Pázmány Péter Catholic University
Faculty of Information Technology and Bionics

"Fides et Ratio"

Physics of Information Technology II
Physics of Molecular Bionics II
2014 Autumn

Lecture 4
Stern-Gerlach Experiment
P.A.M. Dirac's „bra" and „ket" Notation
Hilbert space
Ket Space, Bra Space, Inner product
Operators
Base Kets and Matrix Representation

How electrons behave in magnetic field?

Stern Gerlach Experiment

Electron possesses magnetic „spin” – which is „quantized”

For electrons spin can only take on two values:

up ↑ or down ↓

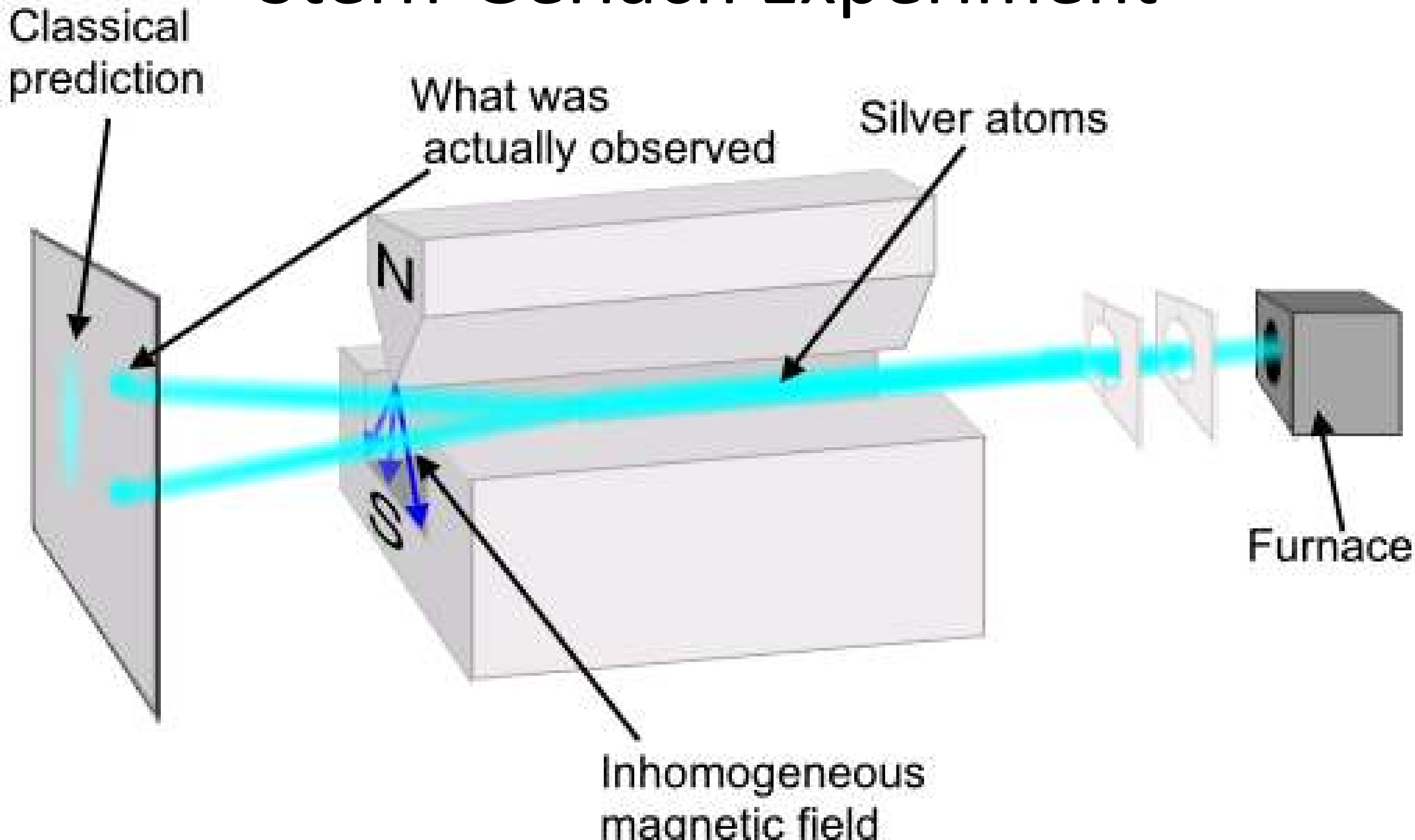
One can measure spin along any axis, spin will be found aligned or anti-aligned with the axis you measure along.

