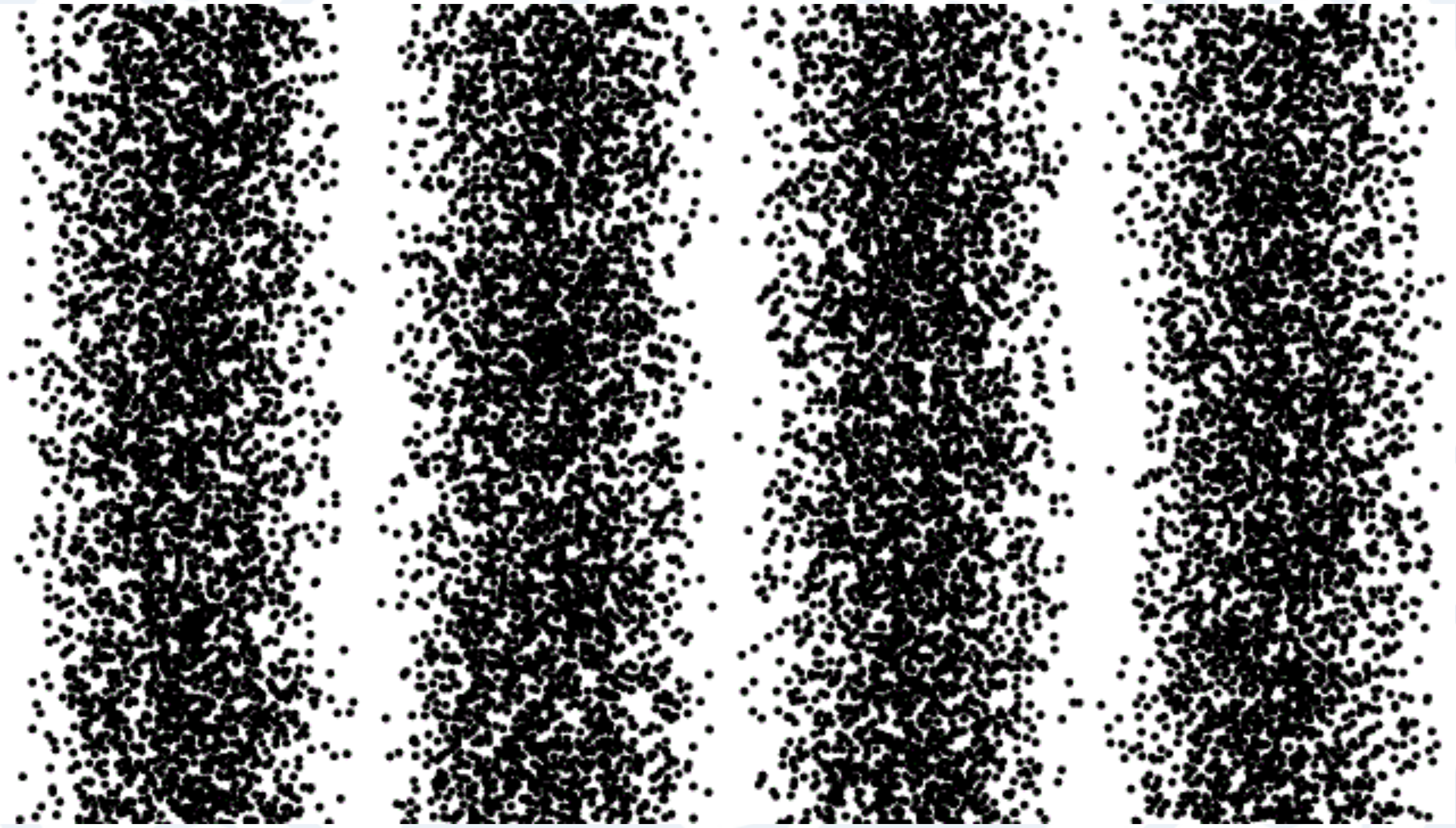
Claus Jönsson

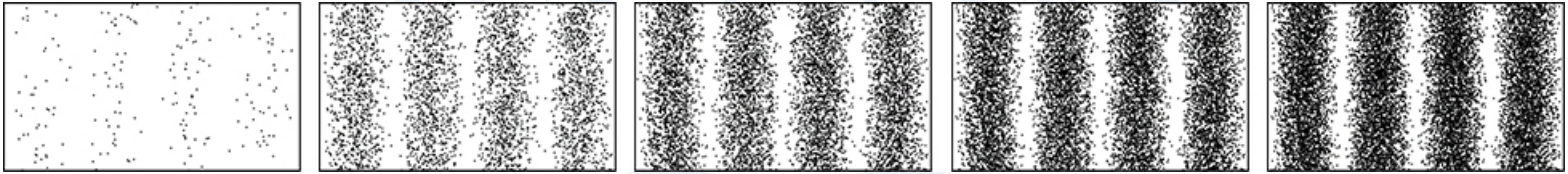
Zeitschrift für Physik **161**, 454–474 (1961) | Cite this article

Circuit is open

波粒二象性（电子散射实验）

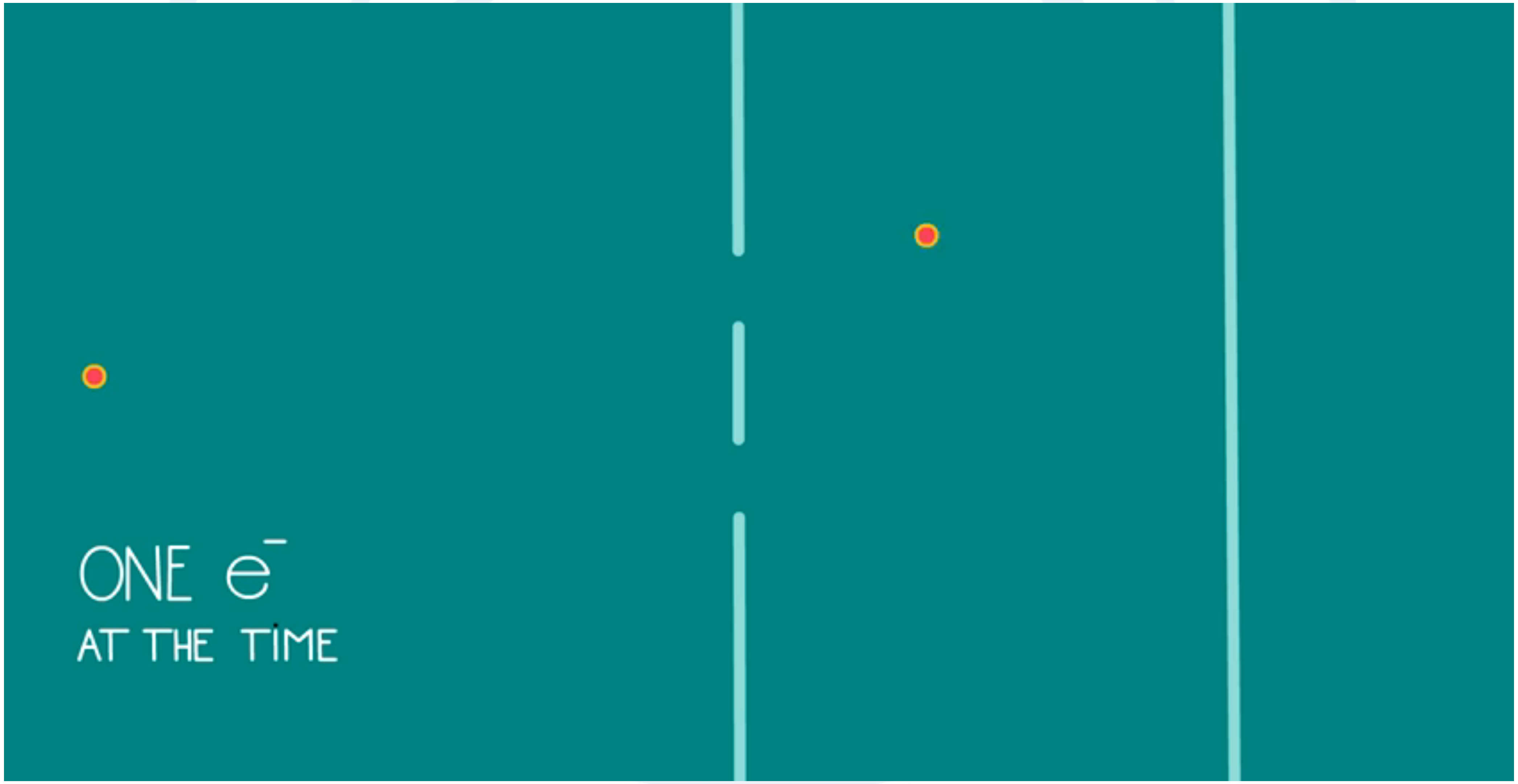
1961年，Claus Jönsson在德国进行了第一个电子束双缝实验，证明电子束确实形成了干涉图案，这意味着电子集体表现为波。



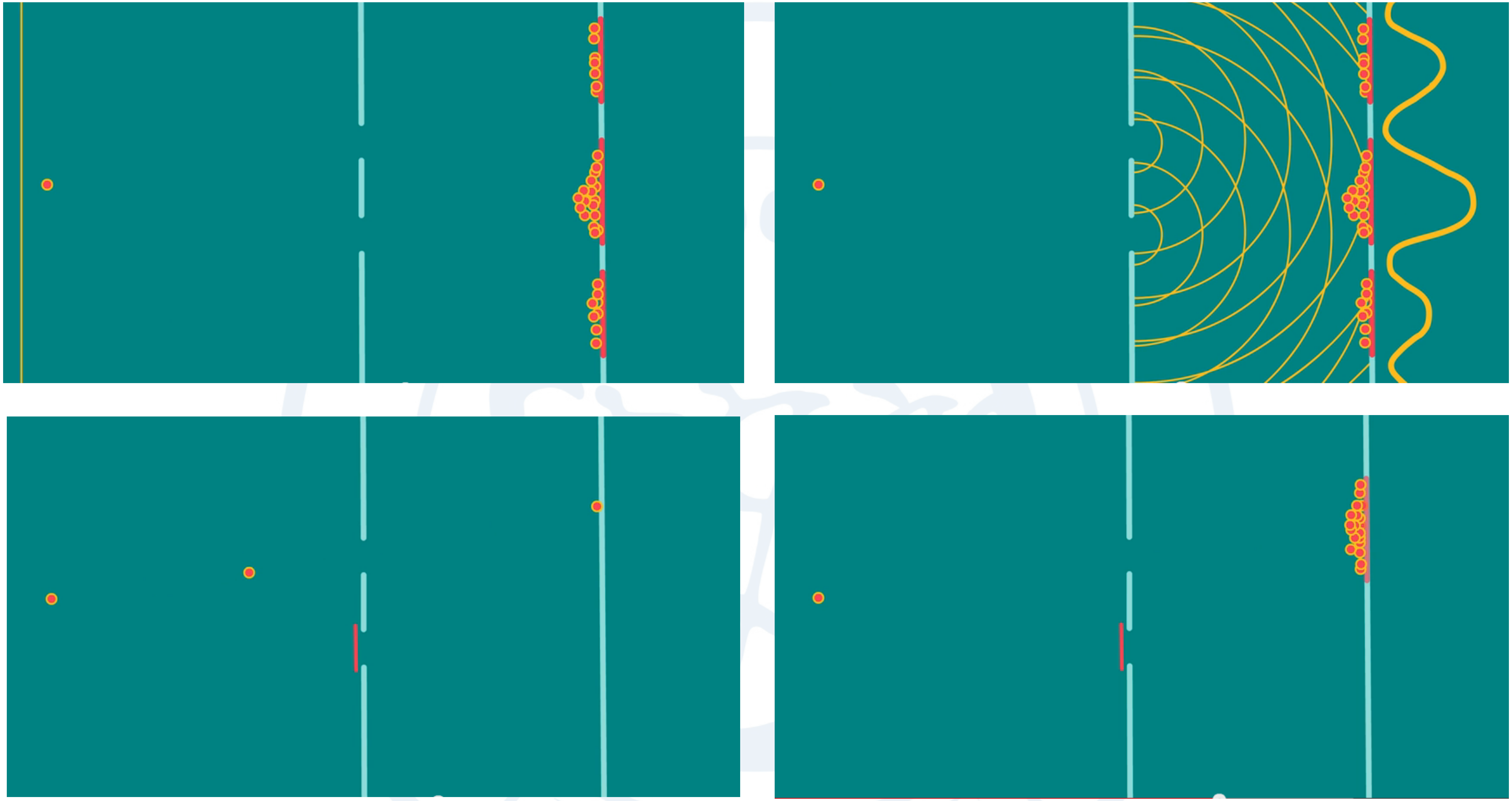


波粒二象性（电子散射实验）

1974 年意大利的Giulio Pozzi和1989年日本的Akira Tonomura进行了第一个单电子通过狭缝的双缝实验。他们表明，即使电子单独通过狭缝，干涉条纹也会逐渐形成。这最终证明了电子衍射图像是由于电子的波动性而形成的。



波粒二象性（电子散射实验）



电子不是每次只是随机通过其中的一条缝，而是“同时”通过了两条缝，并和“自己”发生了干涉。

波粒二象性（电子散射实验）

FEEDBACK

The double-slit experiment with single electrons

John Steeds[1], Pier Giorgio Merli[1], Giulio Pozzi[1], GianFranco Missiroli[1] and Akira Tonomura[1]

