量子力学

王 治 国

同济大学

“人们实在应该为量子力学的成功而感到羞愧，因为它是根据耶稣的格言‘不可让你的左手知道你的右手所做的事的’而获得的。”——爱因斯坦（1919年6月4日给M.玻恩的信）


NIELS BOHR INSTITUTET
1920

波函数是量子力学的基本概念，薛定谔方程是量子力学的核心表达。

本章在与经典力学的质点轨道图像相对比的基础上，

- 引入描述微观粒子运动状态的波函数
- 及描述状态演化规律的薛定谔方程；
- 并详细讨论波函数的性质。

引言

- 任何粒子都是物质波（Any particle is a matter wave） -- 波函数（*wave function*）
- 如何计算这个波函数（How to calculate this wave function）
- 从这个波函数中提取信息是量子力学(或波动力学)的课题。*Extract information* from this wave function is the subject of quantum mechanics (or wave mechanics).

猜测

- 第一步：定义状态描述的波函数
- 第二步：定义物理量，将之与状态波函数相联系。
- 第三步：给出一个控制物质波行为的运动方程。计算各种物理量的表现。

这种非相对论性粒子的物质波波动方程是由Schrödinger在1926年(1933年诺贝尔奖)首次提出的。

表述一种物理理论的方法

(1) 选择有关理论所必需的某些物理概念（selecting certain physical concepts which are essential to the theory concerned）；

(2) 选择一类数学结构（selecting a class of mathematical structures）；

(3) 用选定的数学结构类的理论中的概念来表示选定的物理概念（representing the selected physical concepts in terms of concepts in the theory of the selected class of mathematical structures）。

物理系统，状态，物理量

physical system, state, physical quantities

物理学的基础是实验观察和测量过程，包括用数字表征现实的各个方面，即我们观察到的东西。现实的这些方面被阐述成物理量的概念(例如，速度、能量、电强度等)。The foundation of physics is experimental observation and the measurement process that consists of characterizing aspects of reality, namely what we observe, by numbers. These aspects of reality are elaborated into concepts of physical quantities (for instance, velocity, energy, electric intensity, etc.).

方法论（Methodology）

我们的理论结构有以下要素，我们在**牛顿力学的经典案**例中描述了一个**大质量粒子在力场**——我们假设它来源于势能$V(\boldsymbol{r})$中的作用。

1. 我们必须首先描述系统的状态。这意味着与此状态关联一个从操作角度定义它的数学表示。在牛顿的理论中，空间中一个大质量粒子在时刻t的状态用六个数字来描述;它的位置$\boldsymbol{r}$和速度$\boldsymbol{v}$，或者它的动量$\boldsymbol{p} = m\boldsymbol{v}$.

2. 然后，我们必须知道**在给定条件下控制系统状态时间演化的规律**；也就是说，给定时刻t = 0的状态，我们必须能够预测时刻t的状态。在牛顿的理论中，动力学的基本定律$d\boldsymbol{p}/dt=\boldsymbol{f}$，使我们能够计算轨迹。

3. 其次，我们必须知道使我们能够**计算物理量测量结果的定律**，这些定律**将系统状态的数学表示转化为可测量的数字。**在牛顿的理论中，物理量是状态变量$\boldsymbol{r}$和$\boldsymbol{p}$的函数。

经典物理学:**因果关系或决定论**

classical physics：causality or determinism

"将这些概念结合成事件因果链的单一图景是经典力学的本质"。

"the combination of these concepts into a single picture of a causal chain of events is the essence of classical mechanics".

“在牛顿力学中，一个物质系统的状态是由它们的瞬时位置和速度来定义的，根据众所周知的简单原理，仅仅从系统在给定时间的状态和作用在物体上的力的知识中，就可以推导出系统在任何其他时间的状态。这种显然代表着一种由决定论概念所表示的因果关系的理想形式的描述，其范围更为广泛。因此，在描述电磁现象时，我们必须考虑有限速度的力的传播，如果在状态的定义中不仅包括带电体的位置和速度，而且包括给定时间空间中每一点上的电磁力的方向和强度，就可以维持一种确定性的描述。"

物体可以看作是一个严格定域的粒子，也可以看作是一个在空间中扩展的场，它随时间的变化完全归因于粒子沿着一条确定的路径运动，或者更抽象地说，归因于空间中每一点场强的时间变化。

"经典物理理论的形象化描述代表了一种理想化"

"that the pictorial description of classical physical theories represents an idealization"

“在经典物理学的框架内，对测量仪器的描述和对研究对象的描述在原则上是没有区别的。”

"within the frame of classical physics, there is no difference in principle between the description of the measuring instruments and the objects under investigation "

“在经典物理学的范围内，我们正在处理一种理想化，根据这种理想化，所有现象都可以任意细分，相互作用……”

"within the scope of classical physics we are dealing with an idealization, according to which all phenomena can be *arbitrarily subdivided*, and the interaction . . ."

量子现象的基本条件
The essential conditions for a quantum phenomenon

然而，量子力学说：**物理量具有基本单元，不能无限细分**！

量子假设：**每一种量子现象都具有一个在经典物理学中从未出现过的整体性或个体性的特征，并以普朗克作用量子为代表。**

Quantum postulate. Every quantum phenomenon has a feature of wholeness or individuality which never occurs in classical physics and which is symbolized by the Planck quantum of action.

"**测量只能意味着**将被研究对象的某些特性与作为测量工具的另一个系统的相应特性进行明确的比较"

"a measurement can mean nothing else than the unambiguous comparison of some property of the object under investigation with a corresponding property of another system, serving as a measuring instrument"

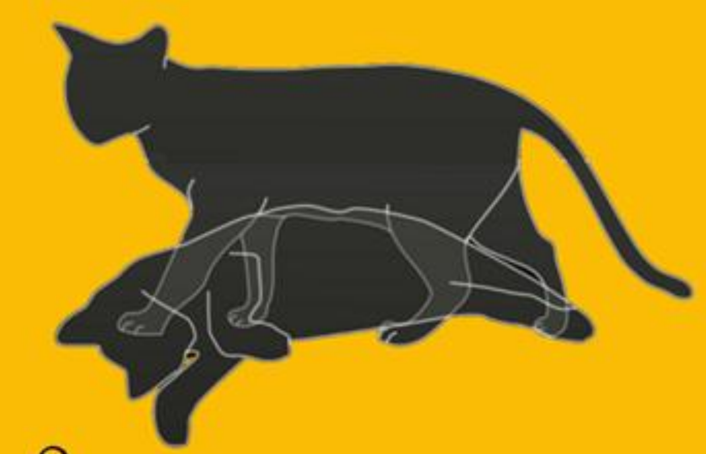
4. 在量子力学中，我们必须解决牛顿理论中没有的一个问题：**测量过程的结果是什么？测量之后我们知道什么？**

Chapter 1 The wave function

- 1 The Schrödinger Equation
- 2 The Statistical Interpretation
- 3 Probability
- 4 Normalization
- 5 Momentum
- 6 The Uncertainty principle
- 7 Brief Review

Chapter 1 The wave function

- 1.1 The Schrödinger Equation

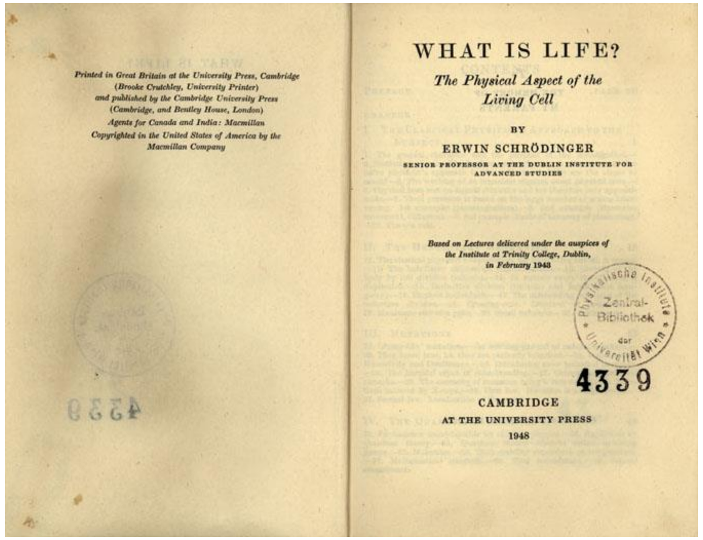


$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \hat{H}\Psi(\mathbf{r},t)$$

1888

1915

1920



1 The Schrödinger Equation in One Dimension

- The Schrödinger equation of the particle

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi$$

- **imaginary number *i***. ——Ψ is generally a complex function of *x* and *t*.
- Time-dependent Schrödinger equation (TDSE) is a partial differential equation for the function Ψ(*x*,*t*). **If Ψ(*x*,0) is known, TDSE determines Ψ(*x*,*t*) at any later time *t* （因果律）.**

- $\hbar=\dfrac{h}{2\pi}=1.054572\times10^{-34}\,\mathrm{J\ s}$

- **Schrödinger equation is *not* derivable**
- It is one of **the laws of quantum physics** (c.f. Newton's laws in classical mechanics).
- As with any law, its "correctness" is tested by the agreement of its predictions with experiment.
- In the approximately 100 years since it was first published in 1926, it has passed such test repeatedly.