Spin along orthogonal axes obeys
Heisenberg uncertainty principle:

$$s_x s_z \geq \hbar / 2; \quad s_y s_z \geq \hbar / 2; \quad s_x s_y \geq \hbar / 2$$

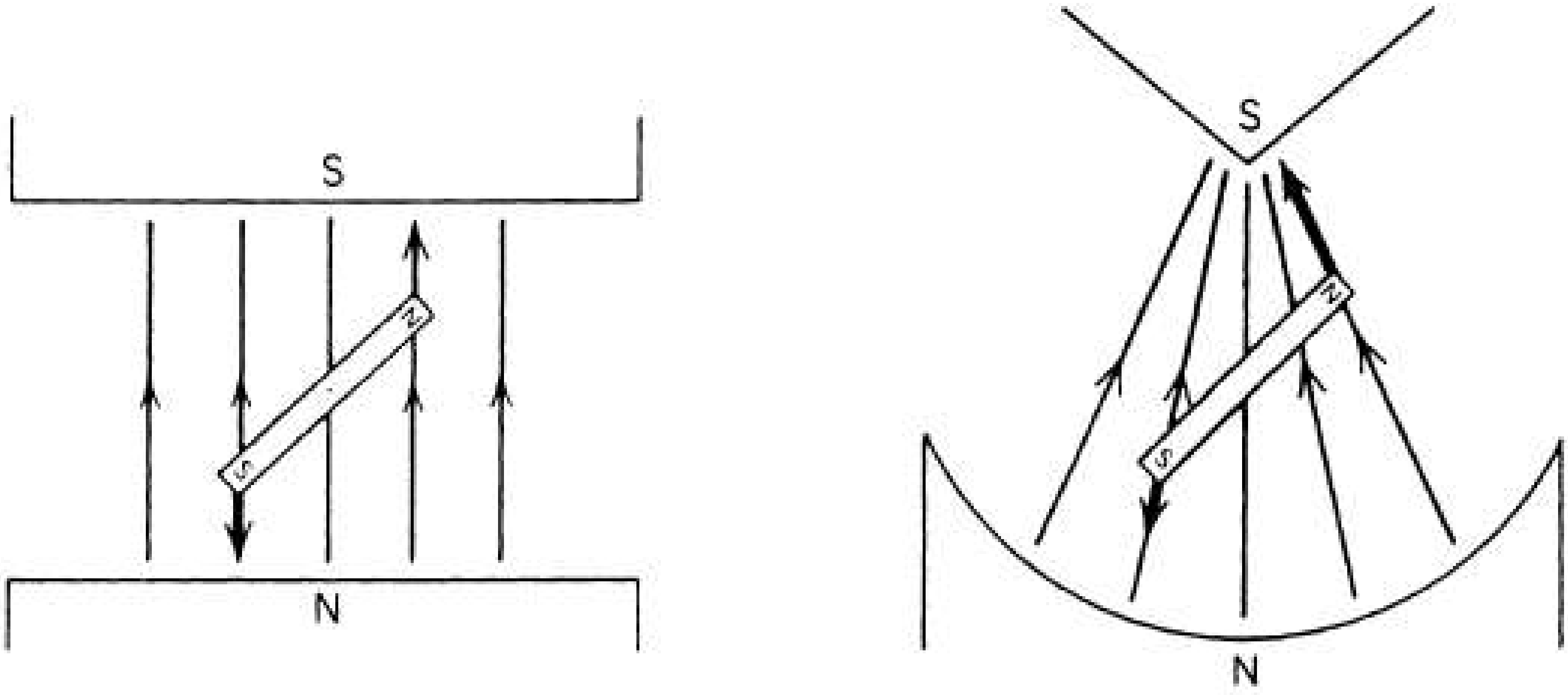
State of definite spin in x direction →
50/50 superposition of up and down in z direction

Stern-Gerlach Experiment



Ag: $\underbrace{1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 4d^{10}}\ 5s^1$