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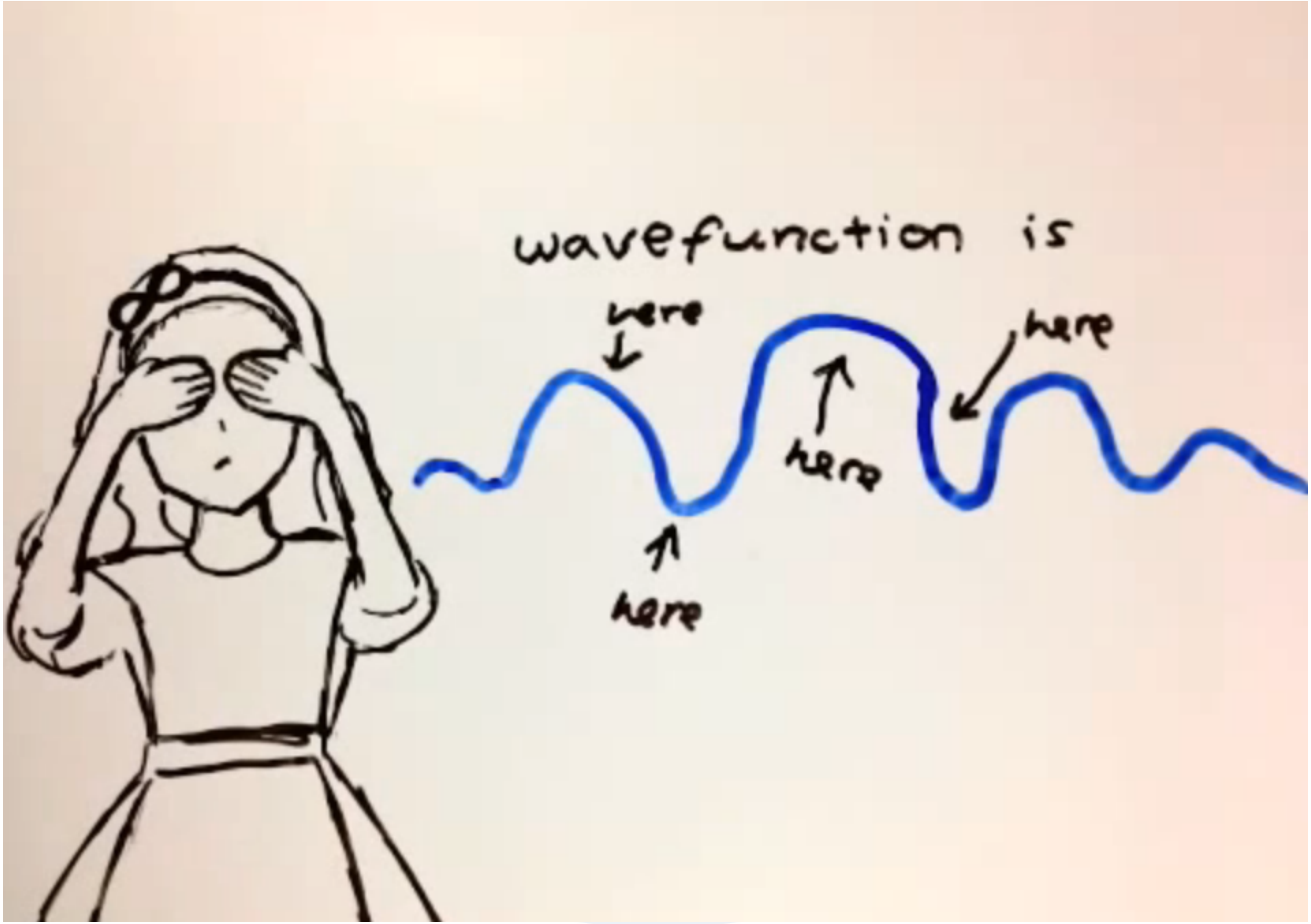
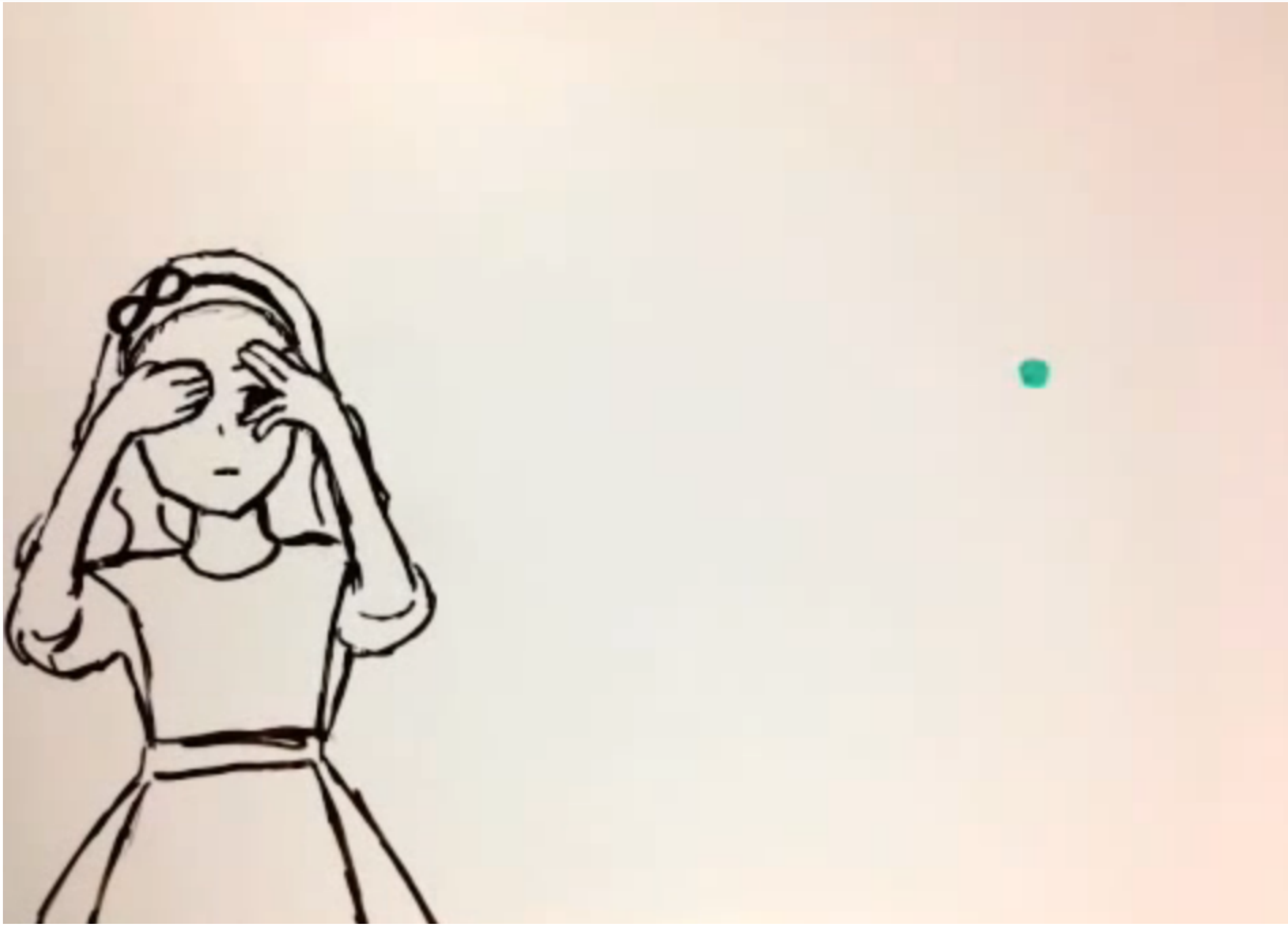
Article PDF

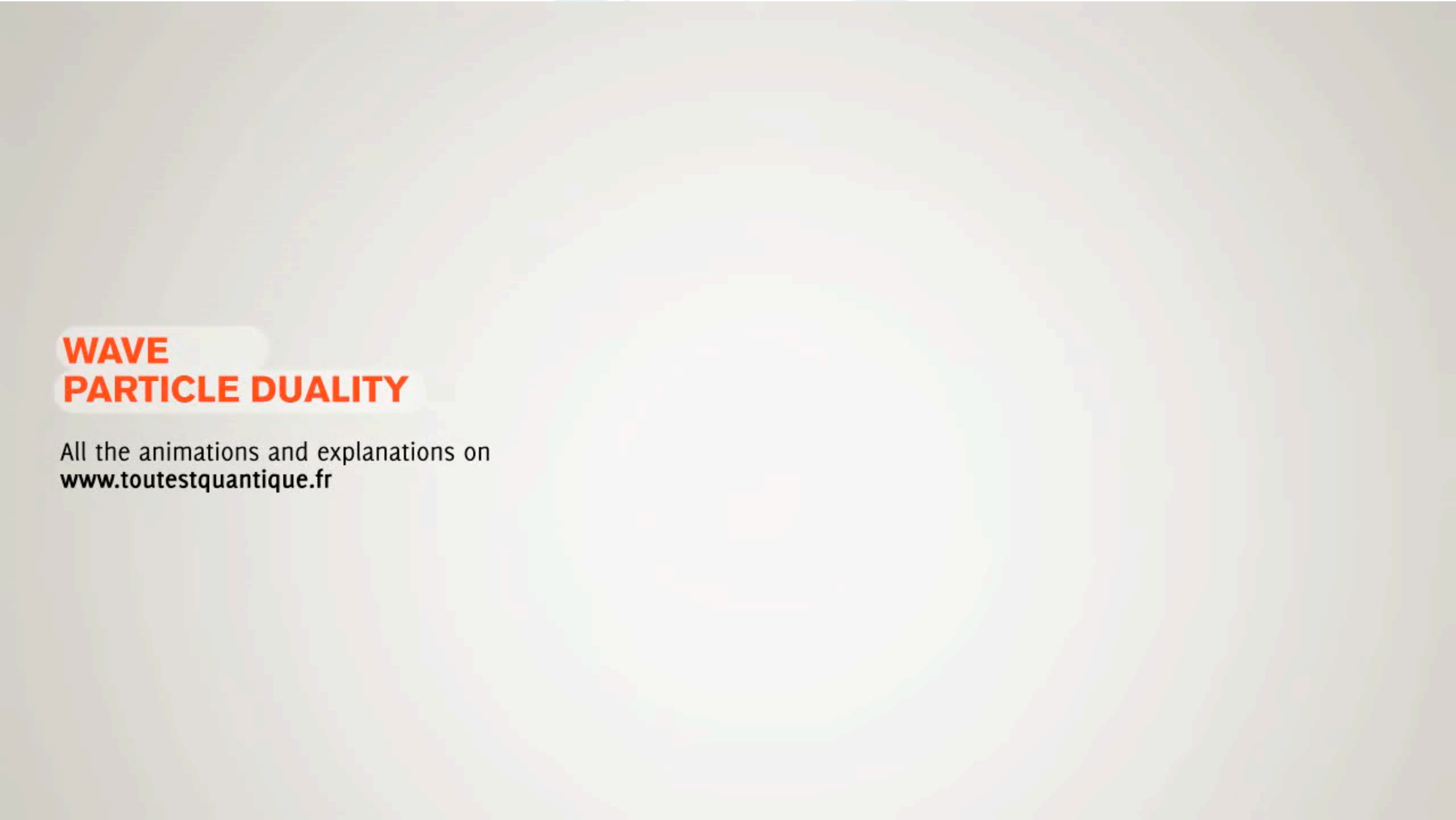
波粒二象性



波粒二象性



波粒二象性


WAVE
PARTICLE DUALITY
All the animations and explanations on
www.toutestquantique.fr

电子显微镜

第一台电子显微镜是由德国鲁斯卡（E·Ruska）研制成功，荣获1986年诺贝尔物理奖。

从波动光学可知，由于显微镜的分辨本领与波长成反比，光学显微镜的最大分辨距离大于0.2 μm，最大放大倍数也只有1000倍左右。

自从发现电子有波动性后，电子束德布罗意波长比光波波长短得多。而且极方便改变电子波的波长。这样就能制造出用电子波代替光波的电子显微镜。


Light Microscopy

小结

(1)德布罗意的物质波假设任何具有动量的粒子也是波。波长与粒子的动量大小成反比。物质波的速度就是粒子的速度。

(2)德布罗意物质波概念为玻尔氢原子模型中电子角动量的量化提供了基本原理。

(3)在戴维孙-革末实验中，电子从结晶镍表面散射。观察到电子物质波的衍射图案。它们是物质波存在的证据。在各种粒子的衍射实验中观察到物质波。

§13 不确定关系

需要掌握的知识点：

（1）描述位置–动量不确定关系的物理意义

（2）解释量子理论中不确定性原理的起源

（3）描述能量–时间不确定性关系的物理意义

唯像的测不准关系(Observer effect)

胎压测量时会导致轮胎内部气体的溢出，无法准确的测量轮胎的胎压

唯像的测不准关系(Observer effect)