- According to the de Brogile relations,

$$k = \frac{p}{\hbar}, \text{and } \omega = \frac{E}{\hbar}$$

- Take $\Psi(x,t)=Ae^{i(kx-\omega t)}$, and consider,
- The crucial link here is the correspondence between E and p and the *operators*:

Original physical quantities
$$\mathrm{E} \rightarrow i\hbar\frac{\partial}{\partial t}$$
$$p \rightarrow -i\hbar\frac{\partial}{\partial x}$$
Mathematical form of operators

- An *operator* is a mathematical procedure (here is a partial differentiation) to be performed on whatever function that follows the operator (here is the wavefunction).
- You will find the Schrödinger equation of a free particle is $E = p^2/2m$
- Consider a particle acted upon by a conservative force

$$F(x) = -\frac{dV(x)}{dx}$$

- Then the energy of the particle is the sum of kinetic and potential energies

$$E = \frac{p^2}{2m} + \mathrm{V}$$

- Assume one can use a wavefunction Ψ to represent such particle. (we don't need to know the exact functional form of Ψ)
- Multiply both sides of $E = \frac{p^2}{2m} + V$ by Ψ, Replace E and p by its corresponding operators,

$$E\Psi \rightarrow \left(i\hbar\frac{\partial}{\partial t}\right)\Psi = E\Psi$$

$$p^2\Psi \rightarrow \left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi = -\hbar^2\frac{\partial^2}{\partial x^2}\Psi$$

We will recover the 1D TDSE

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

1.2 The Schrödinger Equation in Three Dimension

$$p_x \to -i\hbar\frac{\partial}{\partial x},\ p_y \to -i\hbar\frac{\partial}{\partial y},\ p_z \to -i\hbar\frac{\partial}{\partial z}$$

$$\vec{p} \to -i\hbar\nabla$$

(3-D) Schrödinger's equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

- Every *measurable* physical quantity in classical mechanics has a corresponding operator in quantum mechanics.
- – Energy, or the Hamiltonian: $H \rightarrow \widehat{H} = i\hbar\frac{\partial}{\partial t}$, $\hat{H}$ is the *Hamiltonian* operator.
- – Momentum:
- $p_x \rightarrow \hat{p}_x = -i\hbar\frac{\partial}{\partial x}, p_y \rightarrow \hat{p}_y = -i\hbar\frac{\partial}{\partial y}, p_z \rightarrow \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$ or $\vec{p} \rightarrow \hat{\vec{p}} - i\hbar\nabla$
- – Position: $x \rightarrow \hat{x} = x$
- which is simply multiplying *x* to the function that follows the operator, similar procedure for *y* and *z*.
- – Potential energy: $\mathrm{V}(x,t) \rightarrow \hat{V} = V(\hat{x},t) = V(x,t)$
- – Kinetic energy: $T = \frac{p^2}{2m} \rightarrow \hat{T} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi$$

At this point, our real problem is to become familiar with this new concept of a wave function. We want to understand its structure, its properties. We want to understand why we need a whole function in order to describe the state of a particle, whereas for Newton six numbers were sufficient.

现在，我们真正的问题是熟悉波函数的新概念。我们想了解它的结构和性质。我们想要理解为什么我们需要一个完整的函数来描述一个粒子的状态，而对于牛顿来说，六个数字就足够了。

square root of minus one

rate of change

quantum wavefunction

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi$$

Planck's constant

with respect to time

Hamiltonian operator

Song of schrodinger equation

Schrodinger equation is the law of Quantum mechanics,

Don't try to deduce it from Newton's law;

It has the same position as Newton's laws in Classical theory;

For a particular system, it give out a wave function,

Wave function, wave function, what does it mean?

its norm represents the probability for finding the particle for anywhere.

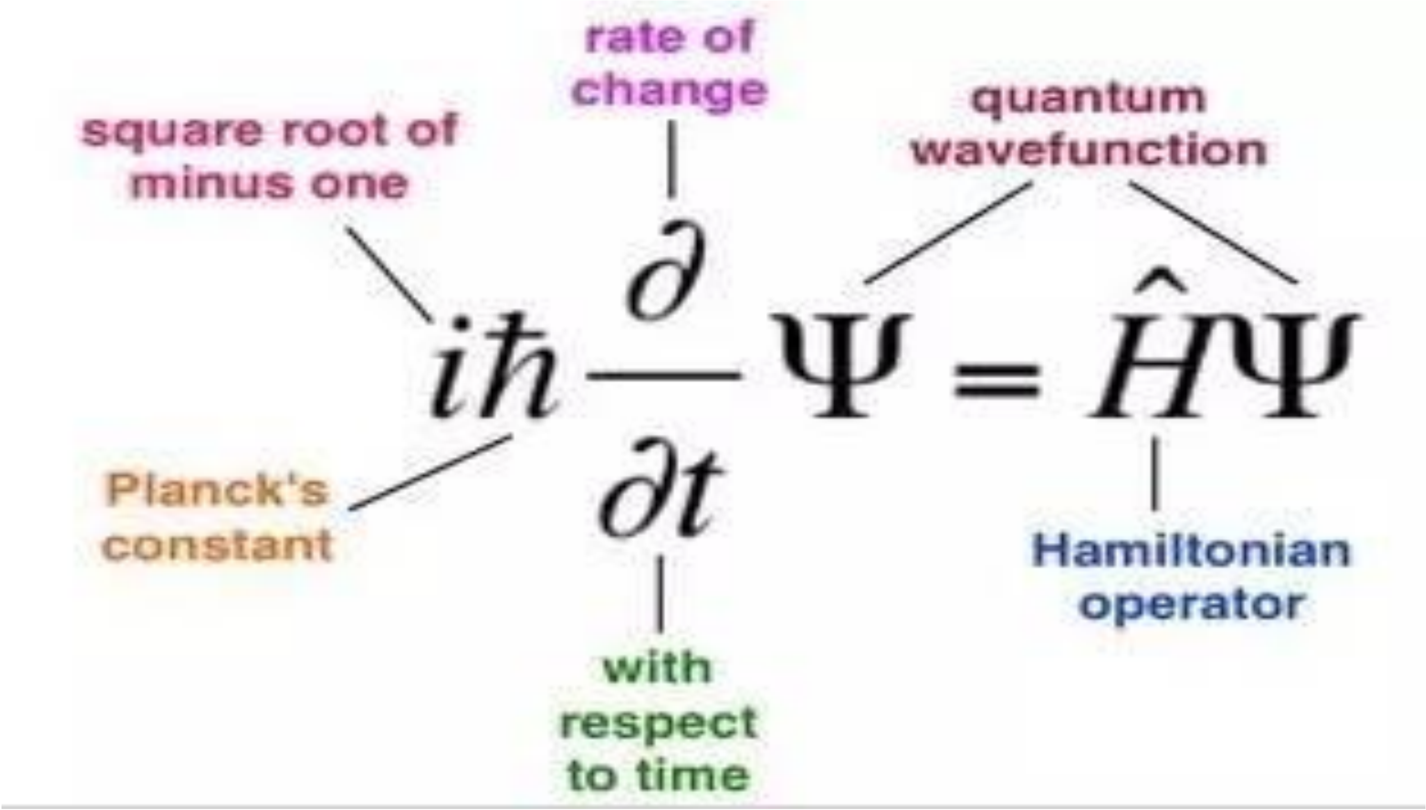
When you have the wavefunction, you know the everything of the world.

The magic of quantum mechanics, magic wave function,

The secret of the universe is inside!

波函数的统计解释

- **1. 2 The Statistical Interpretation**



波动力学的状态描述方式

微观物体运动状态的描述：**波函数**

运动规律的描述：**薛定谔方程**

薛定谔曾断言，ψ在一定程度上反映电子的位置，可看作是一种"影子"波。后来他改变主意，说ψ是电子的电荷密度。他完全陷入了迷途困境。

Max Born，1882—1970

1954年诺贝尔物理学奖

玻恩和波函数的概率解释

玻恩在1926年夏天抛弃了传统物理的因果关系，写了一篇关于碰撞现象的文章，引入了量子力学概率的概念。说到碰撞

“One does not get an answer to the question, What is the state after collision? but only to the question, How probable is a given effect of the collision? From the standpoint of our quantum mechanics, there is no quantity which causally fixes the effect of

“没有人知道碰撞后的状态是什么?但可以回答碰撞的概率是多少？从量子力学的观点来看，没有哪个量可以因果地确定一个事件中碰撞的影响。”

用“概率”观点认识和描述微观世界是物理学的一种进步，是物理思想的一个升华。对于微观粒子运动状态的刻画必须放弃确定性的轨道图像，采用概率的方法（即统计的方法）这样的描述与经典物理学的严格因果律是不相容的，不过玻恩在1926年发布一句名言“粒子的运动遵守概率定律，但概率本身还是受因果律支配的。”这一概述将概率与因果律统一起来，使波函数的统计解释纳入了经典物理学的思路。

“对于一个从状态n散射到状态m的电子而言，ψ代表概率幅度。”

“对它进行平方再取绝对值就成为相应粒子出现(或电荷密度)的 物理概率 ”

玻恩和波函数的概率解释

玻恩引入一个新概念——确定量子态出现的概率：

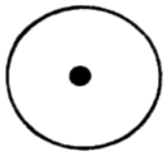
一个状态存在的概率由单个归一化波函数振幅平方来确定。

德布罗意波是概率波：波函数本身无直接物理含意。波函数模的平方是某一时刻粒子在空间某点附近出现的概率密度。

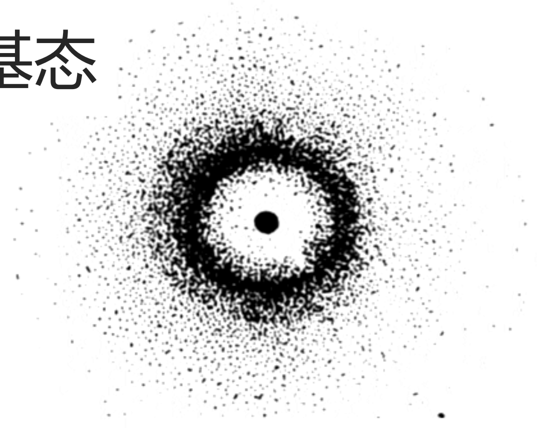
粒子出现在空间某点附近体积元dV内的概率:

$$|\Psi|^2 dV = \Psi\Psi^* dV$$

氢的基态



按照玻尔



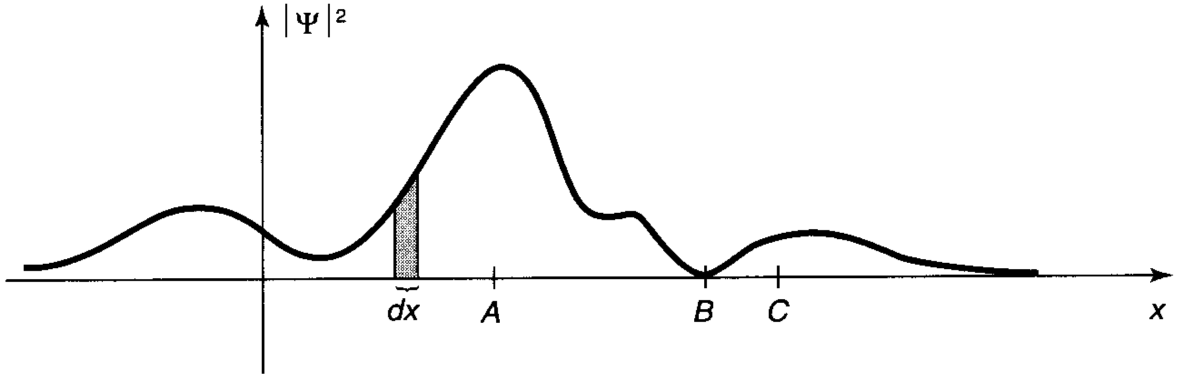
按照玻恩

Schrodinger and Born understood in 1926 that the complete description of a particle in space at time t is performed with a complex wave function ψ(r,t), whose physical interpretation is that the probability dP(r) to find the particle in a vicinity d^3r of the point r is given by