Number of electrons $46 \quad + \quad 1 \quad = 47$

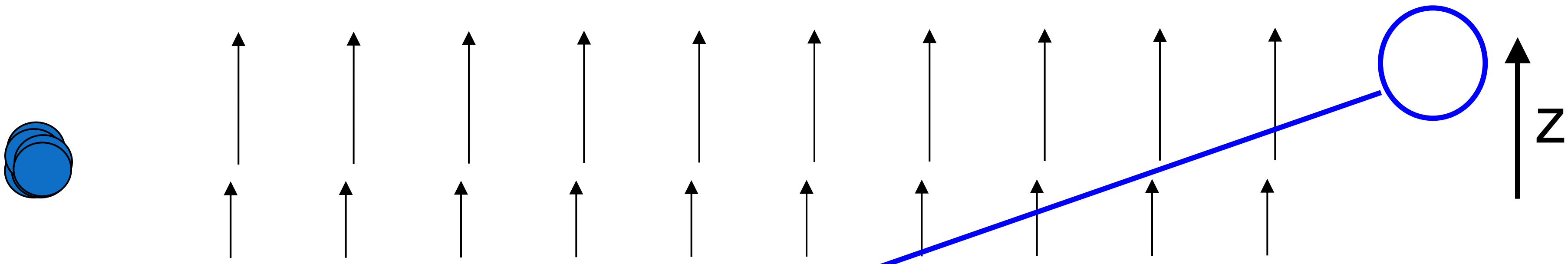


(a) (b)

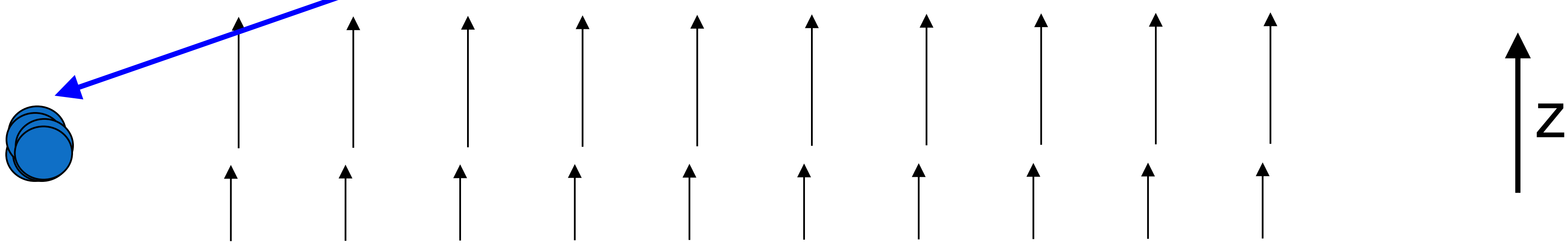
$$W_M = -\bar{\mu} \cdot \bar{B}$$

$$F_z = -\frac{\partial W_M}{\partial z} = \mu \cdot \frac{\partial B}{\partial z} \cos\alpha$$

Put atoms in inhomogeneous magnetic field pointing in z direction – split in two groups – spin up and spin down

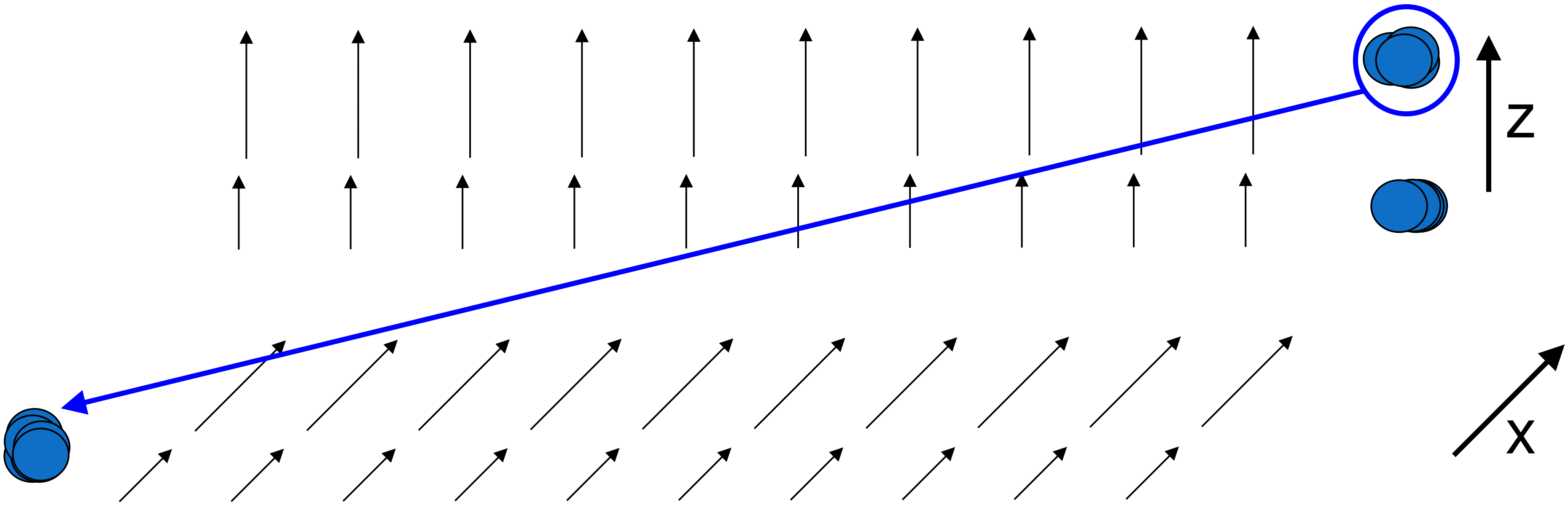


What if I take just atoms that went up, and send them through another, identical magnetic field – What happens?