对位置的测量总是会对运动物体的速度产生干扰，根据动量守恒，粒子受光量子撞击后，它的动量会产生一种测不准性，其大小同光子的动量差不多

运动物体动量的不确定性

$$\Delta p \sim \frac{h}{\lambda}$$

光子的波长

粒子位置的测不准性取决于光量子的波长 $\Delta x \sim \lambda$

$$\Delta p \Delta x \sim h$$

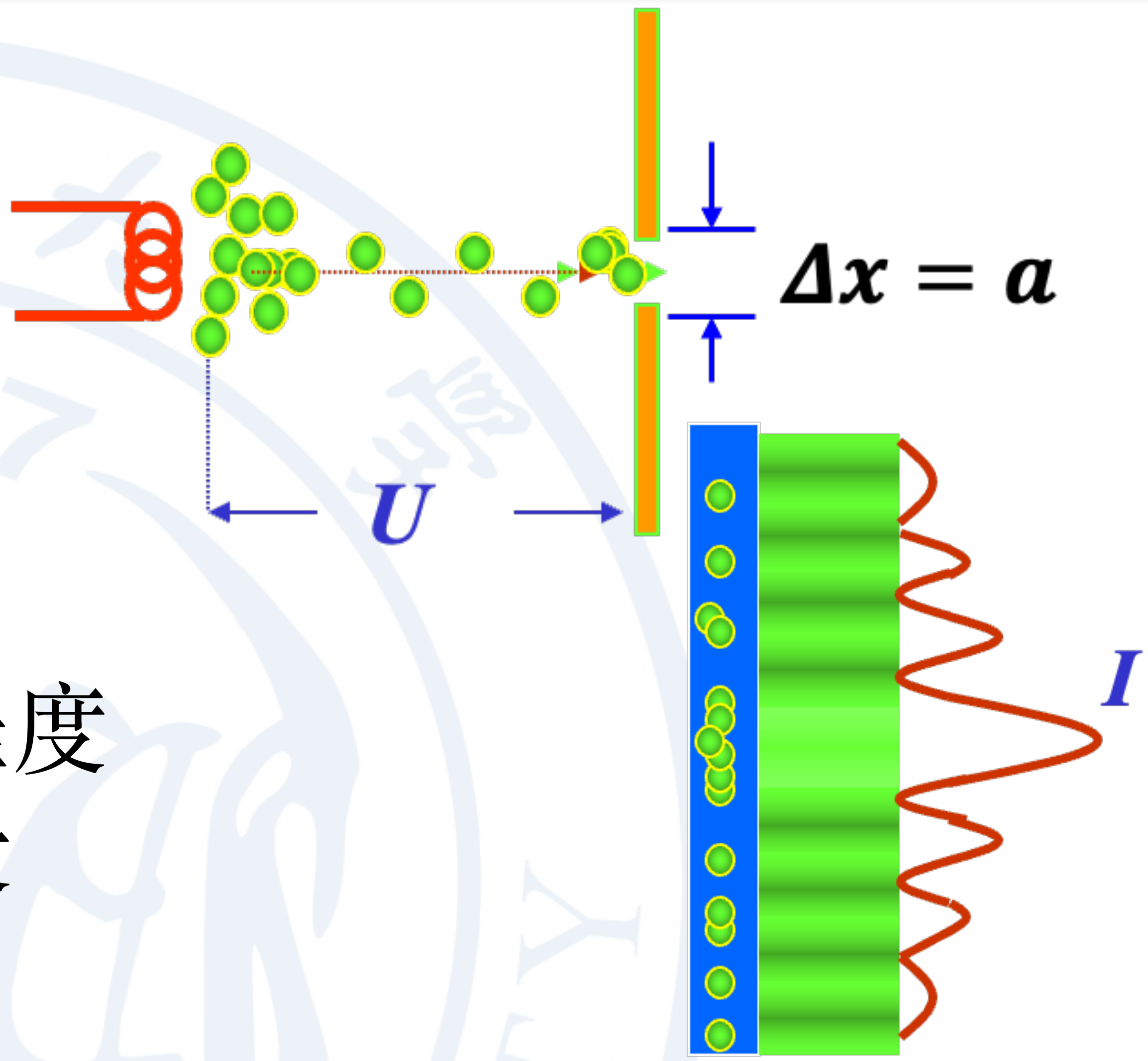
位置测定得越准确，动量就变得越测不准，反之亦然

测不准关系的实验验证（单缝衍射）

1) 位置的不确定程度

电子在单缝处的位置

不确定量为$\Delta x = a$



2）单缝处电子的动量的不确定程度

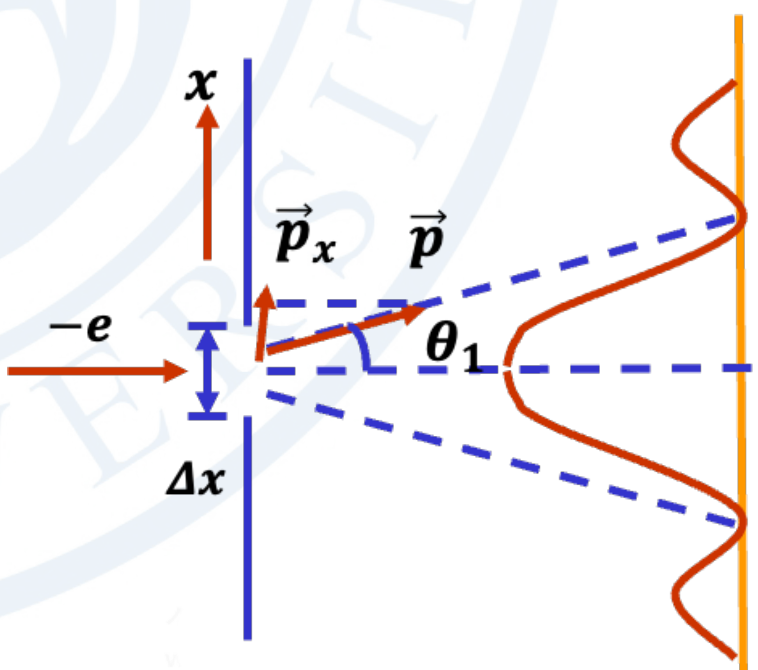
忽略次级极大，认为电子都落

在中央亮纹内，则：

$$0 \le p_x \le p\sin\theta_1 \quad (1)$$

x方向上的动量不确定量为：

$$\Delta p_x = p\sin\theta_1$$



测不准关系的实验验证（单缝衍射）

忽略次级极大，认为电子都落在中央亮纹内，则x方向上的动量不确定量为：

$$\Delta p_x = p\sin\theta_1$$

考虑到衍射条纹的次级极大,可得 $\Delta p_x \geq p\sin\theta_1$ （2）

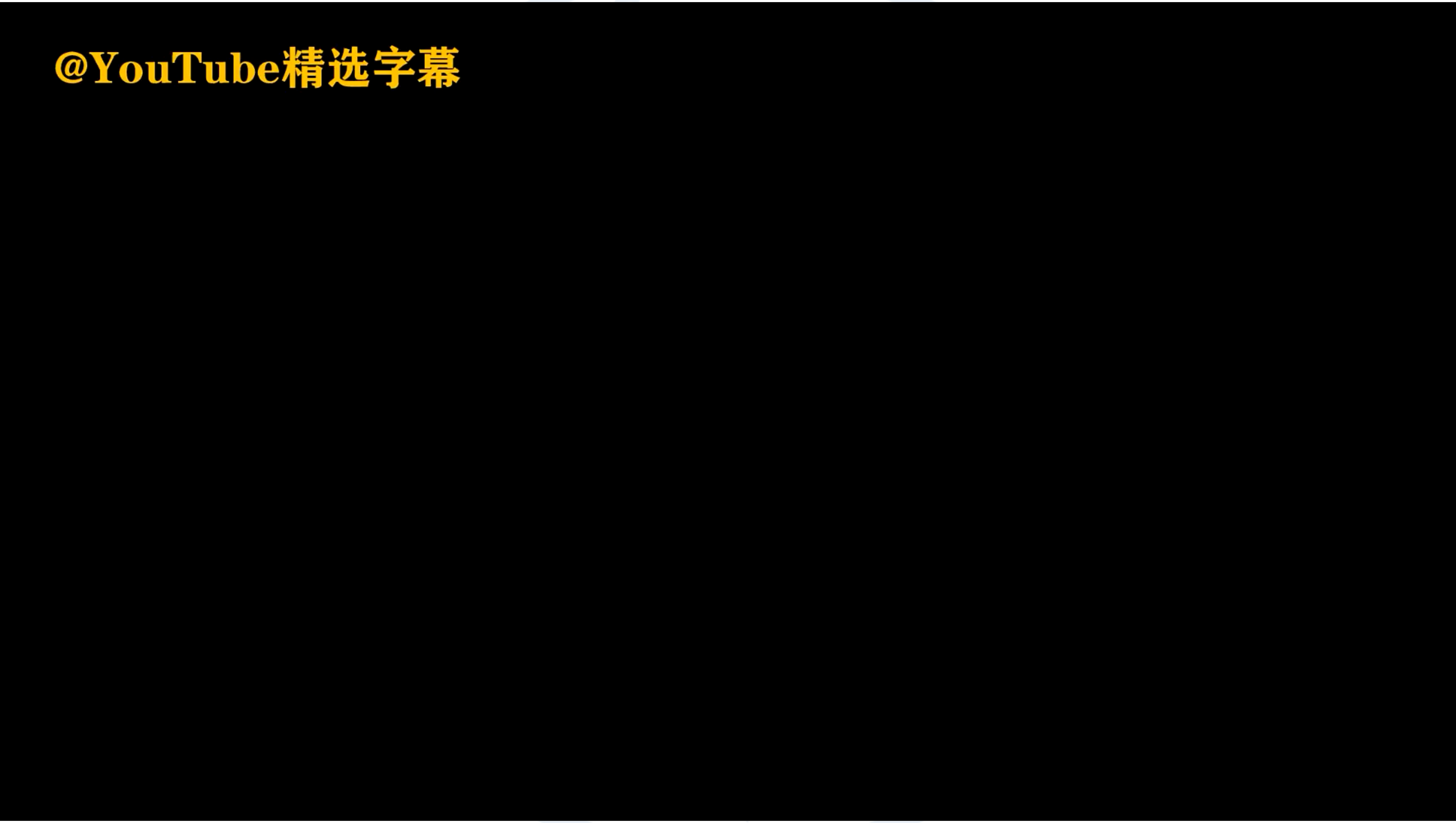
一级最小衍射角 $\sin\theta_1 = \lambda/\Delta x$， 以及 $\lambda = h/p$， 可得

$$\sin\theta_1 = \frac{h}{p\Delta x}$$

代入(2)式有

$$\Delta p \geq \frac{h}{\Delta x}$$ 或： $\Delta x \Delta p \geq h$

测不准关系的实验验证（单缝衍射）



海森堡不确定性原理 1927

1924 波粒二象性（德布罗意物质波） ➡ 测不准

1925 海森堡建立了矩阵力学（量子力学）

1926 薛定谔建立了波动方程（量子力学）

1927 海森堡基于矩阵力学和对易关系 ➡ 不确定性原理

1927 肯纳德基于标准差推导出不确定性关系

1929 罗伯逊更普遍意义的不确定性关系

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

海森堡不确定性原理 1927

Published: March 1927

Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik

W. Heisenberg

Zeitschrift für Physik **43**, 172–198 (1927) | Cite this article

bestimmbar ist, also hier die unstetige Änderung von p beim Comptoneffekt, so stehen nach elementaren Formeln des Comptoneffekts p_1 und q_1 in der Beziehung

$$p_1 q_1 \sim h. \quad (1)$$

Daß diese Beziehung (1) in direkter mathematischer Verbindung mit der Vertauschungsrelation $pq - qp = \frac{h}{\ldots}$ steht, wird später ge-

海森堡不确定性原理 1927

Published: April 1927

Zur Quantenmechanik einfacher Bewegungstypen

E. H. Kennard

Zeitschrift für Physik **44**, 326–352 (1927) | Cite this article

und, da das rechts stehende Integral nicht negativ sein kann, gilt ganz allgemein:

$$p_i\, q_i \geqq \frac{h}{2\pi}. \qquad (27)$$

Dieses ist das etwas verallgemeinerte Unbestimmtheitsgesetz von

海森堡不确定性原理 1927

The Uncertainty Principle

H. P. Robertson
Phys. Rev. **34**, 163 – Published 1 July 1929

The uncertainty principle for two such variables A, B, whose commutator $AB-BA=hC/2\pi i$, is expressed by

$$\Delta A \cdot \Delta B \geqq h|C_0|/4\pi$$

i.e. the product of the uncertainties in A, B is not less than half the absolute value of the mean of their commutator.

能量与时间的不确定性关系

$$p^2c^2 = E^2 - m_0^2c^4 \quad \xrightarrow{\text{两边微分可得}} \quad c^2p\Delta p = E\Delta E$$

可得$\Delta p = \dfrac{E}{c^2p}\Delta E$

粒子可能发生的位移$v\Delta t = \dfrac{p}{m}\Delta t = \Delta x$

$$\Delta x\Delta p = \frac{p}{m}\Delta t\frac{E}{c^2p}\Delta E = \frac{E}{mc^2}\Delta E\Delta t = \Delta E\Delta t \geq \frac{\hbar}{2}$$

$$\Delta E\Delta t \geq \frac{\hbar}{2}$$ 能级自然宽度和寿命

不确定性关系与傅里叶变换

吉他发声可以看成是主弦的频率和腔体反射声音频率的干涉叠加

因此，吉他（以及任何其他乐器，包括你的声音）发出的声音是由具有不同频率和振幅的纯正弦波组成的

不确定性关系与傅里叶变换

当我们描述这样一个复杂的信号时，我们可以选择两种相等的方式来表示它。我们可以选择用一个时间轴来描述所有产生干涉图样的波是如何同时相互作用的，或者我们可以选择用构成它的纯波的频率来描述它。这两种方式被称为双重关系（dual relationship）。

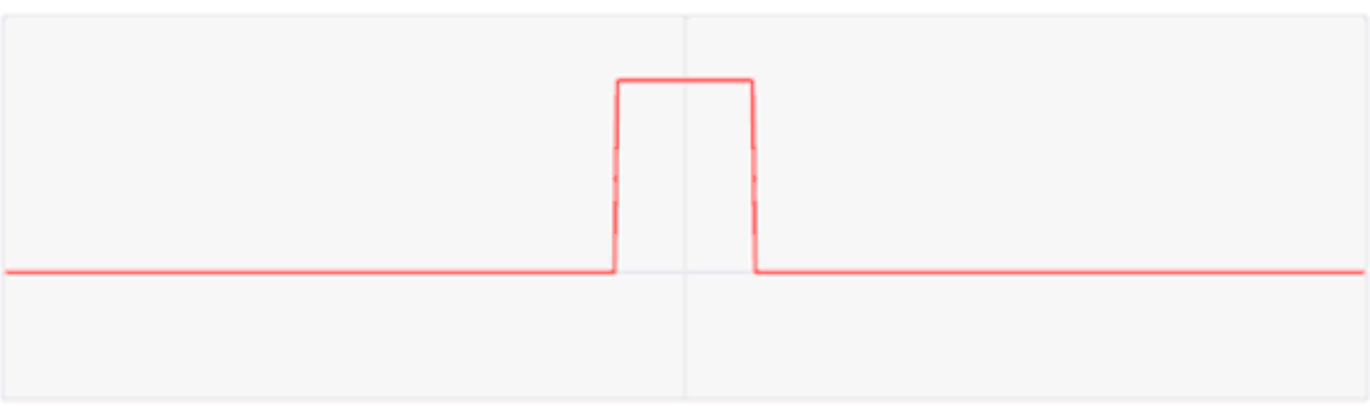
它们之间满足傅里叶变换

$$\hat{f}(s) = \int_{-\infty}^{\infty} f(t)e^{-2\pi ist}dt$$

不确定性关系与傅里叶变换

它们之间满足傅里叶变换

$$\hat{f}(s) = \int_{-\infty}^{\infty} f(t) e^{-2\pi i s t} dt$$



傅里叶逆变换

$$f(t) = \int_{-\infty}^{\infty} \hat{f}(s) e^{2\pi i t s} ds$$

不确定性关系与傅里叶变换

那么对时间的缩放会导致

$$h(t) = f(at) \quad \wedge \quad a > 0 \quad \Rightarrow$$

$$\hat{h}(s) = \int_{-\infty}^{\infty} f(at) e^{-2\pi i s t}\, dt$$

$$= \frac{1}{a} \int_{-\infty}^{\infty} f(u) e^{-2\pi i \left(\frac{s}{a}\right) u}\, du$$

$$= \frac{1}{a} \hat{f}\left(\frac{s}{a}\right).$$

不确定性关系与傅里叶变换

那么对时间的缩放会导致

$$h(t) = f(at) \quad \wedge \quad a < 0 \quad \Rightarrow$$

$$\begin{aligned}
\hat{h}(s) &= \int_{-\infty}^{\infty} f(at) e^{-2\pi i s t}\, dt \\
&= \frac{1}{a} \int_{\infty}^{-\infty} f(u) e^{-2\pi i \left(\frac{s}{a}\right) u}\, du \\
&= -\frac{1}{a} \int_{-\infty}^{\infty} f(u) e^{-2\pi i \left(\frac{s}{a}\right) u}\, du \\
&= \frac{1}{|a|} \int_{-\infty}^{\infty} f(u) e^{-2\pi i \left(\frac{s}{a}\right) u}\, du \\
&= \frac{1}{|a|} \hat{f}\left(\frac{s}{a}\right).
\end{aligned}$$

不确定性关系与傅里叶变换

那么对时间的缩放会导致

$$h(t) = f(at) \quad \Rightarrow$$

$$\hat{h}(s) = \frac{1}{|a|}\hat{f}\left(\frac{s}{a}\right).$$

傅里叶变换的缩放特性意味着如果我们在时间上压缩信号，那么这对应于在频率上扩展信号，反之亦然

练习

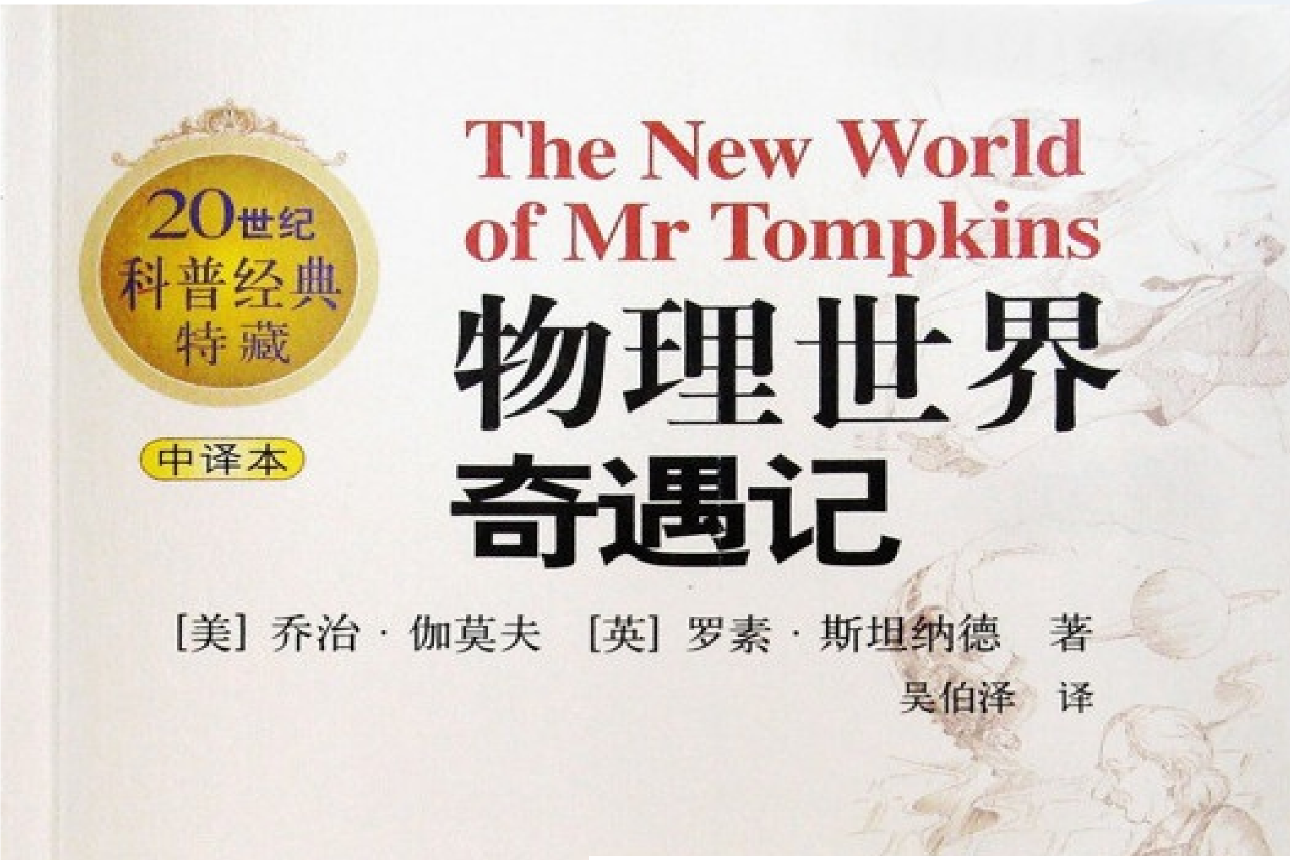
原子的激发态通常存在约$\Delta t = 10^{-8}$ s，估算当原子从激发态跃迁并同时发射平均频率为$\nu = 7.1\times10^{14}$ Hz的光子时，发射光子频率的不确定性，发射的辐射是单色的吗？