$$dP(r)=|\psi(r,t)|^2 d^3r$$

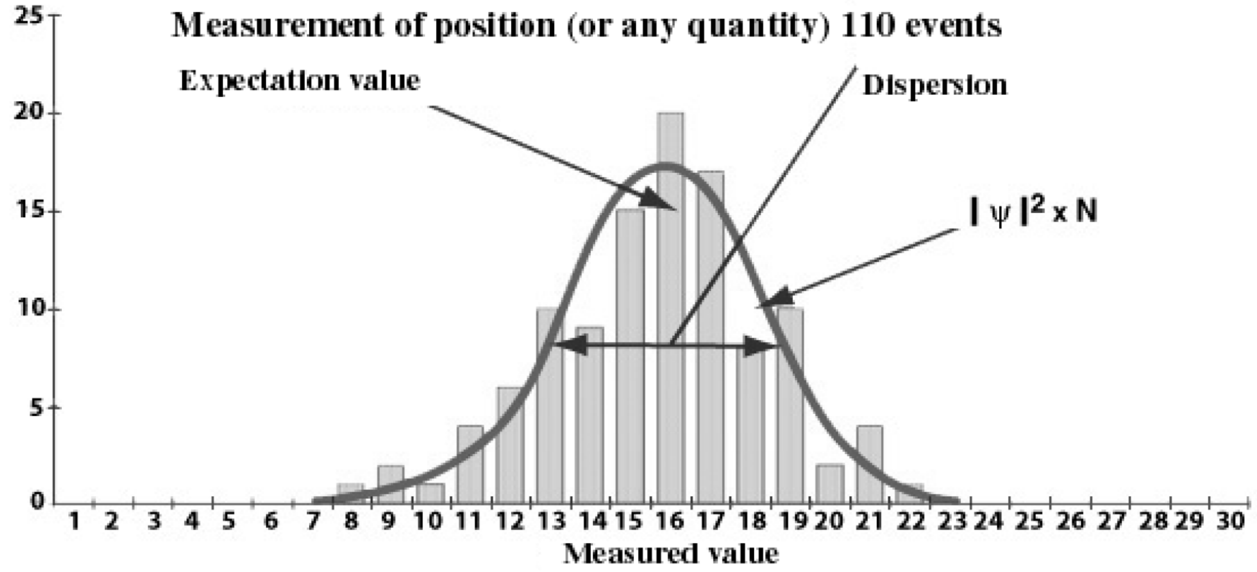
Total probability of finding particle between positions *a* and *b* is

$$\sum_{x=a}^{b} |\Psi(x,t)|^2 \, \delta x \xrightarrow[\delta x \to 0]{} \int_a^b |\Psi(x,t)|^2 \, dx$$



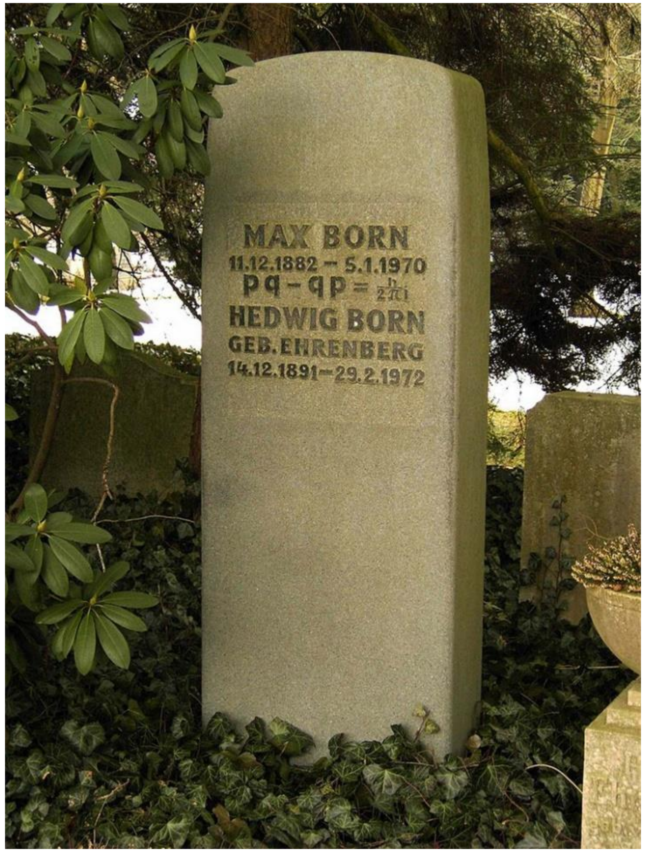
$$\int |\psi(\boldsymbol{r},t)|^2 \, d^3r = 1$$

The meaning of this description is the following. We prepare N atoms independently, in the same state, so that, when each of them is measured, they are described by strictly the same wave function. Then the result of a position measurement is for each of them as accurate as we wish (limited by the accuracy of the measuring apparatus) but is not the same for all. The set of impacts is distributed in space with the probability density $|\psi(r,t)|^2$.



玻恩和波函数的概率解释

- 波函数是什么呢？ $W \propto |\Psi|^2 = \Psi\Psi^*$ 概率密度！
- 物质波是什么呢？物质波既不是机械波，又不是电磁波，而是几率波！
- 波函数本身没有物理含义！
- 对微观粒子，讨论其运动轨道及速度是没有意义的。波函数所反映的只是微观粒子运动的统计规律。



玻恩和波函数的概率解释

经典波	微观粒子几率波
描述某物理量在空间分布的周期变化	微观粒子某力学量的几率分布
波幅增大一倍，相应能量为原来四倍，成另一状态	微观粒子在空间出现的几率只决定于波函数在空间各点的相对强度，增大波幅不改变粒子在空间各点出现的几率
附加相因子$e^{i\delta}$改变状态	相因子$e^{i\delta}$不会引起状态改变

波函数要求

- 单值：一定时刻，在空间某点附近，单位体积内，粒子出现的几率应有一定的量值.
- 连续、有限　　（保证其平方可积）
- 归一化　　$W=\int dW=\int |\Psi|^2 dV=1$

波函数要求

量子力学公理：

对于一个微观体系，它的任何一个状态都可以用一个坐标和时间的连续、单值、平方可积的函数Ψ来描述。Ψ是体系的状态函数，它是所有粒子的坐标函数，也是时间函数。$\Psi^*\Psi d\tau$为时刻t在体积元$d\tau$内出现的概率。Ψ是归一化的：$\int\Psi^*\Psi d\tau=1$式是对坐标的全部变化区域积分。

- It is important to note that $\Psi(x,t)$ itself is *NOT* a measurable quantity; only $|\Psi(x,t)|^2$ is measurable, which is the *probability density* for finding the particle at point x and time t.
- This probability wave is to be contrasted with typical waves encountered in classical mechanics. For example, consider transverse waves in a string; the wavefunction $y(x,t)$ is the displacement of the string at position x and time t and is a measurable quantity.

- An important consequence is that $\Psi(x,t)$ in quantum mechanics can be, and is generally, a *complex* function of x and t. Of course, $|\Psi(x, t)|^2$ is always **real**, as it should be.

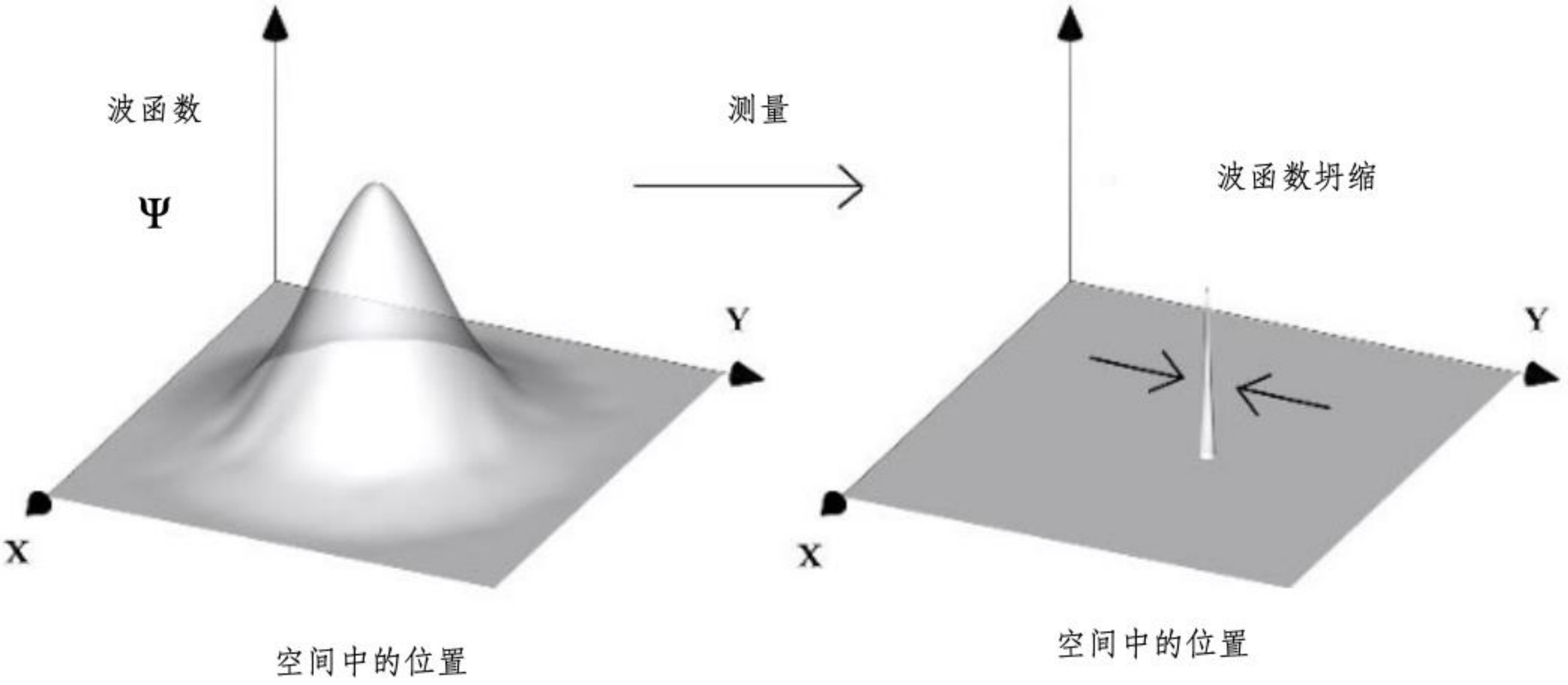
- The statistical interpretation introduces a kind of indeterminacy into quantum mechanics.