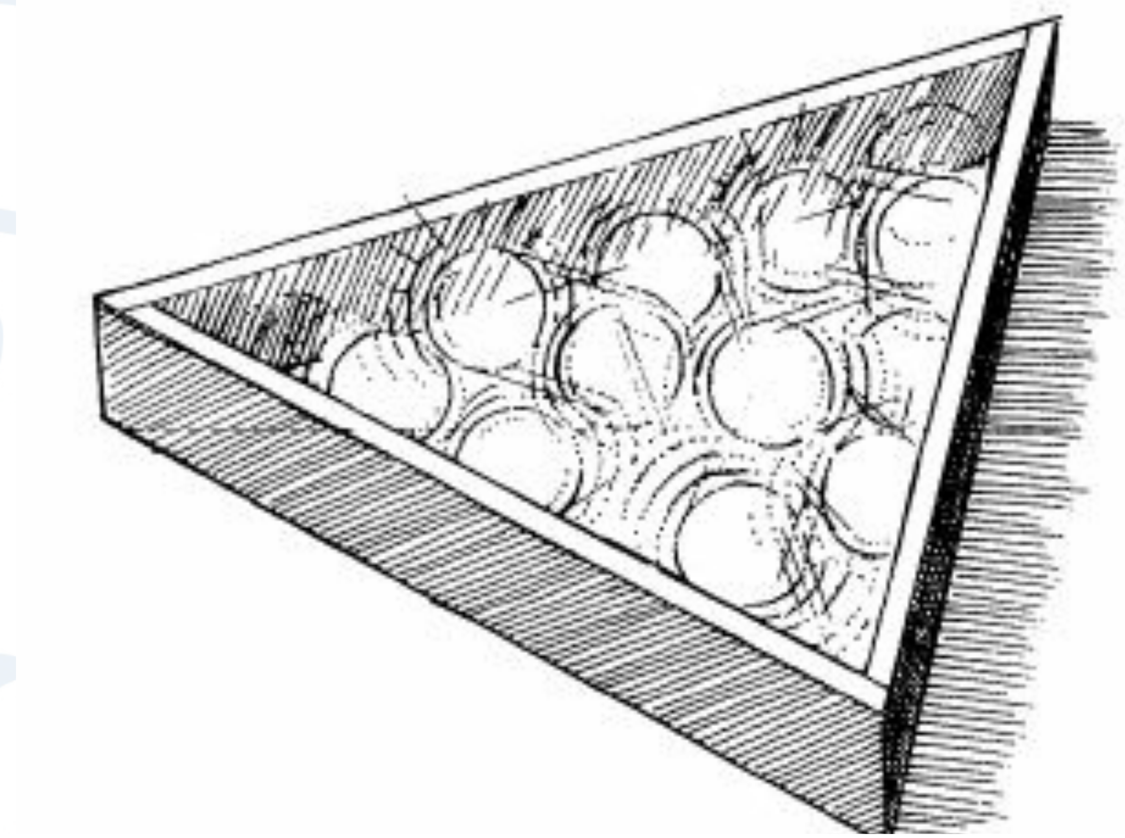
$$\Delta E \approx \frac{\hbar}{2\Delta t} \Rightarrow h\Delta f \approx \frac{\hbar}{2\Delta t} \Rightarrow \Delta f \approx \frac{1}{4\pi\Delta t} = \frac{1}{4\pi\left(10^{-8}\ \mathrm{s}\right)} = 8.0\times10^{6}\ \mathrm{Hz}$$

$$\frac{\Delta f}{f} = \frac{8.0\times10^{6}\ \mathrm{Hz}}{7.1\times10^{14}\ \mathrm{Hz}} = 1.1\times10^{-8}$$

能量–时间不确定性原理表达了实验观察到，仅存在很短时间的量子态不能具有确定的能量。

当h=1时





台球被限定在三角框里

“你看，”教授说，“我把台球的位置限定在三角框里几分米范围内了，这就使速度产生了相当可观的测不准性，所以台球在木框里迅速地运动。”

“你能让它停下吗？”汤普金斯先生问道。

“不，从物理学上说，这是不可能的。任何一个处在封闭空间内的物体都有一定的运动——我们物理学家把它称为零点运动。举个例子吧，任何原子中的电子的运动都属于这一类。”

课外阅读

§14 波函数

需要掌握的知识点：

(1)描述波函数的统计解释

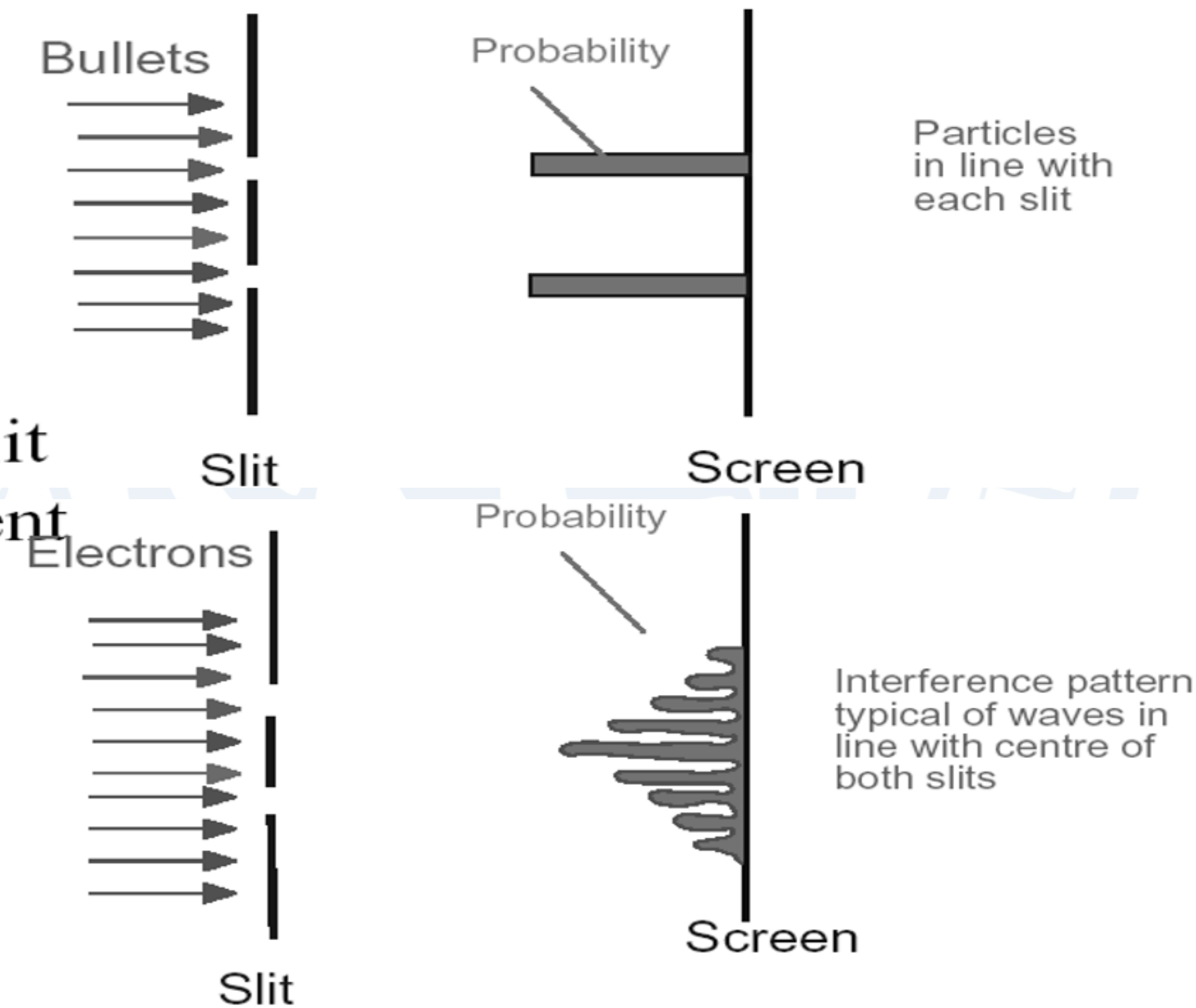
(2)使用波函数来确定概率

(3)计算位置的期望值

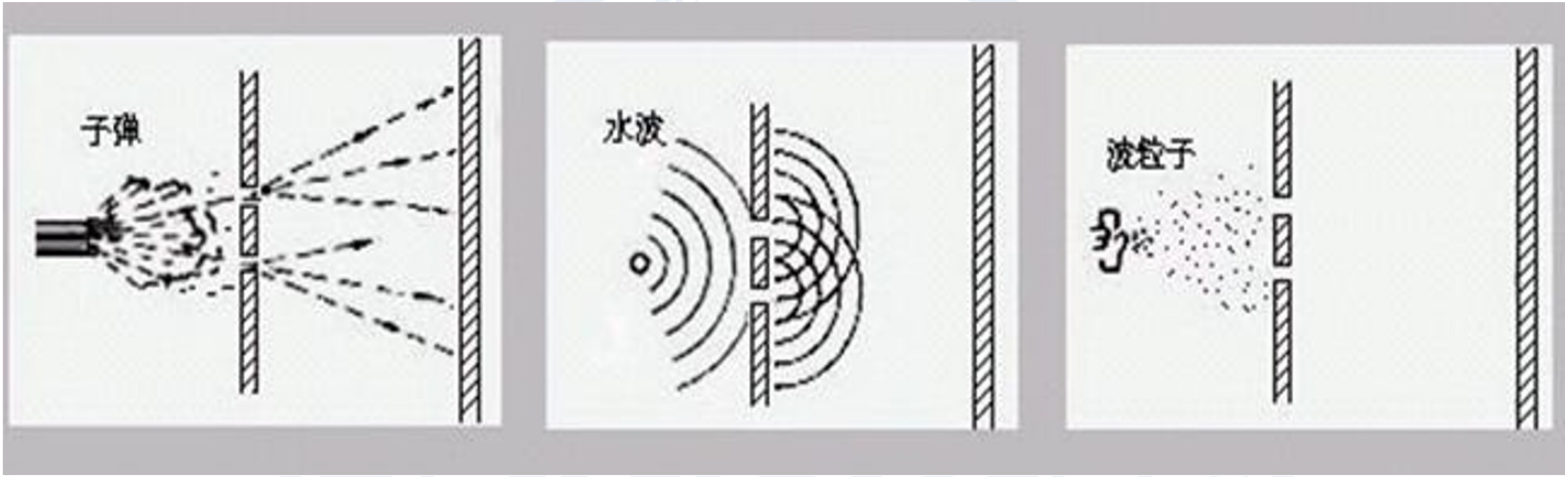
波函数

问题：那么，粒子性和波动性这两个完全不同的性质又是如何统一到了微观粒子上呢?