- Even you know everything about the particle, you still cannot predict its position.

- All quantum mechanics has to offer is statistical information about the possible results.

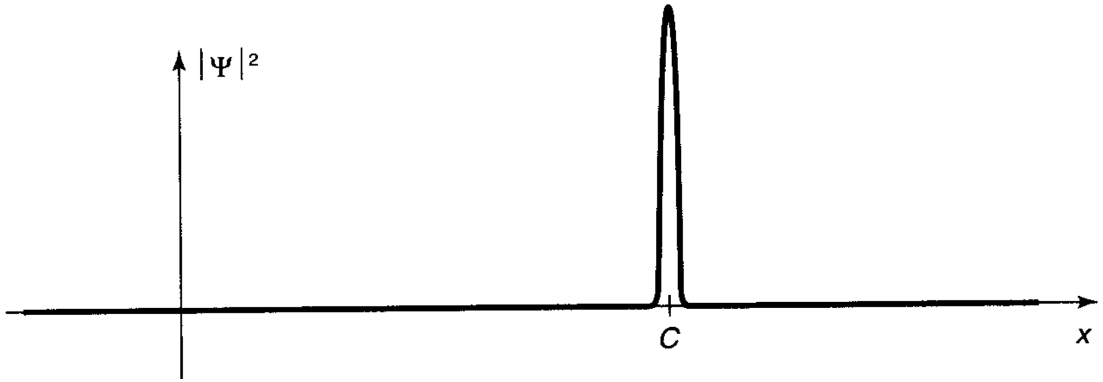
- Suppose I do measure the position of the particle, and I find it to be at the point C. Question: Where was the particle just before I made the measurement?
- **Three plausible answers:**
- 1. The realist (现实主义者) position: The particle was at C.
- 2. The orthodox (传统的) position: The particle wasn't really anywhere. (the so-called Copenhagen interpretation is associated with Bohr and his followers)
- 3. The agnostic (不可知论者) position: Refuse to answer.
- 1964 John Bell confirmed the **orthodox interpretation**: A particle does not have a precise position prior to measurement.

哥本哈根诠释



自哥白尼以来，量子物理学首次将人类思维重新恢复到物理学的中心地位。甚至有人认真地提出，要想从量子世界中出现正常的物理现实，人类的意识是必不可少的。

阐明了测量对于理解量子物理如何引导我们的世界经验确实是至关重要的。



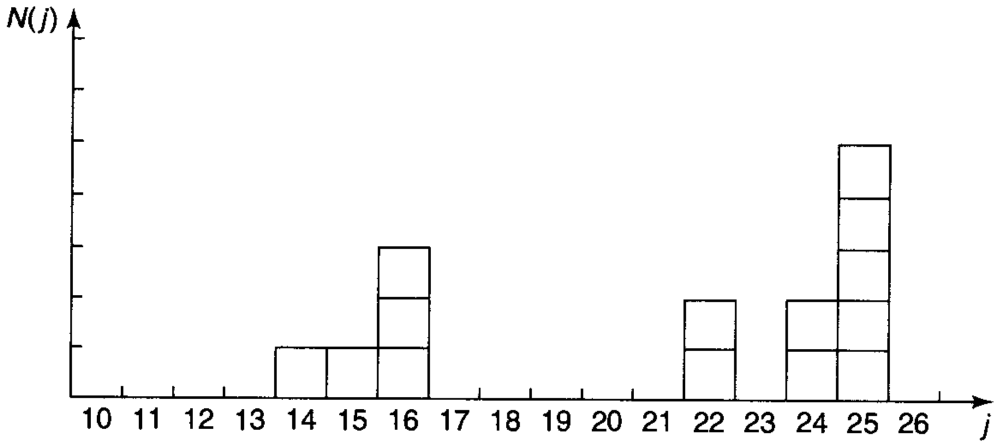
Collapse of the wave function: graph of $|\Psi|^2$ mmediately after a measurement has found the particle at point C.

- Then, two entirely distinct kinds of physical processes:
- "ordinary" ones, in which the wave function evolves under the Schrodinger equation,
- "measurements", in which Ψ suddenly and discontinuously collapses.

- If I made a second measurement, immediately after the first? Would I get C again, or new position?
- Everyone is in agreement: A repeated measurement (on the same particle) must return the same value.
- **orthodox interpretation**: the **wave function collapses upon measurement**, to a spike at the point C (it soon spreads out again, in accordance with the Schrodinger equation, so the second measurement must be made quickly).

- **3 Probability**

3.1 Discrete variables



Histogram showing the number of people, N(j), with age j.

$$N = \sum_{j=0}^{\infty} N(j)$$

the probability $$P(j) = N(j)/N$$

all the probabilities $$\sum_{j=0}^{\infty} P(j) = 1$$

1. The average (or mean) value: $\langle j \rangle = \sum_{j=0}^{\infty} jP(j)$
2. Most probable value: whereas P(j) is a maximum.
3. The median value : the probability of getting a larger result is the same as the probability of getting a smaller result.

- Notice that there need not be anyone with the average age or the median age.
- In quantum mechanics the average is usually called the expectation value. It's a misleading term, since it suggests that this is the outcome you would be most likely to get if you made a single measurement (that would be the most probable value, not the average value.

- The average of the squares

$$\langle j^2 \rangle = \sum_{j=0}^{\infty} j^2 P(j)$$

- In general, the average value of some function of j is given by

$$\langle f(j) \rangle = \sum_{j=0}^{\infty} f(j) P(j)$$

- Each individual deviates from the average, $\Delta j = j - \langle j \rangle$

$$\langle \Delta j \rangle = \sum_{j=0}^{\infty} (j - \langle j \rangle) P(j) = \sum_{j=0}^{\infty} j P(j) - \sum_{j=0}^{\infty} \langle j \rangle P(j) = \langle j \rangle - \langle j \rangle = 0$$

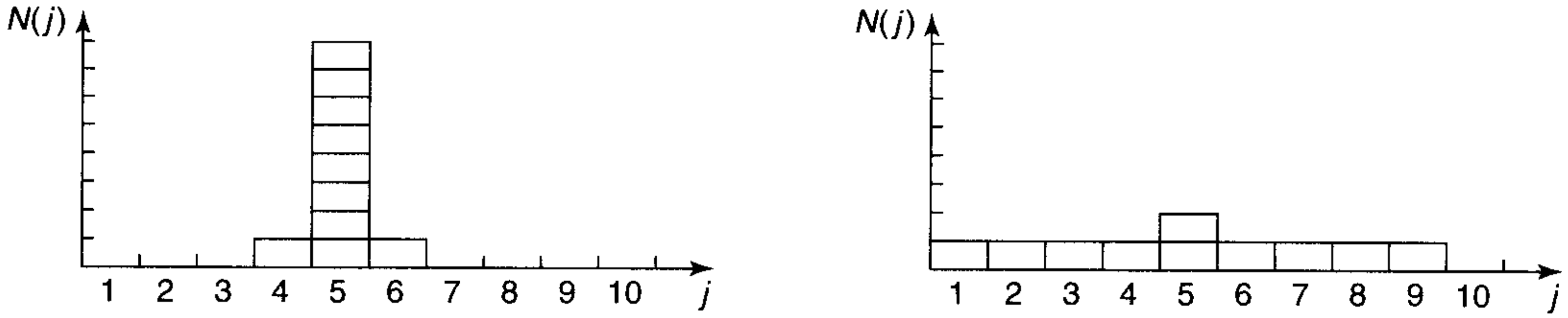
- Standard deviation

$$\sigma^2 \equiv \langle (\Delta j)^2 \rangle$$

$$\sigma^2 \equiv \langle (\Delta j)^2 \rangle = \sum_{j=0}^{\infty} (\Delta j)^2 P(j) = \sum_{j=0}^{\infty} (j - \langle j \rangle)^2 P(j) = \sum_{j=0}^{\infty} (j^2 - 2j\langle j \rangle + \langle j \rangle^2) P(j)$$

$$= \sum_{j=0}^{\infty} j^2 P(j) - 2\langle j \rangle \sum_{j=0}^{\infty} j P(j) + \langle j \rangle^2 \sum_{j=0}^{\infty} P(j) = \langle j^2 \rangle - 2\langle j \rangle\langle j \rangle + \langle j \rangle^2 = \langle j^2 \rangle - \langle j \rangle^2$$

$$\boldsymbol{\langle j^2 \rangle \geq \langle j \rangle^2}$$



Two histograms with the same median, same average, and same most probable value, but different standard deviations.

2. 2 continuous Variables

If the interval is sufficiently short, the probability is proportional to the length of the interval.

$$\text{probability that individual (chosen at random)lies between } x \text{ and } (x + dx) = \rho(x)dx$$

The proportionality factor,$\rho(x)$ is called probability density.

The *probability* of finding the particle in any finite interval $a \leq x \leq b$ is

$$\int_a^b \rho(x)dx$$

Thus, we have the result that

$$\int_{-\infty}^{+\infty} \rho(x)dx = 1,$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} x\rho(x)dx\,,$$

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} f(x)\rho(x)dx\,, \qquad \sigma^2 \equiv \langle (\Delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

Example 1.1 Suppose I drop a rock off a c1iff of height *h*. As it falls, I snap a million photographs, at random intervals. On each picture I measure the distance the rock has fallen. Question: What is the average of all these distances? That is to say, what is the time average of the distance traveled?

Solution: The rock starts out at rest, and picks up speed as it falls; it spends more time near the top, so the average distance must be less than h /2. Ignoring air resistance, the distance x at time t is

$$x(t) = \frac{1}{2}gt^2$$

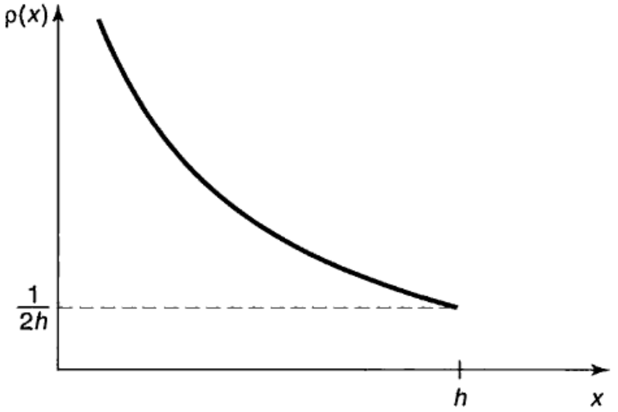
The velocity is $\frac{dx}{dt} = gt$, and the total flight time is $T = \sqrt{2h/g}$.

The probability that the camera flashes in the intervals dt is $\frac{dt}{\mathrm{T}}$, so the probability that a given photograph shows a distance in the corresponding range dt is

$$\frac{dt}{T} = \frac{dx}{gt}\sqrt{\frac{g}{2h}} = \frac{1}{2\sqrt{hx}}dx$$

Evidently the probability *density* $\rho(x) = \frac{1}{2\sqrt{hx}}, \quad (0 \le x \le h)$

We can check this result satisfying the normalization



$$\int_0^h \frac{1}{2\sqrt{hx}}dx = \frac{1}{2\sqrt{h}}(2\sqrt{x})|_0^h = 1$$

The average distance is

$$\langle x \rangle = \int_0^h x\frac{1}{2\sqrt{hx}}dx = \frac{1}{2\sqrt{h}}\left(\frac{2}{3}x\sqrt{x}\right)|_0^h = \frac{h}{3}$$

problem 1.3

1.4 归一化（Normalization）

- With the wave function Ψ, the probability density of finding the particle at point x, at time t is $|\Psi|^2$, then the *probability* of finding the particle in any finite interval $a \le x \le b$ is

$$P = \int_a^b |\Psi(x,t)|^2 \, dx$$

- Thus, we have the result that

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

- This is called the *normalization* condition and a wavefunction satisfying this is said to be *normalized*.

1. The wave function is supposed to be determined by the Schrodinger equation.
2. We can't impose an extraneous condition on Ψ.
3. If $\Psi(x, t)$ is a solution of Schrodinger equation, so too is $A\Psi(x, t)$, where A is any (complex) constant.
4. Then, we pick this undetermined multiplicative factor so as to ensure the normalization satisfied.
5. This process is called normalizing the wave function.

1. For some solutions to the Schrodinger equation, the integral is infinite; in that case no multiplicative factor is going to make it 1. The same goes for the trivial solution $\Psi = 0$. Such non-normalizable solutions cannot represent particles, and must be rejected.
2. Physically realizable states correspond to the "square-integrable" solutions to Schrodinger's equation.
3. Suppose the wave function is normalized at time $t = 0$. How do I know that it will stay normalized, as time goes on and Ψ evolves?

The Schrodinger equation has the property that it automatically preserves the normalization of the wave.

Proof：

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x,t)|^2 dx = \int_{-\infty}^{+\infty}\frac{\partial}{\partial t}|\Psi(x,t)|^2 dx$$

$$\frac{\partial}{\partial t}|\Psi(x,t)|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^*\frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t}\Psi$$

Since

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi, \qquad \frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*$$

So

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

$$\frac{\partial}{\partial t}\rho + \nabla\cdot\vec{j} = 0 \quad \left(\vec{j} = -\frac{i\hbar}{2m}(\Psi^*\nabla\Psi - \nabla\Psi^*\Psi)\right)$$

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x,t)|^2 dx = \frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\Big|_{-\infty}^{+\infty}$$

But $|\Psi(x,t)|^2$must go to zero as $x \to \pm\infty$ --otherwise the wave function would not be normalizable. It follows that

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x,t)|^2 dx = 0$$

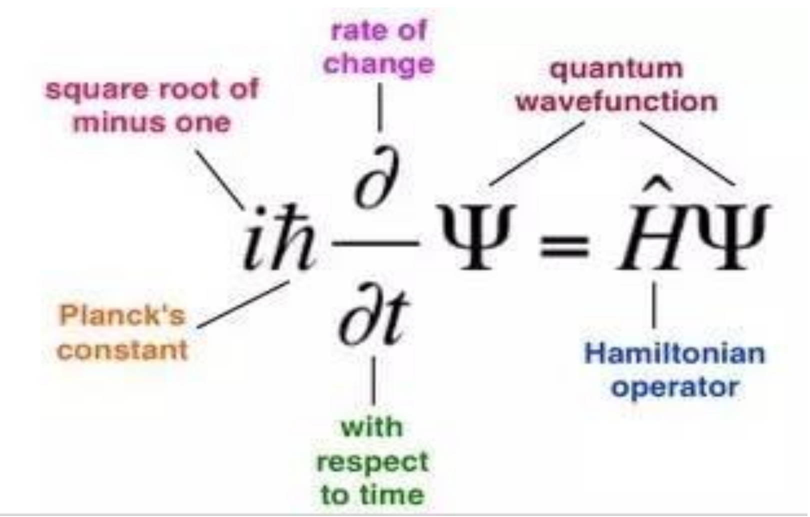
Then if $|\Psi|^2$ is normalized at t = 0, it stays normalized for all time.

The **wavefunction** must:

1. Be a continuous and single-valued function of both *x* and *t* (in order that the probability density be uniquely defined)
2. Have a continuous first derivative (unless the potential goes to infinity)
3. Have a finite normalization integral.

- **Problem 1.4**
- **Problem 1.5**

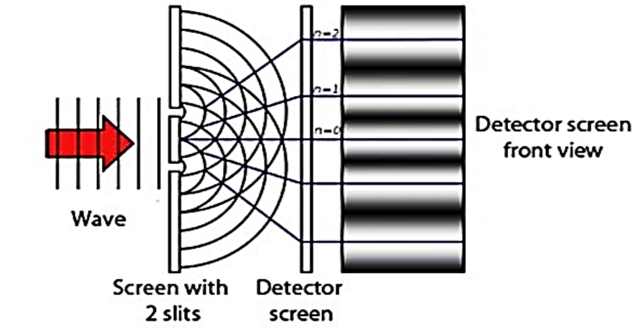
分析：态叠加原理（**Superposition principle**）



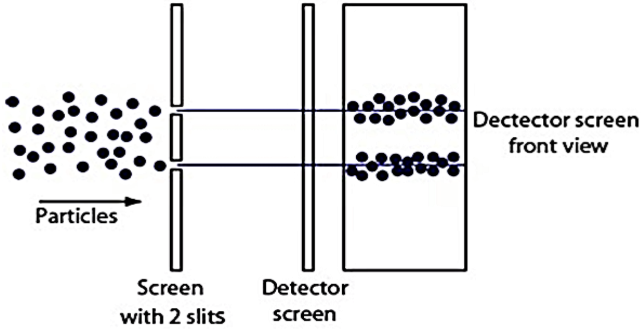
$$P = \int_a^b |\Psi(x,t)|^2\, dx$$

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

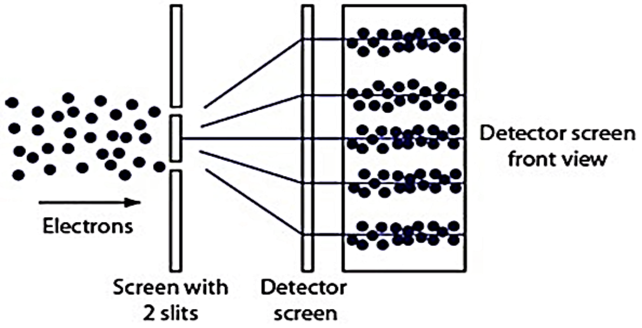
双缝实验



- 波的干涉图案



- 预期粒子穿过狭缝后形成的图案



- 电子穿过狭缝后实际图案——干涉图案

电子在到达光屏时被认为是粒子？！

- 微观粒子的波粒二象性隐含其满足态迭加原理

$$\Psi = \alpha\psi_1 + \beta\psi_2$$

- 迭加原理：干涉、衍射的物理机制

- 线性迭加 若体系具有一系列互异的可能状态 $\{\Psi_1, \Psi_2, \cdots\}$，则 $\Psi = C_1\Psi_1 + C_2\Psi_2 + \cdots$ 也是可能的状态。

If a measurement of the observable corresponding to the operator A is made on the normalized quantum state ψ, given by,

$$\Psi = \sum_n c_n \psi_n$$

$$\sum_n |c_n|^2 = 1$$

› 几率波的特性

$\{c_n\}$的含义、归一化

$\psi_p = A e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}$ 情况、相对密度概念

状态的不同描述、平面波叠加

$$\Psi(\boldsymbol{x},t)=\frac{1}{\left(\sqrt{2\pi\hbar}\right)^{d}}\int_{-\infty}^{+\infty}c(\boldsymbol{p},t)e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}}d\boldsymbol{p}\,,$$

$$c(\boldsymbol{p},t)=\frac{1}{\left(\sqrt{2\pi\hbar}\right)^{d}}\int_{-\infty}^{+\infty}\Psi(\boldsymbol{x},t)e^{-\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{x}}d\boldsymbol{x}$$