Double Slit Experiment



子弹、水波和电子分别通过双缝的理想实验



理查德·费曼Richard Feynman

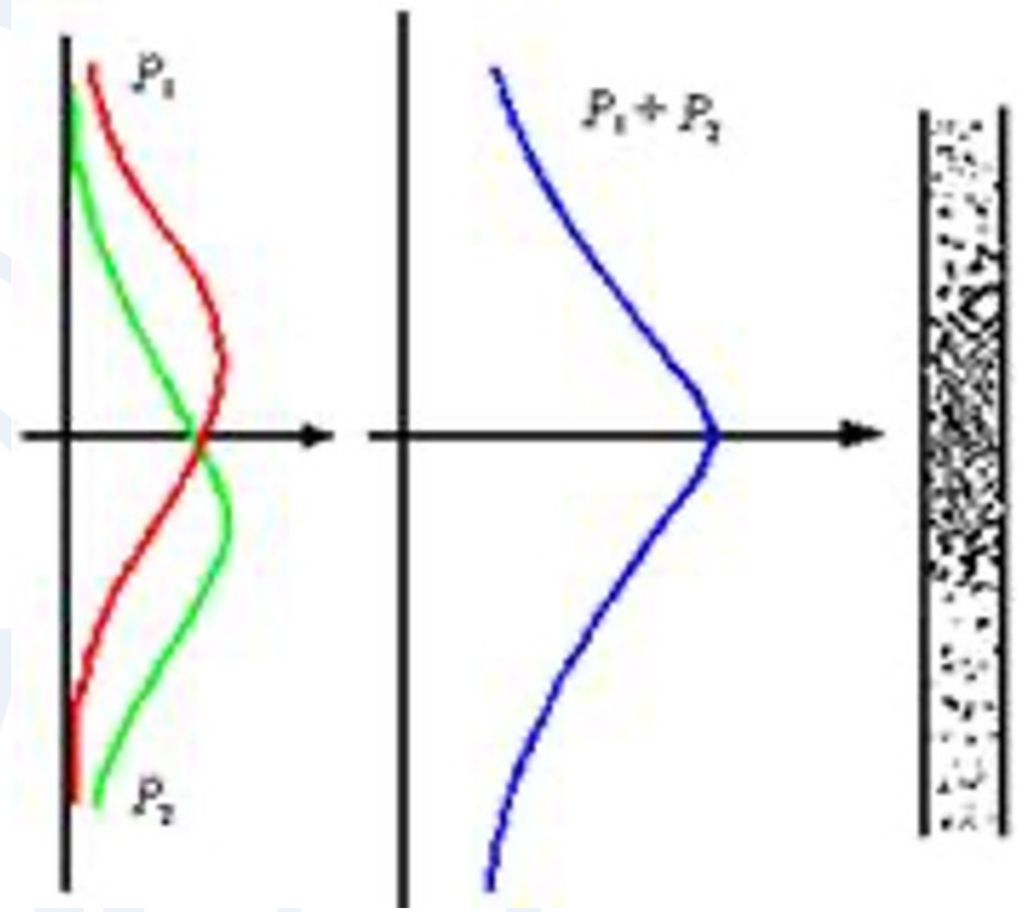
（1918－1988）美国物理学家。

1965年诺贝尔物理奖得主。

子弹的双缝实验

开单缝：

子弹密度分布曲线：P1 和P2。



开双缝：

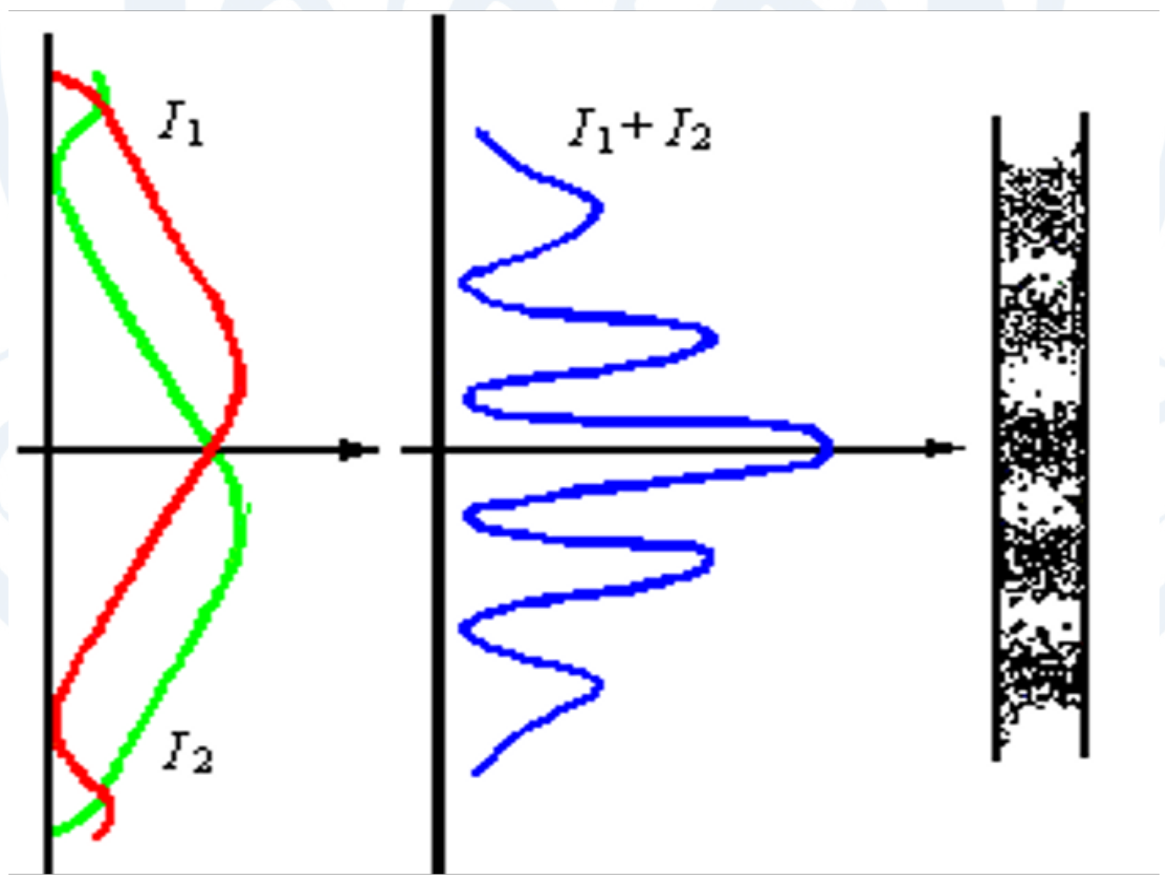
曲线P1 ＋P2。

“非相干叠加”。即主要表现了粒子性。

水波的双缝实验

水波的双缝实验，屏上观察到的分布是否与子弹实验结果一样？

因为水波通过双缝时被分为两个相干的次波源，它们在空间将进行相干叠加，所以在屏上将呈现出双缝干涉图样。

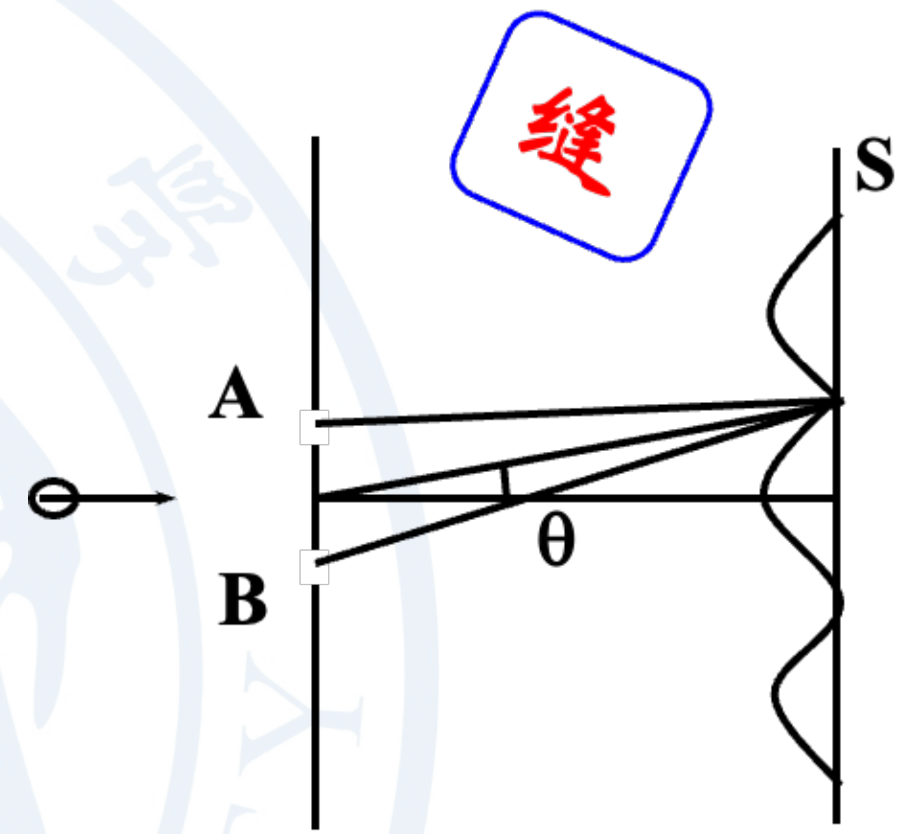


电子的双缝实验

每个电子是如何从两个缝通过的，它们又是如何逐渐形成干涉花样的?

1). 通过缝时电子是粒子?

双缝干涉花样就应该是两个单缝花样的简单叠加。存在干涉就表明每个电子似乎都是从两个缝通过的。



2). 通过缝时电子已散开成波?

不可能在到达屏的一瞬间收缩成一个亮点 。

经典物理学无法解释

经典物理学无法说明粒子性和波动性之间的关系

概率波

在量子力学建立的初期，人们对德布罗意波的意义曾提出过各种各样的猜测，例如:

电子波是一个代表电子实体的波包，

电子本身是弥散于空间的物质波动，

电子的波动性是大量电子之间的相互作用等。

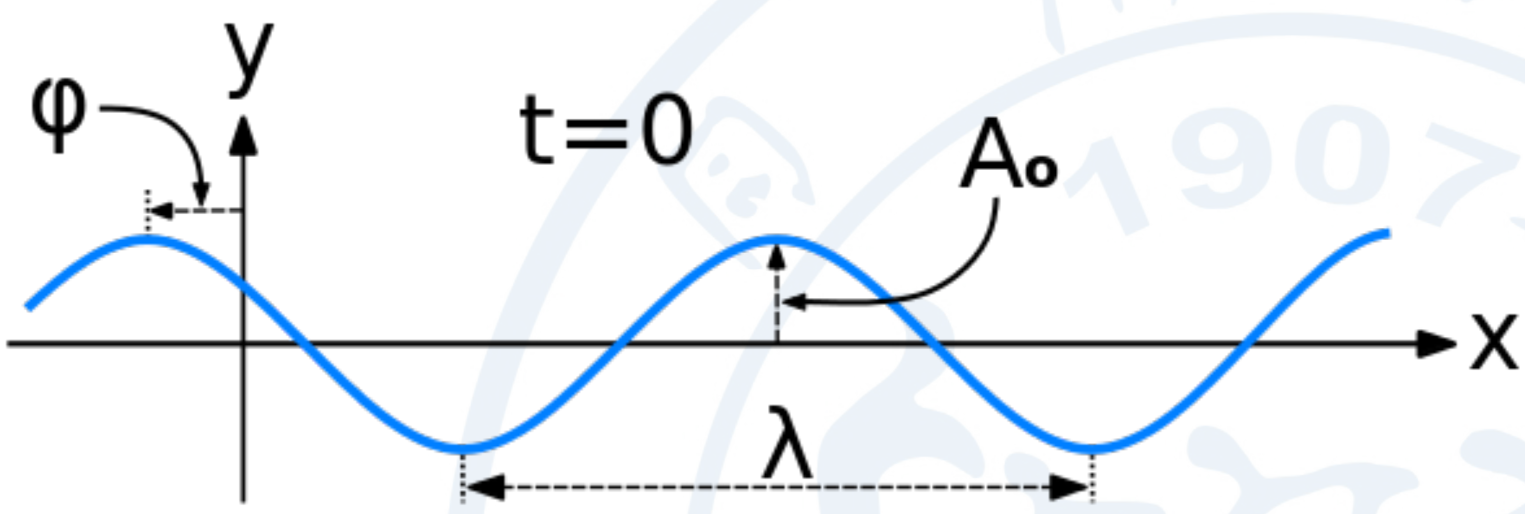
但是，这些猜测最终都因不能圆满地解释实验现象而不得不放弃。

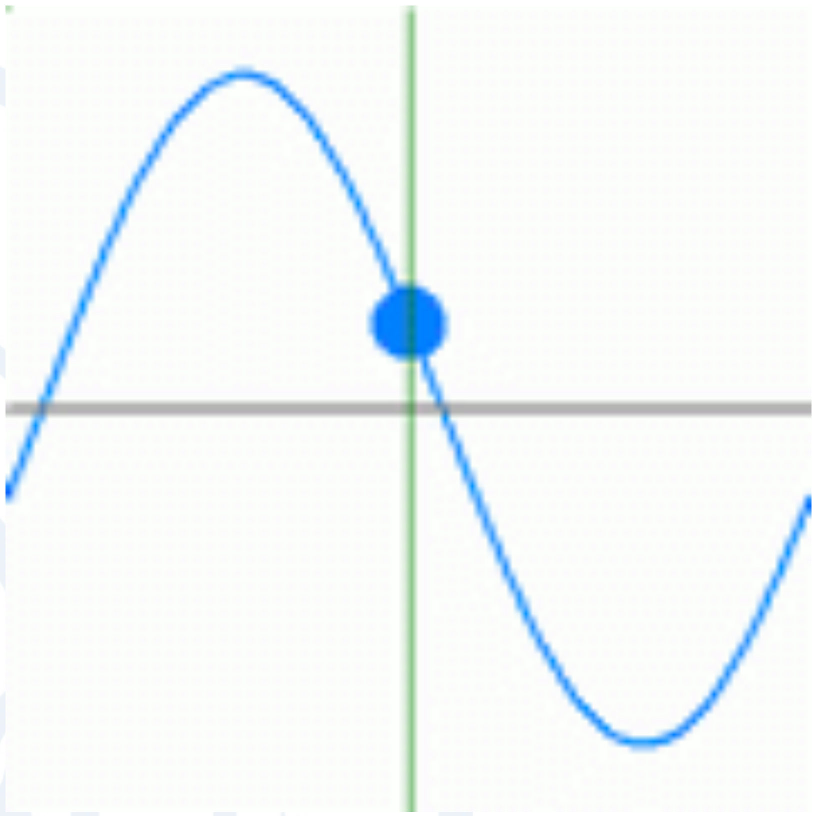
1926年，玻恩（M.Born）对波粒二象性给出了一种统计诠释，他认为

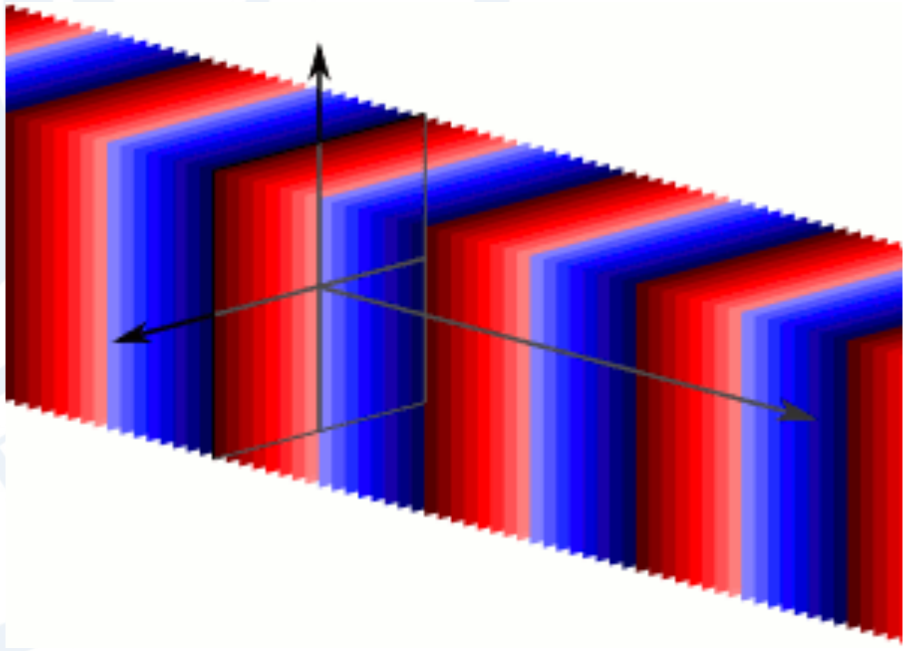
德布罗意波：是概率波

什么是波函数

宏观上





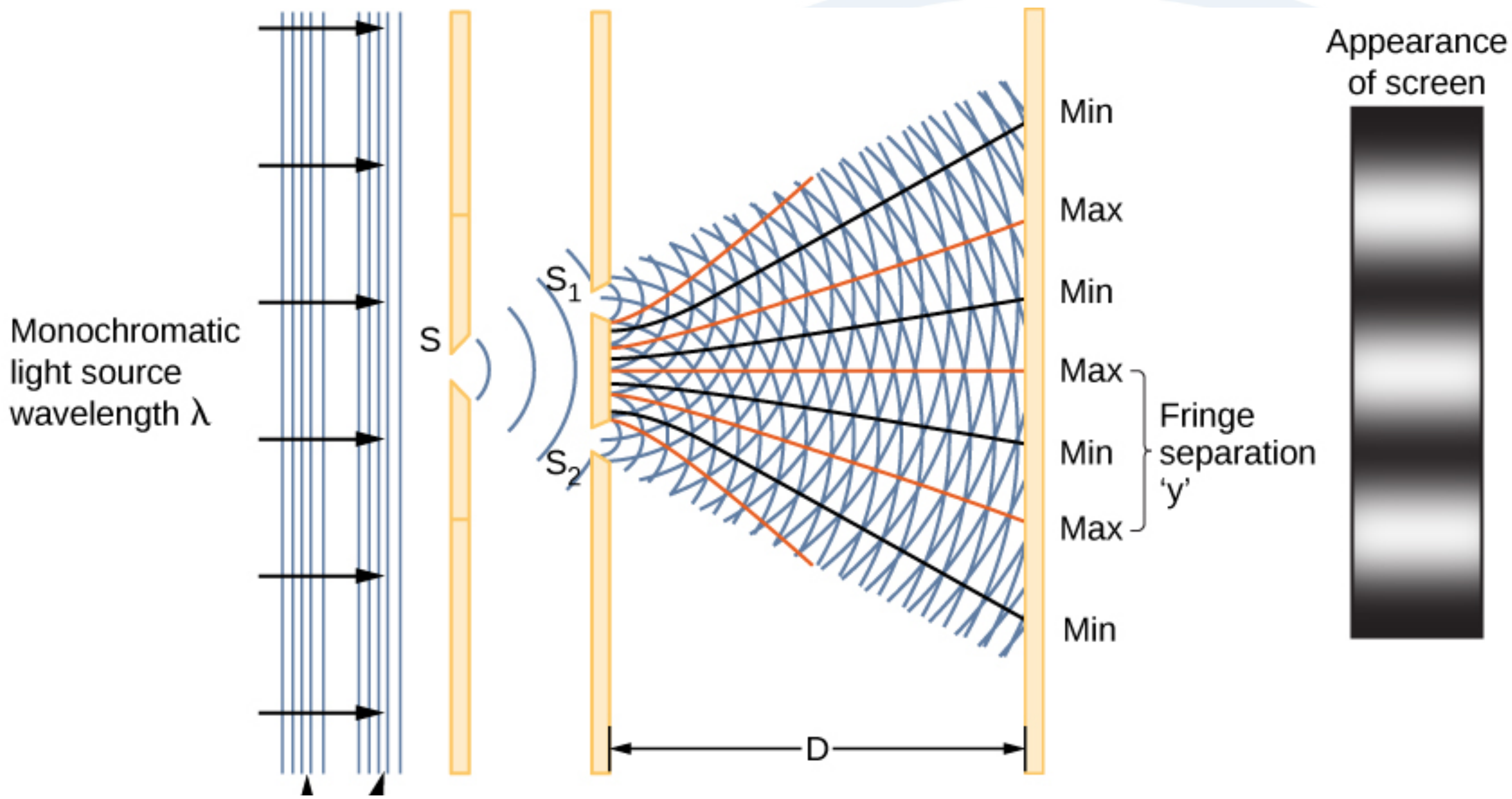


波函数需要的信息有相位，波长，振幅，含时演化

考虑到物质波也是波的一种，也应该具备上述信息

但是位置和动量不能同时确定

光的波函数



波函数$E(x,t)$

能量密度$|E|^2$

E为电场强度

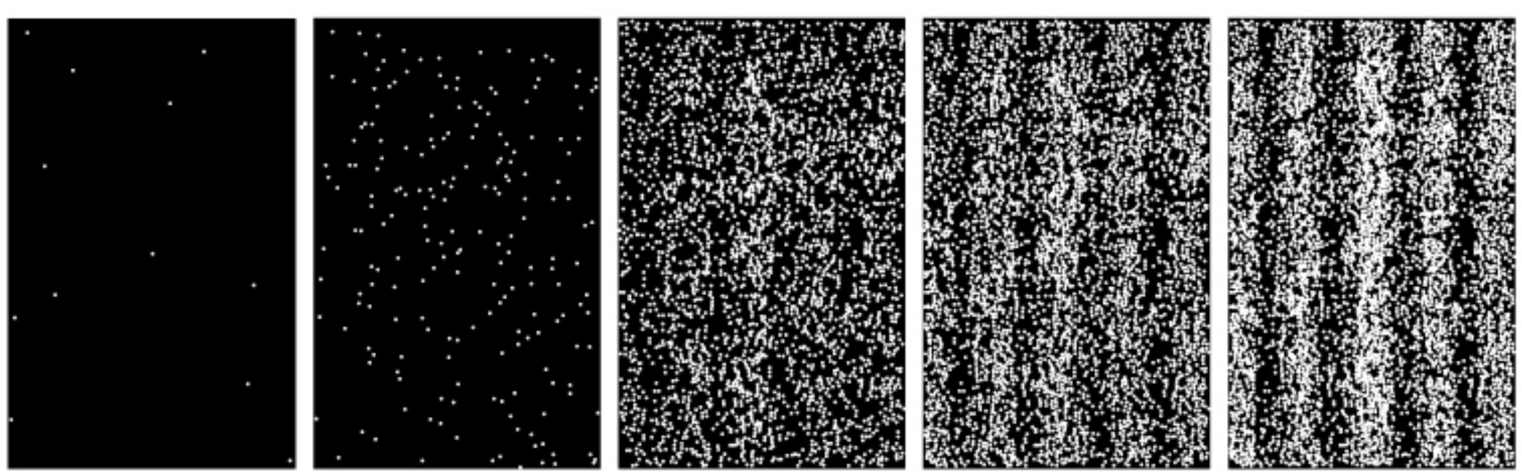
单个光子的能量

$\varepsilon_{\text{photon}} = h\nu$

光打在屏幕上某点的概率
正比于电场在该点的强度的平方

$|E|^2$正比于光子数量

(b)



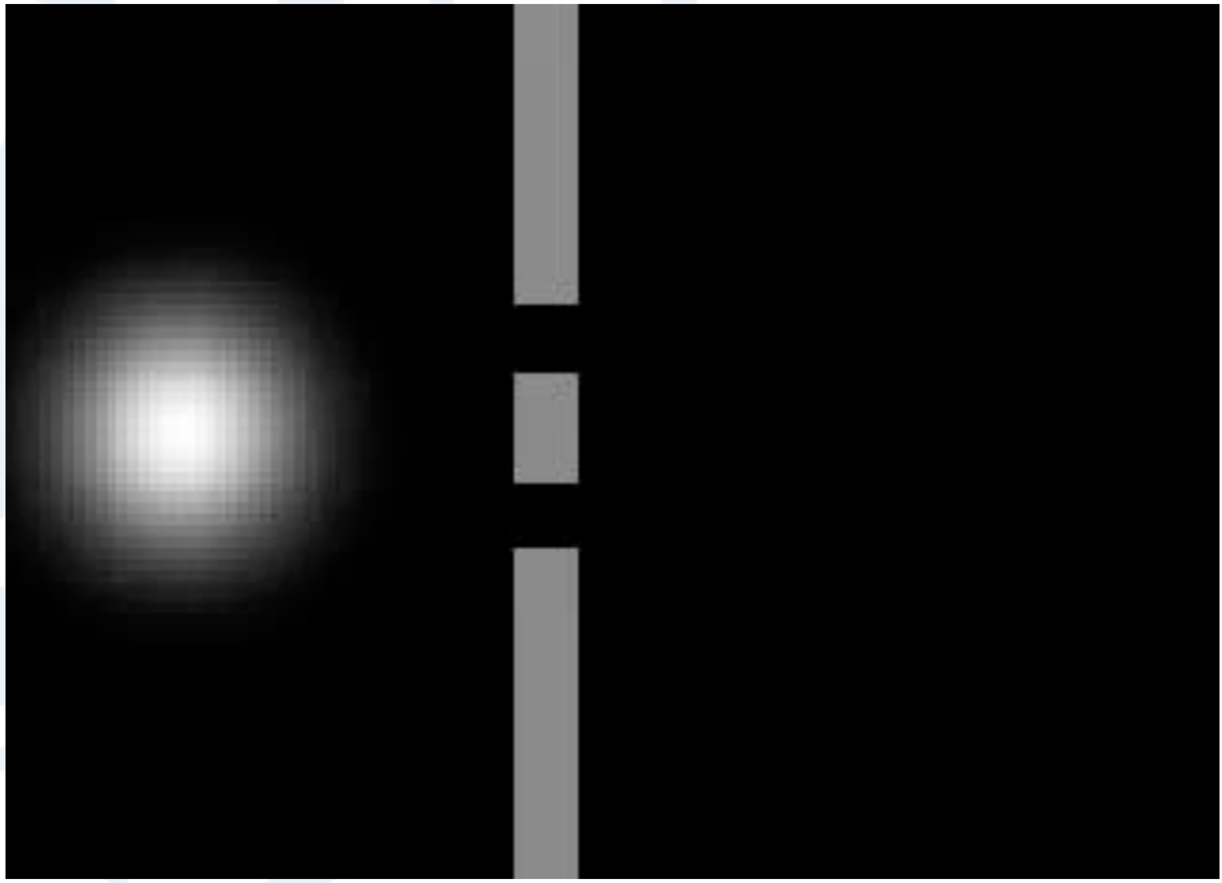
(c)

波函数的统计解释（M.Born，1926）

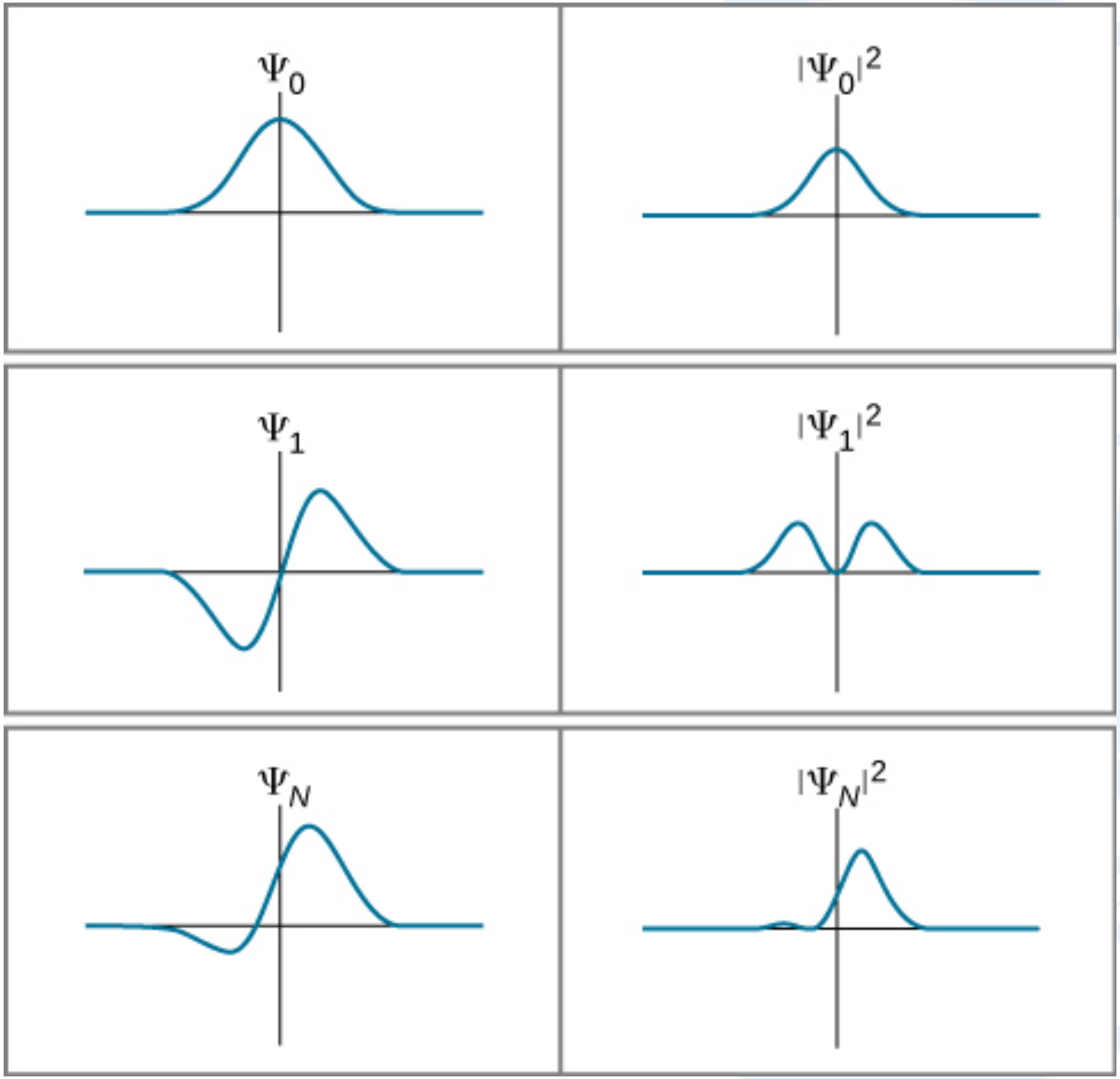
直到1926年，M.Born在认真研究波粒二象性之后，才意识到，类似于爱因斯坦"光振幅的平方为光子密度的概率量度"，波函数的模方是粒子的几率密度！

即：波函数的模方 $|\Psi(x,t)|^2$ (波在空间某点的强度)与t时刻在空间某点x处单位体积内发现粒子的几率成正比

或，t时刻在x到$x+dx$的区间内找到粒子的几率$P(x, x+dx)$与$|\Psi(x,t)|^2 dx$成正比



波函数的统计解释（M.Born，1926）



波恩的波函数几率解释是量子力学基本原理之一

波函数是几率幅，是不可测量，可测量是几率

1954年Nobel物理奖

波函数的统计解释（M.Born，1926）

Published: December 1926

Zur Quantenmechanik der Stoßvorgänge

Max Born

Zeitschrift für Physik **37**, 863–867 (1926) | Cite this article

Zusammenfassung

Durch eine Untersuchung der Stoßvorgänge wird die Auffassung entwickelt, daß die Quantenmechanik in der Schrödingerschen Form nicht nur die stationären Zustände, sondern auch die Quantensprünge zu beschreiben gestattet.

波函数的统计解释（M.Born，1926）

Published: November 1926

Quantenmechanik der Stoßvorgänge

Max Born

Zeitschrift für Physik **38**, 803–827 (1926) | Cite this article

Zusammenfassung

Die Schrödingersche Form der Quantenmechanik erlaubt in natürlicher Weise die Häufigkeit eines Zustandes zu definieren mit Hilfe der Intensität der zugeordneten Eigenschwingung. Diese Auffassung führt zu einer Theorie der Stoß-vorgänge, bei der die Übergangswahrscheinlichkeiten durch das asymptotische Verhalten aperiodischer Lösungen bestimmt werden.

波函数的统计解释（M.Born，1926）

In a letter to Born on 4 December 1926, Einstein made his famous remark regarding quantum mechanics:

Quantum mechanics is certainly imposing. But an inner voice tells me that it is not yet the real thing. The theory says a lot, but does not really bring us any closer to the secret of the 'old one'. I, at any rate, am convinced that *He* is not playing at dice.

This quotation is often paraphrased as 'God does not play dice'.

Niels Bohr reportedly replied to Einstein's later expression of this sentiment by advising him to "stop telling God what to do."

波函数的统计解释（M.Born，1926）

课外阅读

MAX BORN

The statistical interpretation of quantum mechanics

Nobel Lecture, December 11, 1954

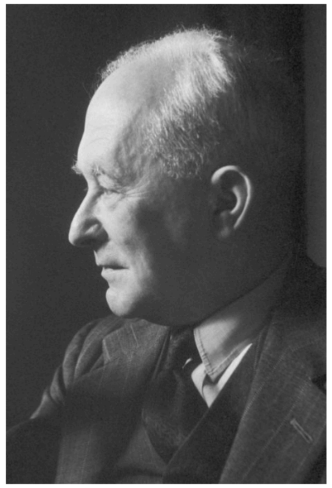


Photo from the Nobel Foundation archive.

Max Born
The Nobel Prize in Physics 1954

Born: 11 December 1882, Breslau, Germany (now Wroclaw, Poland)

Died: 5 January 1970, Göttingen, West Germany (now Germany)

Affiliation at the time of the award: Edinburgh University, Edinburgh, United Kingdom

Prize motivation: “for his fundamental research in quantum mechanics, especially for his statistical interpretation of the wavefunction”

波函数的性质

波函数必须单值、有限、连续

单值：在任何一点，几率只能有一个值。

有限：几率不能无限大。

连续：几率一般不发生突变。

归一化条件：由于粒子总在空间某处出现，故在整个空间出现的总几率应当为1

$$P(-\infty,+\infty)=\int_{-\infty}^{\infty}|\Psi(x,t)|^2dx=1$$

波函数的归一化

由于波函数$\psi(\vec{r},t)$的概率解释，粒子在整个空间出现的概率为1，所以ψ应该满足波函数的归一化条件：

$$\int_{\Omega} |\Psi|^2 dV = 1 \quad (\Omega - \text{全空间})$$

已知$\phi(\vec{r},t)$是未归一化的波函数，则令$\psi = A\phi$，它们描述同一个状态，有

$$\int |\psi|^2 dV = \int |A\phi|^2 dV = |A|^2 \int |\phi|^2 dV = 1$$

所以

$$A = \frac{1}{\sqrt{\int |\phi|^2 dV}}, \quad \psi = \frac{1}{\sqrt{\int |\phi|^2 dV}}\phi$$

波函数的物理意义

在空间很小的区域 $[x, x+\Delta x]$，$[y, y+\Delta y]$，$[z, z+\Delta z]$ 内，波函数可视为不变，粒子在$dV = dxdydz$内出现的概率，正比于$|\Psi|^2$和dV。

$|\psi|^2$ – 在t时刻粒子出现在(x, y, z)点处单位体积内出现的概率密度。

$|\psi|^2 dV$ – 在t时刻粒子出现在(x, y, z)点附近 dV 体积元内出现的概率。

$\int_V |\psi|^2 dV$ – 在t时刻粒子出现在V体积内的概率。

当α为实数时，ψ与$e^{i\alpha}\psi$代表同一个态

电子双缝干涉实验的统计学解释

在电子双缝干涉实验中，用波函数$\psi_A(r,t)$和$\psi_B(r,t)$分别表示从A、B缝通过电子的状态。两缝同时开启时，电子的波函数为$\psi(r,t)=\psi_A(r,t)+\psi_B(r,t)$