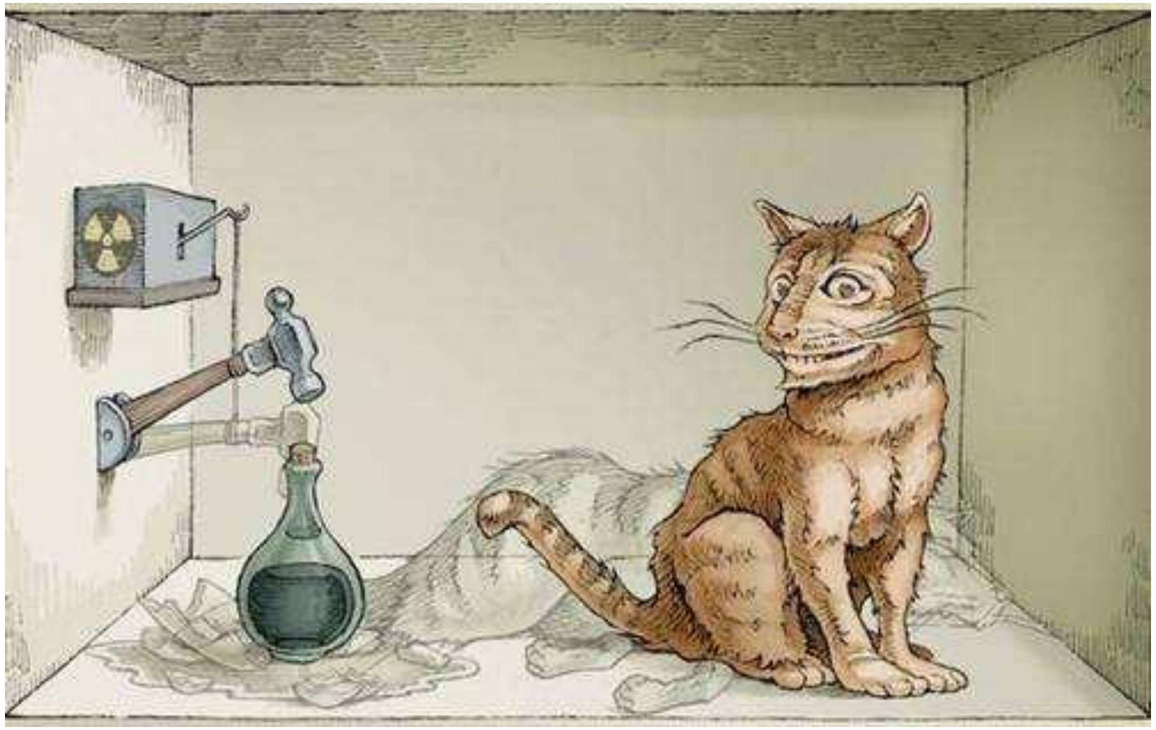
态叠加原理带来的……

状态测量：造成波函数的决定性塌缩

当一个系统开始处于状态ψ时，测量它以查明它是否处于一种状态φ，那么测量后，状态ψ就塌缩到状态φ，测量结果发现系统处于状态φ的概率是$|\varphi^*\psi|^2$.

态叠加原理带来的……

- 一次测量前后的状态
- 二次测量前后的状态



态叠加原理带来的……

测量问题的真实解答是什么？

量子世界中究竟发生了什么？

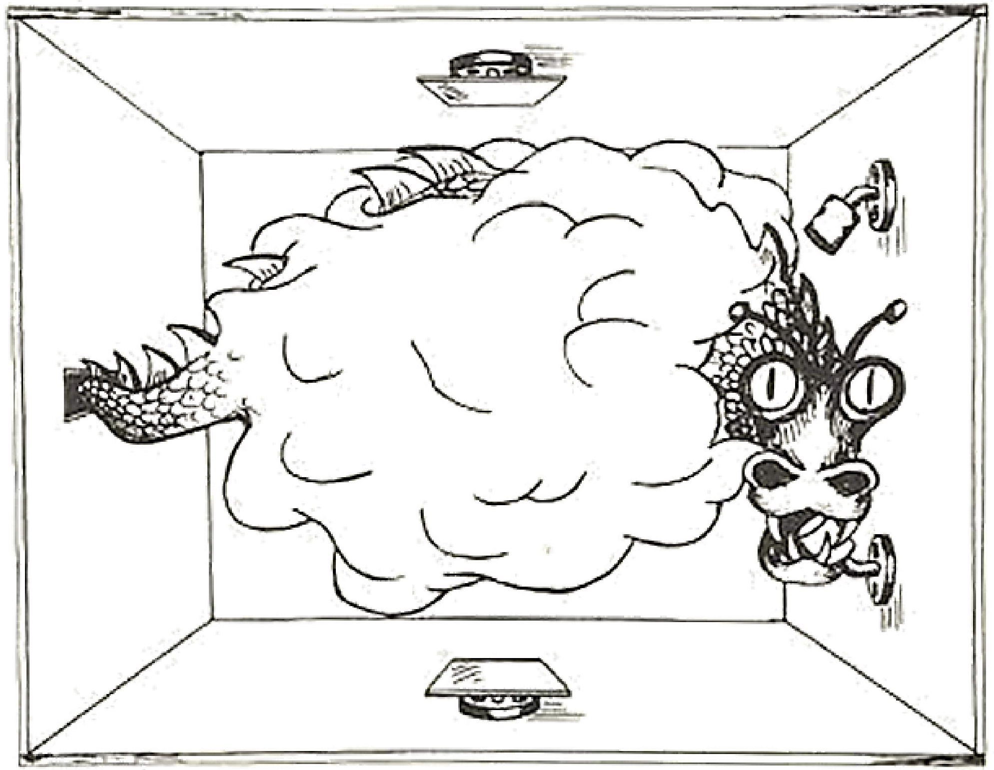
从历史上看，曾经的标准答案应该是——测量问题并不存在，因为在没有人观测的时候问询发生了什么是没有意义的。那些发生在无人观测时候的事是不可观测的，从而谈论不可观测的事也就毫无意义。这种见解被称为量子物理学的“哥本哈根诠释”

态叠加原理带来的……

惠勒：

“任何一种基本量子现象只在其被记录之后才是一种现象”

——“延迟双缝干涉实验”



The song for wave function

The great schrodinger gives an equation;

It has imaginary parameters;

It accurately describes the microscopic world;

Wave functions determine everything in nature;

Born said: It represents the probability of finding a particle;

The expected physical quantities are averaged with it as a weight;

There are statistical fluctuations;

But the system's behavior is unique!

波函数之歌

伟大的薛定谔给出了一个方程;

里面有着虚幻的参数;

准确的描绘了微观世界;

波函数决定了自然界的一切;

玻恩说：它代表了寻找粒子的概率;

期待的物理量都以它作为权重进行平均;

里面有着统计的涨落;

但是系统的行为还是唯一!

例题　将波函数$\psi(x)=e^{-\alpha^2x^2/2}$归一化

解　设归一化因子为C，

则归一化的波函数为$\psi(x)=Ce^{-\alpha^2x^2/2}$, 由

$$\int_{-\infty}^{+\infty}|\Psi|^2dx=1$$

计算积分得$|C|^2=\alpha/\sqrt{\pi}$, $C=(\alpha/\sqrt{\pi})^{1/2}e^{i\delta}$

取$\delta=0$，则归一化的波函数为

$$\psi(x)=Ce^{-\alpha^2x^2/2}e^{-\alpha^2x^2/2}$$

狄拉克说：“量子力学的主要特征是什么？现在我倾向于认为，量子力学的主要特征不是不对易代数，而是波函数（概率幅、几率幅）的存在，波函数的模方是观测到某个量的概率，但此外还有个**相位**，它是模为1的数，其变化不影响模方，但**此相位是极其重要的，它是所有干涉现象的根源，而其物理含义极其隐晦难解。**”

- **1. 5 (Momentum)** Expectation Values

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

$$\hat{H} = i\hbar\frac{\partial}{\partial t}$$

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

$$\langle p\rangle = \ ?$$

- Recall that for the position x, as $|\Psi(x,t)|^2 dx$ gives the probability of finding the particle at $(x, x + dx)$ at time t, the expectation value of the position is:

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

- Similarly, the expectation value for any function f of x is:

$$\langle f(x(t))\rangle = \int_{-\infty}^{+\infty} f(x)|\Psi(x,t)|^2 dx$$

- In particular, the expectation value of the potential energy of the particle is

$$\langle V(x(t))\rangle = \int_{-\infty}^{+\infty} V(x)|\Psi(x,t)|^2 dx$$

Notes: The expectation value is the average of repeated measurements on an ensemble of identical prepared systems, not the average of repeated measurements on one and the same system.

What about other dynamical variables?

$$\langle p \rangle = \int_{-\infty}^{+\infty} p|\Psi(x,t)|^2 dx$$

$$\langle T \rangle = \int_{-\infty}^{+\infty} \frac{p^2}{2m}|\Psi(x,t)|^2 dx$$

Wrong!

– The situation is, however, not as simple. To carry out the integrations, one needs to express *p* in terms of *x* and *t*. But it is *impossible* to do so in quantum mechanics precisely because of the uncertainty principle!

– Thus, we must try a different approach. A natural way is to define

$$\langle p_x \rangle = m \frac{d\langle x \rangle}{dt}$$

– Now x can be written as

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \Psi^* \Psi dx$$

Differentiating this with respect to time t gives

$$\frac{d\langle x \rangle}{dt} = \int_{-\infty}^{+\infty} x \frac{\partial}{\partial t} (\Psi^* \Psi) dx = \int_{-\infty}^{+\infty} x \left(\frac{\partial \Psi^*}{\partial t} \Psi + \Psi^* \frac{\partial \Psi}{\partial t} \right) dx$$

Using the time dependent Schrodinger equation, one gets

$$\frac{d\langle x \rangle}{dt} = \frac{i\hbar}{2m} \int_{-\infty}^{+\infty} x \left(\Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \Psi^*}{\partial x^2} \Psi \right) dx$$

Using integration parts twice on the second term and **the boundary sonditions on $\boldsymbol{\Psi}$ and $\boldsymbol{\frac{\partial \Psi}{\partial x}}$ at infinity**, we obtain

$$\frac{d\langle x\rangle}{dt} = -\frac{i\hbar}{m}\int_{-\infty}^{+\infty} \Psi^* \frac{\partial \Psi}{\partial x} dx$$

Hence,

$$\langle p_x\rangle = -i\hbar \int_{-\infty}^{+\infty} \Psi^* \frac{\partial \Psi}{\partial x} dx = \int_{-\infty}^{+\infty} \Psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \Psi dx = \int_{-\infty}^{+\infty} \Psi^* \hat{p}_x \Psi dx$$

例：证明一维自由粒子的速度v可以表示为

$$v = J/\rho$$

其中，ρ和J分别是一维自由粒子的概率密度和概率流密度。

证明： 一维自由粒子波函数及其复共轭为

$$\Psi(x,t) = Ae^{i/\hbar(px-Et)}, \Psi^*(x,t) = A^*e^{-i/\hbar(px-Et)}$$

则其概率密度和概率流密度分别为

$$\rho = \Psi^*\Psi = A^*A = |\mathrm{A}|^2$$

$$\hat{\mathrm{j}} = \frac{i\hbar}{2m}\left(\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right) = \frac{\mathrm{p}}{\mathrm{m}}|\mathrm{A}|^2 = v\rho$$

What about other dynamical variables?