屏上发现电子的概率分布为

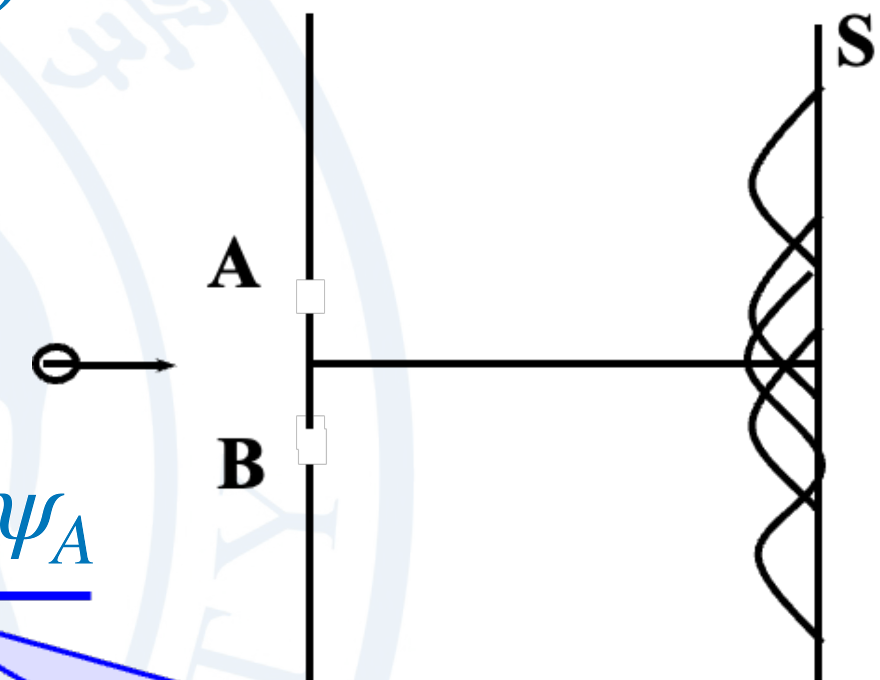
$$|\psi(\mathbf{r},t)|^2 = |\psi_A+\psi_B|^2$$

$$= |\psi_A|^2 + |\psi_B|^2 + \psi_A^*\psi_B + \psi_B^*\psi_A$$

只开A缝时电子出现的概率密度

只开B缝时电子出现的概率密度

两缝同时打开时还有干涉项，正是产生双缝干涉的原因



玻恩用概率解释把微观粒子的波动性和粒子性统一起来，玻恩的统计诠释成为量子力学的一个基本假设。

如何理解微观粒子的波粒二象性

1) 粒子性

- 整体性
- 不是经典的粒子 没有“轨道”概念

2) 波动性

- “可叠加性”
- 有“干涉”“衍射”“偏振”现象
- 不是经典的波 不代表实在物理量的波动

电子云

用密或稀表示空间各处概率密度的大小，很像在原子核外有一层疏密不等的“云”，人们把它形象地叫做“电子云”。

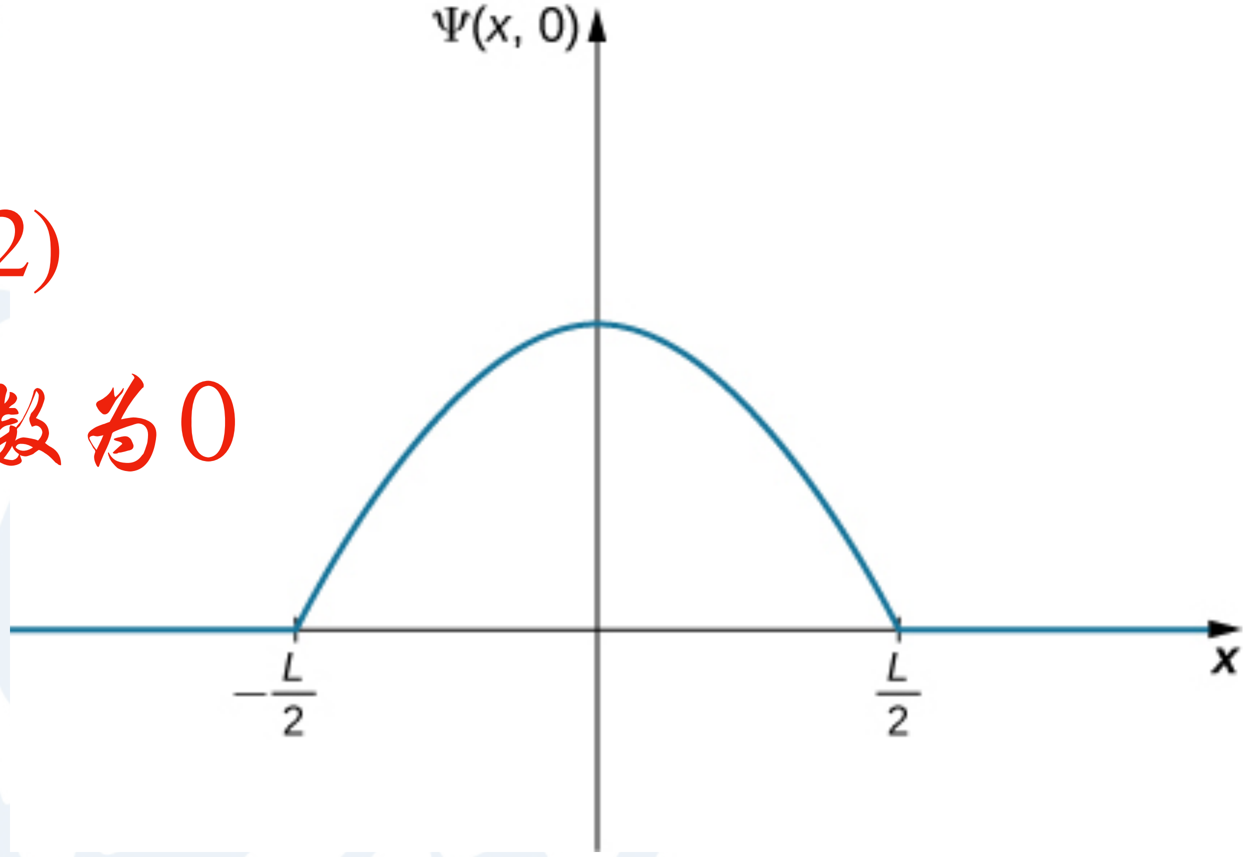
习题

球被限制在长度为L的管内移动，球优先位于管的中间。表示其波函数的一种方法是使用简单的余弦函数。在管子的最后四分之一处找到球的概率是多少？

波函数可以写为

$$\Psi(x,0) = A\cos(kx) \ (-L/2 < x < L/2)$$

$k = 2\pi/\lambda$为波数，区间外波函数为0



$$A\cos(kL/2) = 0$$

$$\frac{kL}{2} = \frac{\pi}{2}$$

应用归一化条件可得$A = \sqrt{2/L}$，可得

$$\Psi(x,0) = \sqrt{\frac{2}{L}}\cos(\pi x/L), \quad -L/2 < x < L/2$$

习题

球被限制在长度为L的管内移动，球优先位于管的中间。表示其波函数的一种方法是使用简单的余弦函数。在管子的最后四分之一处找到球的概率是多少？

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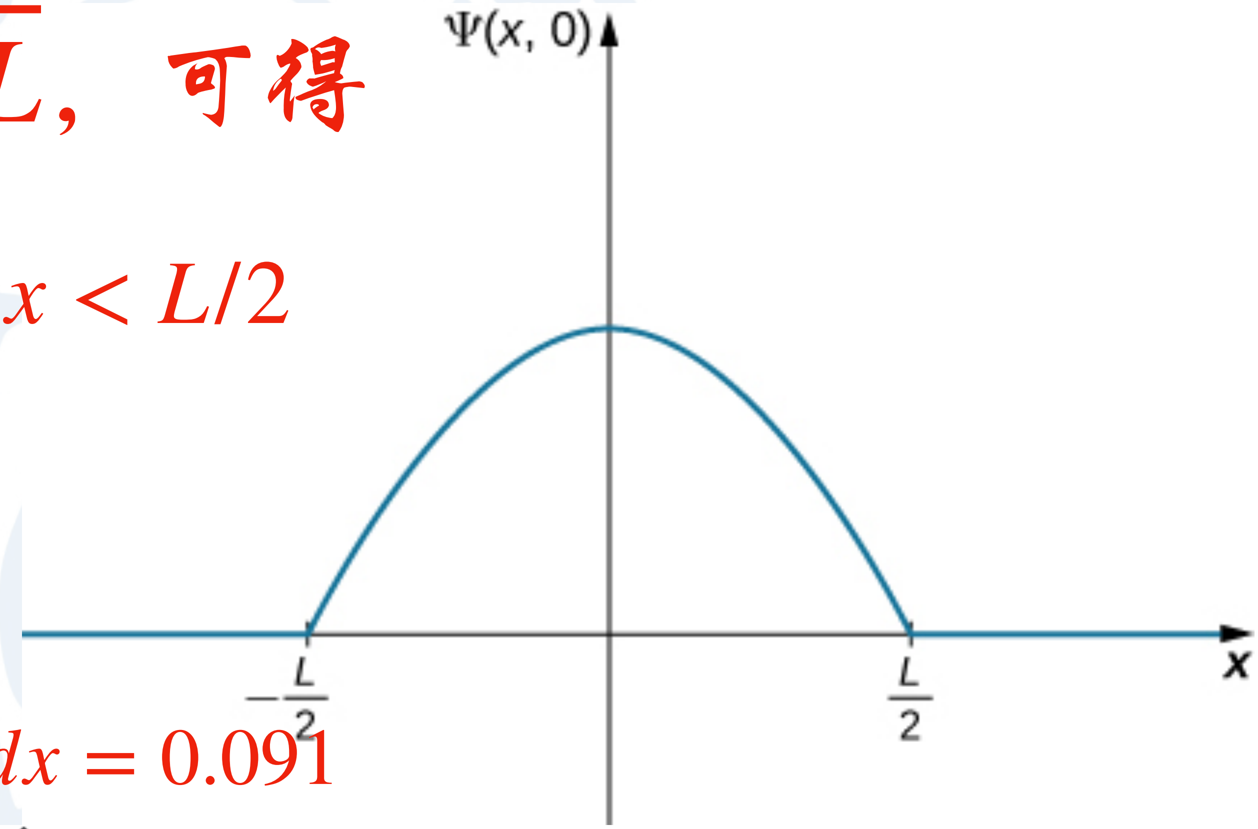
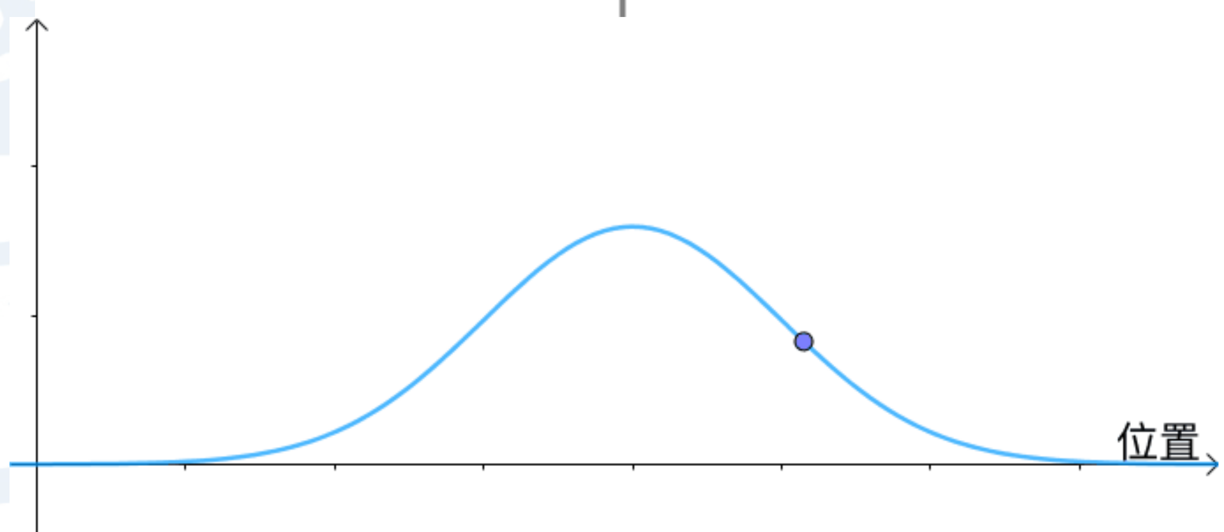


最后四分之一处找到球的概率

$$P(x=L/4,L/2)=\int_{L/4}^{L/2}\left|\sqrt{\frac{2}{L}}\cos\left(\frac{\pi x}{L}\right)\right|^2 dx=0.091$$

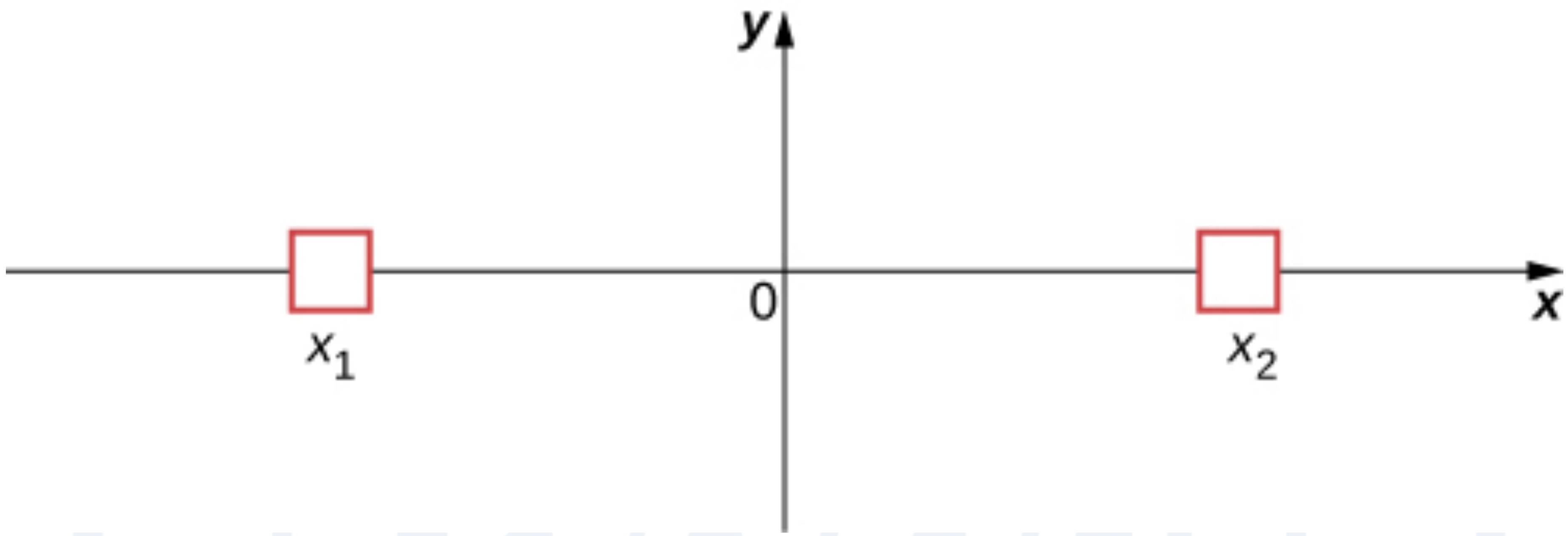
小球的波长

$$\lambda=\frac{h}{p}=\frac{h}{\hbar k}=\frac{2\pi}{k}=2L$$



态叠加原理

考虑一个粒子可以在盒子x_1或x_2处



宏观上，粒子不是在x_1就是在x_2

量子力学中，当不被测量时，粒子既在x_1，又在x_2，处于x_1与x_2的叠加态

→ 薛定谔的猫

什么是波函数

量子上$\Psi(x,t)=A\sin(kx-\omega t)$

1.一个数学函数，它可用于确定做位置测量时粒子可能在哪里。

2.波函数如何用于预测？如果有必要找出在某个区间内发现粒子的概率，则对波函数求平方并在感兴趣的区间上积分。

3.如果物质波波函数为$\Psi(x,t)$，那么粒子究竟在哪？

I.当不被观测时，粒子无处不在$(x=-\infty,+\infty)$

II.当被观测时，粒子“跳入”特定的状态$(x,x+dx)$，概率为$P(x,x+dx)=|\Psi(x,t)|^2dx$，这个过程叫做“坍缩”

波函数的复数形式

量子力学的平面波波函数可以写为

$$\Psi(x,t) = A\cos(kx-\omega t) + iA\sin(kx-\omega t) = Ae^{i(kx-\omega t)} = Ae^{i\phi}$$