All such quantities can be written in terms of position and momentum. For examples,

$$T = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

$$\vec{L} = \vec{r} \times \vec{p}$$

- An *observable* is any particle property that can be measured. The position and momentum of a particle are observables, as its kinetic and potential energies.

[Question: Is the wavefunction Ψ an observable?]

- In quantum mechanics, we associate an *operator* Q with each observable Q. Above anaslysis suggests that we identify the expectation value of any observable Q as

$$\langle Q(x,p)\rangle = \int_{-\infty}^{+\infty} \Psi^* \hat{Q}\,(x, -i\hbar\frac{\partial}{\partial x})\Psi dx$$

Problem 1.6, 1.7, 1.8

For the concept of Schrodinger equation

- **Law of probability conservation**
- **Energy conservation law**
- Repeated measurement（可能你会迷糊）
- **Classical mechanics for space average**
- **Classical laws for angular motion**

Law of probability conservation

If the normalization relation $\int \psi^* \psi d^3x = 1$ is interpreted in the sense of probability theory, so that $\psi^* \psi d^3x$ is the probability of finding the particle under consideration in the volume element d^3x, then there must be a conservation law. This is to be derived. How may it be interpreted classically?

Solution: The conservation law sought must have the form of an equation of continuity, $\nabla \cdot \vec{j} + \frac{\partial \rho}{\partial t} = 0$ with $\rho = \psi^* \psi$ the probability density, and $\vec{s}$ the probability current density. As ρ is the bilinear form of ψ and its complex conjugate, from Schrodinger equations

$$H\psi = i\hbar \frac{\partial \psi}{\partial t}; \quad H\psi^* = -i\hbar \frac{\partial \psi^*}{\partial t}$$

we find

$$\psi^* H\psi - \psi H\psi^* = i\hbar \frac{\partial \rho}{\partial t}$$

With the Hamiltonian $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$, we write the left-hand side in the form of a divergence

$$\psi^* H\psi - \psi H\psi^* = -\frac{\hbar^2}{2m}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) = -\frac{\hbar^2}{2m}\nabla(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

So that we may identify

$$\vec{j} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*) = \frac{1}{2m}\left(\psi^*\frac{\hbar}{i}\nabla\psi - \psi\frac{\hbar}{i}\nabla\psi^*\right)$$

Compare with $\psi^* H\psi - \psi H\psi^* = i\hbar\frac{\partial\rho}{\partial t}$,

$$\therefore \nabla\cdot\vec{j} + \frac{\partial\rho}{\partial t} = 0$$

Classical interpretations may be arrived at as follows. If the quantities $\rho\ and\ \vec{J}$ are both multiplied by m, the mass of the particle, we obtain

$$\text{mass density } \rho_m = m\rho \text{ and momentum density } \vec{g} = m\vec{J}$$

the law of mass conservation.

In the same way,

$$\rho_e = e\rho\ ; \vec{j}_e = e\vec{J},$$

it is the law of charge conservation.

It is remarkable that the conservation laws of both mass and charge are essentially identical.

The expression for the total momentum of the Schrodinger field,

$$\vec{p} = \int d^3x\,\vec{g} = m\int d^3x\,\vec{J} = \frac{-i\hbar}{2}\int d^3x\,(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

May by partial integration on the second term be reduced to

$$\vec{p} = \int d^3x\,(\psi^*(-i\hbar\nabla)\psi)$$

Corresponding to its explanation as the expectation value of the momentum operator $\frac{\hbar}{i}\nabla$ in the quantum state ψ.

Energy conservation law

The energy conservation law is of the form $\frac{\partial W}{\partial t} + \nabla \cdot \vec{S} = 0$, with W the energy density and $\vec{S}$ the energy flux vector. Please derived it by constructing the flux vector in quantum mechanics.

Solution: since $\mathrm{E} = \int d^3 x W$, with $\mathrm{W} = \frac{\hbar^2}{2m} (\nabla\psi^* \cdot \nabla\psi) + \psi^* V \psi$, where the first term is the kinetic, the second the potential energy density. We have

$$\dot{\mathrm{W}} = \frac{\hbar^2}{2m} \left(\nabla\dot{\psi}^* \cdot \nabla\psi + \nabla\psi^* \cdot \nabla\dot{\psi}\right) + V(\dot{\psi}^*\psi + \psi^*\dot{\psi})$$

Since $\nabla\dot{\psi}^* \cdot \nabla\psi = \nabla(\dot{\psi}^*\nabla\psi) - \dot{\psi}^*\nabla^2\psi$, $\nabla\psi^* \cdot \nabla\dot{\psi} = \nabla(\dot{\psi}\nabla\psi^*) - \dot{\psi}\nabla^2\psi^*$ then

$$\dot{\mathrm{W}} = \nabla\frac{\hbar^2}{2m}\{\dot{\psi}^*\nabla\psi + \dot{\psi}\nabla\psi^*\} - \frac{\hbar^2}{2m}\dot{\psi}^*\nabla^2\psi - \frac{\hbar^2}{2m}\dot{\psi}\nabla^2\psi^*$$

$$+\dot{\psi}^*V\psi \qquad +\dot{\psi}V\psi^*$$

In the last terms, use of the Schrodinger equation permits us to replace space derivatives

and potential by time derivatives. The resulting terms $\dot{\psi}^*\left(-\frac{\hbar}{\mathrm{i}}\dot{\psi}\right) + \dot{\psi}\left(\frac{\hbar}{\mathrm{i}}\dot{\psi}^*\right) = 0$

exactly cancel so that indeed is of the form of conservation to be proved with

$$\vec{S} = -\frac{\hbar^2}{2m}\{\dot{\psi}^*\nabla\psi + \dot{\psi}\nabla\psi^*\}$$

The energy flux vector.

Repeated measurement

The time-independent Hamiltonian H of a system has eigenvectors $|\nu\rangle$ with non-degenerate eigenvalues $\hbar\omega_\nu$.

Let an observable A be defined by the equally non-degenerate eigenvalue problem $A|n\rangle = a_n|n\rangle$ in the same Hilbert space.

Let the system initially have been in the state $|\nu\rangle$ and then let a measurement of the observable A be performed on this system.

What is the expectation value of A and what is the probability of finding the value a_m of A by this measurement?---If the measurement leads to the value a_m and is them repeated a time interval t later, what is the probability that the value a_m will again be found?

solution: The expectation value of A in the initial state is $\langle v|A|v\rangle$. With the expectations

$|v\rangle = \sum_n |n\rangle\langle n|\,|v\rangle$; $\langle v| = \sum_{n'}\langle v||n'\rangle\langle n'|$, it becomes

$\langle v|A|v\rangle = \sum_{nn'}\langle v||n'\rangle\langle n'|A|n\rangle\langle n|\,|v\rangle$

With $\langle n'|A|n\rangle = a_n\delta_{nn'}$, this simplifies to

$$\langle v|A|v\rangle = \sum_n a_n\langle v|n\rangle^2$$

The probability of finding the value a_m as the result of the first measurement therefore is

$$P_m = |\langle v|m\rangle|^2$$

Afterwards, the system is no longer in the initial state $|\nu\rangle$, but in the state $|m\rangle$.

Its further development follows from the Schrodinger equation $H|t\rangle = i\hbar\frac{\partial}{\partial t}|t\rangle$, where $|t\rangle$ denotes the state vector at time t, with the initial condition $|0>=|m>$.

Since H does not depend on time, this leads to the solution $|t\rangle = e^{-\frac{it}{\hbar}H}|m\rangle$, or if |m> is expanded in eigenfunctions of H, $|m\rangle = \sum_\mu |\mu\rangle\langle\mu|\,|m\rangle$ and using $e^{-\frac{it}{\hbar}H}|\mu\rangle = e^{-i\omega_\mu t}|\mu\rangle$, it leads on to

$$|t\rangle = \sum_\mu e^{-i\omega_\mu t}|\mu\rangle\langle\mu|\,|m\rangle$$

We find that the probability again to measurement a_m at the time t is $P'_m = |\langle m|t\rangle|^2$

With

$$\langle m|t\rangle = \sum_\mu e^{-i\omega_\mu t}|\langle\mu|m\rangle|^2$$

Classical mechanics for space average

The fundamental equation of classical dynamics is Newton's second law

$$\frac{d\vec{p}}{dt} = \vec{F}$$

with $\vec{p}$ the momentum of, and $\vec{F}$ the force acting upon the particle. Please show it still holds for the space averages (expectation values) of the corresponding operators in quantum mechanics.

Solution: If the force $\vec{F}$ derives from a potential, $\vec{F} = -\nabla V$, and momentum is replaced by the operator $\frac{\hbar}{i}\nabla$, them the two space averages are defined by

$$\vec{F} = -\frac{\hbar}{i}\int d^3x\,\psi^{*(}\nabla V)\psi\vec{p} = \frac{\hbar}{i}\int d^3x\,\psi^{*}\nabla\psi$$

since ψ and ψ^* satisfy the Schrodinger equations

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi^* + V(\vec{r})\psi^* = \frac{\hbar}{i}\frac{\partial\psi^*}{\partial t}$$

We get

$$\dot{\vec{p}} = \frac{\hbar}{i}\int d^3x\,(\dot{\psi}^*\nabla\psi + \psi^*\nabla\dot{\psi}) = \frac{\hbar}{i}\int d^3x\,(\dot{\psi}^*\nabla\psi - \dot{\psi}\nabla\psi^*)$$

Where the surface contribution of the partial integration in the last term vanishes and has been omitted. Replacing ψ and ψ^*according to Schrodinger equations, we may proceed to

$$\dot{\vec{p}} = -\frac{\hbar^2}{2m}\int d^3x\,(\nabla^2\psi^*\nabla\psi + \nabla^2\psi\nabla\psi^* + \int d^3x\,(\psi^* V\nabla\psi + V\psi\nabla\psi^*)$$

A partial integration

$$\int d^3x\, \nabla^2\psi^*\nabla\psi = -\int d^3x\, \nabla\psi^*\nabla^2\psi$$

shows that the two terms of the first integral cancel each other out. We perform a partial integration in the last term,

$$\dot{\vec{p}} = \int d^3x\, \psi^*\{V\nabla\psi - \nabla(V\psi)\} = -\int d^3x\, \psi^*(\nabla V)\psi = \vec{F}$$

It is ok.