相对于宏观的机械波、声波，物质波波函数不可测，因此需要写成复数形式

用复共轭的方式计算概率

$$P(x,x+dx) = |\Psi(x,t)|^2 dx = \Psi^*(x,t)\Psi(x,t)dx$$

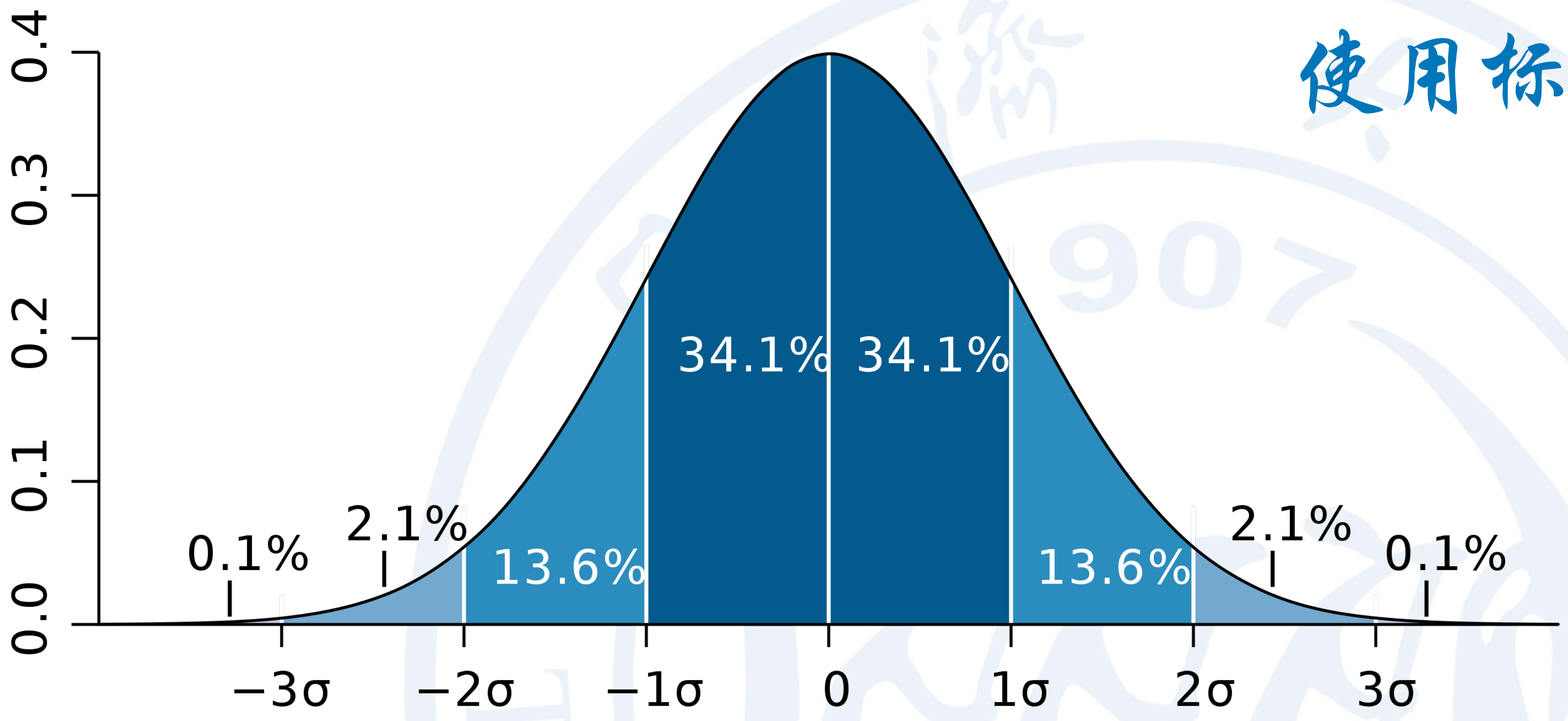
期望值计算

宏观上，运动方程的解是一个可测量量的函数，例如$x(t)$，其中x是位置，t是时间。请注意，粒子在任何时间t都有一个位置值。

在量子力学中，运动方程的解是波函数$\Psi(x,t)$。粒子在任何时间t都有许多位置值，并且只能知道找到粒子的概率密度$|\Psi(x,t)|^2$。粒子的位置平均值为

$$\langle x\rangle = \int_{-\infty}^{\infty} xP(x,t)dx = \int_{-\infty}^{\infty} x\Psi^*(x,t)\Psi(x,t)dx$$

不确定性原理的统计学解释



使用标准差代替不确定度

$$\Delta x \rightarrow \sigma_x$$

$$\Delta p \rightarrow \sigma_p$$

$$\sigma \equiv \sqrt{E[X^2] - (E[X])^2}$$

$$\mathrm{E}[X] \equiv \int_{-\infty}^{+\infty} X f(X) dX$$

习题

利用不确定性原理估算氢原子的基态能量（假设氢原子的直径为0.1 nm）

$$\sigma_x \sigma_p = \frac{\hbar}{2}$$

其中

$$\sigma_x^2 = x^2 - \bar{x}^2 \text{ and } \sigma_p^2 = p^2 - \bar{p}^2$$

电子在左右来回运动，$\bar{p} = 0$；位置的不确定性近似为原子的半径$\sigma_x = L$，因此基态能量可以估算为

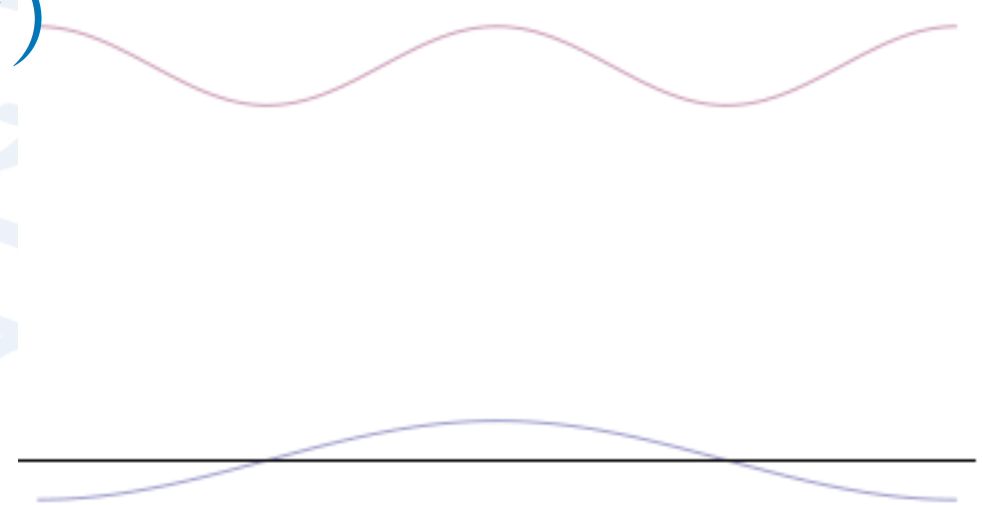
$$E_0 = E_{\text{Gaussian}} = \frac{\sigma_p^2}{2m} = \frac{1}{2m}\left(\frac{\hbar}{2\sigma_x}\right)^2 = \frac{1}{2m}\left(\frac{\hbar}{2L}\right)^2 = \frac{\hbar^2}{8mL^2}$$

为了方便计算，

$$E_0 = \frac{(\hbar c)^2}{8\left(mc^2\right)L^2} = \frac{(197.3\text{eV}\cdot\text{nm})^2}{8\left(0.511\cdot 10^6\text{eV}\right)(0.1\ \text{nm})^2} = 0.952\text{eV} \approx 1\text{eV}$$

波包

平面波波函数（确定动量$p = \hbar k$）



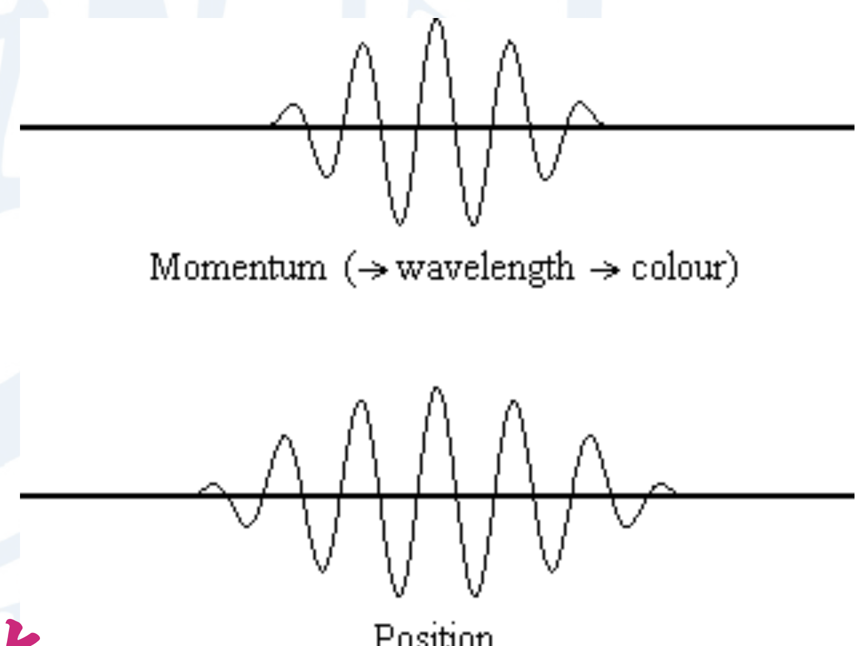
$$\Psi(x,t) = Ae^{i(kx-\omega t)}$$

$$|\Psi(x,t)|^2 = |A|^2$$

确定动量时，粒子完全无法确定位置，无处不在

$$\Delta p \rightarrow \Delta x$$

$$\psi(x,t) = \int_p^{p+\Delta p} \Psi_p(x,t)dp$$



波包是平面波在Δp区间内的叠加态

小结

(1)在量子力学中，系统的状态由波函数表示。

(2)在玻恩的解释中，粒子波函数的平方表示在空间中特定位置附近找到粒子的概率密度。

(3)在使用波函数进行预测之前，必须首先对波函数进行归一化。

(4)期望值是一种平均值，它的计算需要波函数的形式和进行积分运算

小结（GPT总结）

(1)量子世界玄妙多，

(2)波函数描态真奥妙。

(3)粒子波函数平方值，

(4)概率密度空间表。

(5)预测前须归一化，

(6)期望值积分求平均。

§15 薛定谔方程

需要掌握的知识点：

(1)描述薛定谔方程在量子力学中的作用

(2)解释与时间依赖和与时间无关的薛定谔方程之间的区别

(3)解释薛定谔方程的解

薛定谔方程

宏观上

- 经典的波：用波函数描述，满足经典的波动方程
- 经典的波、经典粒子都满足牛顿力学
- 那么，具有波粒二象性的粒子呢？

用什么描述？满足什么方程？

- 这是1925年维也纳大学的P.Debye和E.Schrodinger遇到的问题，也是玻尔的弟子们W.Heisenberg等人的问题！

问题的提出

德拜:问薛定谔能不能讲一讲De Broglie的那篇学位论文呢?

德拜提醒薛定谔:“对于波,应该有一个波动方程”

物理讨论会(1925)

薛定谔(1926)提出了非相对论性的薛定谔方程:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}\right)+U(x,y,z,t)\Psi=i\hbar\frac{\partial\Psi}{\partial t}$$

薛定谔方程

FIGURE 1. The Villa Herwig–Frisia (right), Arosa, where it is believed wave mechanics was discovered during the Christmas holidays 1925–26.

薛定谔方程

annalen der physik

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Quantisierung als Eigenwertproblem

E. Schrödinger

First published: 1926 | https://doi.org/10.1002/andp.19263840404 | Citations: 1,113

Es muß also erstens

$$\Delta\psi + \frac{2m}{K^2}\left(E + \frac{e^2}{r}\right)\psi = 0 \tag{5}$$

1) Es entgeht mir nicht, daß diese Formulierung nicht ganz eindeutig ist.

自由粒子的波动方程

与经典波相似，自由粒子波函数分别对时间、空间求偏导，可以得到其满足的波动方程：$\Psi(x,t)=Ae^{i(kx-\omega t)}$

$$\frac{\partial^2\Psi}{\partial x^2}=-k^2\Psi(x,t),\quad \frac{\partial\Psi}{\partial t}=\frac{E}{i\hbar}\Psi(x,t)$$

或$E\Psi(x,t)=i\hbar\frac{\partial\Psi}{\partial t}$

考虑到：$E=\frac{(\hbar k)^2}{2m}$，有

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)$$

自由粒子的波动方程

非自由粒子的波函数

◆对非自由粒子，由于受外场作用，其波函数与自由粒子的不同。

◆一般情况下，是一个坐标与时间的函数$\Psi(x, y, z, t)$，但具体形式要根据具体问题来确定。

◆用波函数描述微观粒子的状态，这是量子力学的基本假设之一，这种新的描述方法，充分体现了粒子的波粒二象性。

非自由粒子的波动方程

非自由粒子受到势场作用，其波函数$\Psi(x,t)$的形式与具体的势场有关，其满足的波动方程应加势能项：

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x,t)\right]\Psi(x,t)$$

三维情况下，波动方程变为：

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r},t)\right]\Psi(\vec{r},t)$$

薛定谔方程是量子力学的基本方程

类比牛顿第二定律在宏观的作用

经典力学与量子力学的对比

	经典力学	量子力学
特点	粒子性	波粒二象性
状态描述	坐标和动量	波函数
运动方程	牛顿方程 $\frac{d\vec{p}}{dt}=m\frac{d^2\vec{r}}{dt^2}$	薛定谔方程 $i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r},t)\right]\Psi(\vec{r},t)$
联系	$E\rightarrow i\hbar\frac{\partial}{\partial t}$	$\vec{p}\rightarrow -i\hbar\nabla$

定态薛定谔方程

当势能项U不依赖于时间时，我们可以根据平面波波函数的形式$\Psi(x,t)=Ae^{i(kx-\omega t)}$，猜测（ansatz）

$$\Psi(x,t)=\psi(x)e^{-i\omega t}$$

$e^{-i\omega t}$ → 不依赖于空间

$\psi(x)$ → 不依赖于时间

满足定态薛定谔方程

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+U(x)\psi(x)=E\psi(x)$$

波函数$\psi(x)$：单值、有限、连续、可归一

Ansatz

is an educated guess or an additional assumption made to help solve a problem, and which may later be verified to be part of the solution by its results.

$$y''(x) + 2y'(x) + 3y(x) = x^3$$

假设

$$y(x) = ax^3 + bx^2 + cx + d$$

代入上式求解系数a, b, c, d

定态薛定谔方程

解出定态波函数$\psi(x)$后可得总波函数为：

$$\Psi(x,t)=\psi(x)e^{-i\omega t}$$

概率密度为

$$|\Psi|^2=\Psi^*\Psi=\psi^* e^{iEt/\hbar}\psi e^{-iEt/\hbar}=\psi^*\psi=|\psi|^2$$

概率密度与时间无关

即在定态下概率分布不随时间改变，这正是定态这一名称的由来。

定态薛定谔方程的意义：$-\frac{\hbar^2}{2m}\nabla^2\psi+U\psi=E\psi$

对波函数进行某种运算或作用的符号称为算符。

若$H\psi=\lambda\psi$，则ψ是算符H的本征函数，数值λ称为算符 H 的本征值，$H\psi=\lambda\psi$称为算符H的本征方程。因此，定态薛定谔方程也称为哈密顿算符的本征方程，或能量算符的本征方程。

利用薛定谔方程，再加上波函数标准条件，可以“自然地”得到微观粒子的重要特征—量子化结果，而不须象普朗克假设那样强制假定量子化。薛定谔方程的结果，已被无数实验所证实。

态叠加原理

如果$\psi_1,\psi_2,\cdots,\psi_n$等都是体系的可能状态或称基矢，那么，它们的线性叠加态也是这个体系的一个可能状态。

即

$$\Psi = C_1\psi_1 + C_2\psi_2 + \cdots + C_n\psi_n$$

其中的系数$C_1, C_2, \ldots, C_n$ 为复数，它们模平方是在对应态粒子出现的概率。

它们满足：

$$1 = \sum_n C_n^2$$

为什么波函数用复数表示

考虑定态薛谔方程$(E-H)\Psi=0$，其中$H=T+V$

通过变换可得$(E-T)\Psi=V\Psi$

当$E<0$时，$\Psi=\dfrac{1}{E-T}V\Psi$

当$E>0$时，$\Psi=\lim\limits_{\epsilon->0}\dfrac{1}{E-T+i\epsilon}V\Psi$

总结

德布罗意关系式：$E = h\nu$ and $p = h/\lambda$

德布罗意对角动量量子化的解释：局域内的波函数⇒波长的量子化⇒角动量的量子化

戴维孙-革末实验：物质波的第一个证据

波函数的统计解释：$|\Psi|^2 =$ 概率密度

正弦波的参数：$\lambda = 2\pi/k, \quad \nu = \omega/2\pi = 1/T, \quad v = \lambda\nu$

ω和k表达下的德布罗意关系：$E = \hbar\omega, \quad p = \hbar k$

波包：在某个有限区域之外为零（或极小）的波

总结

波函数的性质以及归一化：$\int_{\Omega} |\Psi|^2 dV = 1 \quad (\Omega -$ 全空间 $)$

不确定性关系：

$$\Delta x \Delta k \geq 1/2, \quad \Delta t \Delta \omega \geq 1/2$$

$$\Delta x \Delta p \geq \hbar/2, \quad \Delta t \Delta E \geq \hbar/2$$

不确定性原理的统计学解释：$\sigma \equiv \sqrt{E[X^2] - (E[X])^2}$

经典力学与量子力学的对比：特点，状态描述，运动方程，联系