Classical laws for angular motion

The classical relation between angular momentum $\vec{L} = \vec{r} \times \vec{p}$ and torque $\vec{T} = \vec{r} \times \vec{F}$ is

$$\frac{d\vec{L}}{dt} = \vec{T}$$

please show it still holds for the space averages in quantum mechanics.

Solution: we start by constructing the space averages

$$\vec{L} = \frac{\hbar}{i} \int d^3x\, \psi^* (\vec{r} \times \nabla) \psi$$

$$\vec{T} = -\int d^3x\, \psi^* (\vec{r} \times \nabla V) \psi$$

We begin the proof by differentiating $\vec{L}$

$$\dot{\vec{L}} = \frac{\hbar}{i}\int d^3x\,\{\dot{\psi}^*(\vec{r}\times\nabla)\psi + \psi^*(\vec{r}\times\nabla\dot{\psi})\}$$

In the second term we use the identity

$$\psi^*\nabla\dot{\psi} = \nabla(\psi^*\dot{\psi}) - \nabla\psi^*\dot{\psi}$$

to the first term of which we apply the general vector rule $\int d^3x\,\vec{r}\times\nabla f$=0 with f=$\psi^*\psi$. Thus we arrive at

$$\dot{\vec{L}} = \frac{\hbar}{i}\int d^3x\vec{r}\times(\dot{\psi}^*\nabla\psi - \dot{\psi}\nabla\psi^*)$$

Use the Schrodinger equations, we get

$$\dot{\vec{L}} = -\frac{\hbar^2}{2m}\int d^3x\,\vec{r} \times (\nabla^2\psi^*\nabla\psi + \nabla^2\psi\nabla\psi^*) + \int d^3x\,V\vec{r} \times (\psi^*\nabla\psi + \psi\nabla\psi^*)$$

Now, in the first integral, the bracket $\nabla^2\psi^*\nabla\psi + \nabla^2\psi\nabla\psi^* = \nabla(\nabla\psi \cdot \nabla\psi^*)$ is the gradient of a scaler function, so that this integral vanishes.

In the second integral, the bracket is equal to $\nabla(\psi\psi^*)$. We them use the identity

$$V\nabla(\psi\psi^*) = \nabla(V\psi\psi^*) - \psi\psi^*\nabla V$$

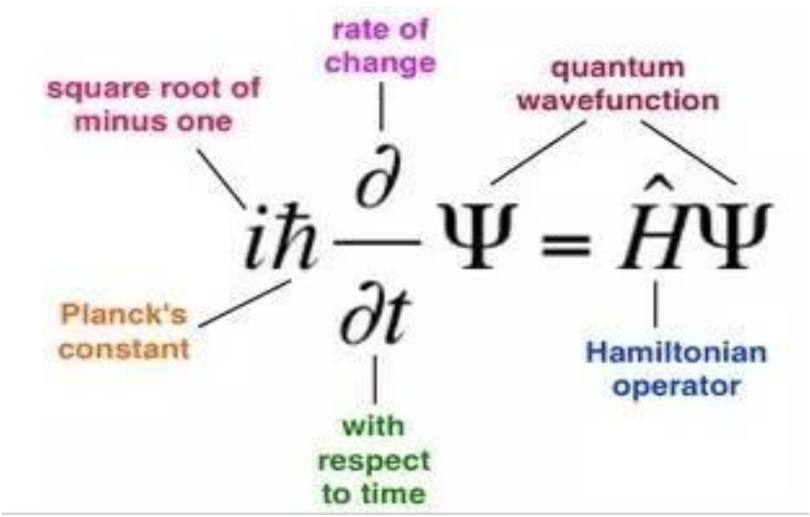
and for

$$f\text{=}V\psi^*\psi,$$

$$\Longrightarrow \int d^3x\,\vec{r} \times [V\nabla(\psi^*\psi)] = -\int d^3x\,\vec{r} \times [\psi^*\psi\nabla V].$$

So it is proved.

Review



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

$$\vec{j} = \frac{\hbar}{2mi}(\psi^* \nabla \psi - \psi \nabla \psi^*)$$

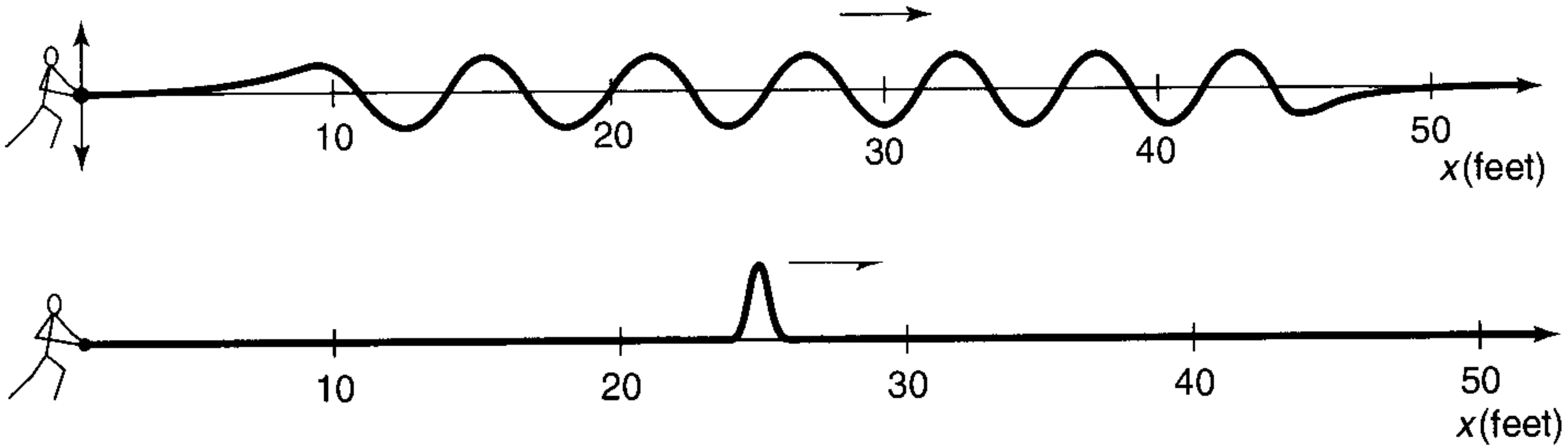
$$\nabla \cdot \vec{j} + \frac{\partial \rho}{\partial t} = 0$$

$$\vec{p} \rightarrow -i\hbar\nabla$$

$$\vec{p} = \int d^3x \left(\psi^* (\frac{\hbar}{i} \nabla) \psi \right)$$

$$\dot{\vec{p}} = \int d^3x \, \psi^* \{ V \nabla \psi - \nabla (V \psi) \} = -\int d^3x \, \psi^* (\nabla V) \psi = \vec{F}$$

1.6 The Uncertainty principle



Heisenberg

Where precisely is the wave? What is its avelength?

To any wave phenomenon, and hence in particular to the quantum mechanical wave function. Now the wavelength of Ψ is related to the momentum of the particle by the de Broglie formula:

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

Thus a spread in wavelength corresponds to a spread in momentum, and our general observation now says that the more precisely determined a particle's position is, the less precisely its momentum is determined. Quantitatively,

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

爱因斯坦(Albert Einstein)在听到维尔纳·海森堡(Werner Heisenberg)在1927年的演讲中宣布他的不确定性原理时表示: **“太棒了，现在的年轻人有这么多想法。可我一个字也不信。”**

Example :

If a **flying speck** of dust (sufficiently small from an everyday point of view) with mass $m \sim 10^{-7}$ kg and velocity in the x-direction $v_x \sim 0.1 ms^{-1}$. We can define this velocity by a standard optical methods with a precision $\Delta v_x \approx 10^{-5} ms^{-1}$, then the unavoidable uncertainty in measurements of the particle's coordinate is $\Delta x \approx h/\Delta p_x = h/m\Delta v_x \approx 10^{-21}$ m.

The size of a speck of dust with mass 0.1 mg depends on the material composing this speck and is of the order of **10^{-5}m.** The uncertainty of measurement of its location (10^{-21} m) **is 16 orders of magnitude less** than its dimensions, and it lies far beyond our possibility to make measurements of a coordinate with such precision. In this case the behavior of the particle is entirely described by **the classical laws of physics**.

For example, in an **electron tube** with an accelerating potential difference $U \sim 10^4$ V, an electron acquires momentum $p = (2m_e eU)^{1/2} \approx 5.4 \times 10^{-23}$ kgms^{-1}. This momentum is directed along the tube's axis.

The diameter of the focused beam can reach values of $d \approx 10^{-5}$m. This magnitude defines the uncertainty in the electron's position on the screen.

According to the uncertainty relations the electron has non-controllable momentum in the transverse direction $\Delta p_{\perp} \approx h/d \approx 10^{-29}$ kgms^{-1}.

Since $\Delta p_{\perp}/p << 1$ **the motion of the electron follows a specific trajectory and can be described by the laws of classical physics.**

For **the electron in a hydrogen atom** the radius of the first Bohr orbit is equal to $r \approx 5 \times 10^{-11}$ m.

the magnitude of the electron's momentum: $\mathbf{p} = e(k_e m_e/r)^{1/2} \approx 2 \times 10^{-24}$ kg ms^{-1}.

Since the electron is localized in an atom, the uncertainty of its coordinate is equal to the dimension of an atom, i.e., $\Delta r \approx 2r$. The corresponding uncertainty of momentum is $\mathbf{\Delta p} \approx h/\Delta r \approx 6.6 \times 10^{-24}$ kgms^{-1}.

The uncertainty of momentum, Δp, is comparable to the magnitude of the momentum, p. Thus, the laws of classical physics cannot describe the behavior of such a particle and it is necessary to apply the quantum approach instead.

We can say since $\Delta x \geq h/\ \ p_x \geq h/p_x = \lambda_{Br}$. This means that the notion of a particle’s trajectory can be used only when the uncertainty of its coordinate is small compared with the characteristic dimension of the region where it moves, i.e., $\Delta x \ll L$. Therefore, the condition for correctness of the classical description of a particle’s behavior is $\lambda_{Br} \ll L$. When the size of the region, L, becomes of the order ofλ_{Br} the quantum effects cannot be neglected.

Homework

- Problem 1.11
- Problem 1.12
- Problem 1.14
- Problem 1.15
- Problem 1.16
- Problem 1.17
- Problem 1.18