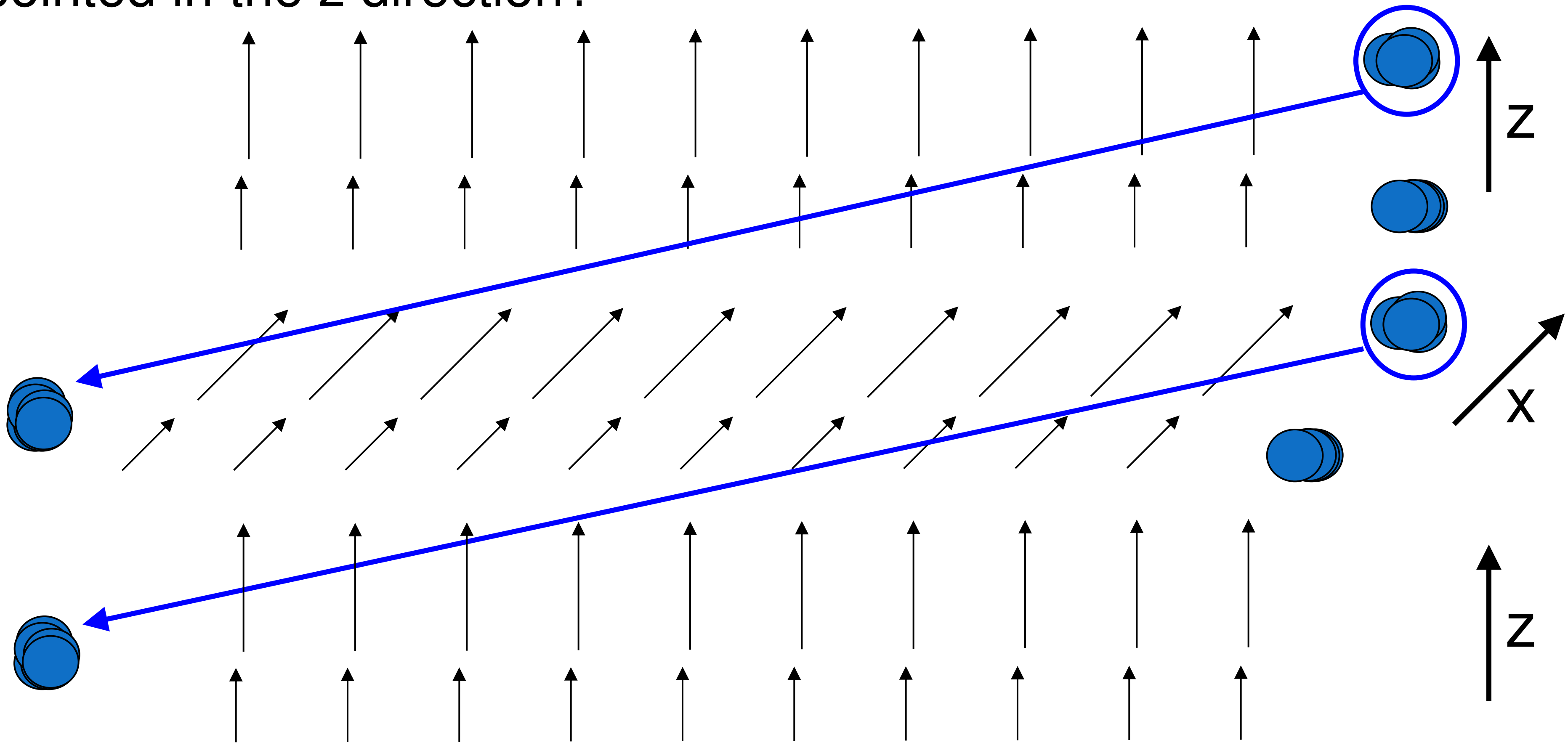
All go up (+z)

Second Experiment: What if I take just atoms that went up, and send them through a magnetic field pointed in the x direction – <u>perpendicular</u> to first field (pointing into the screen)?

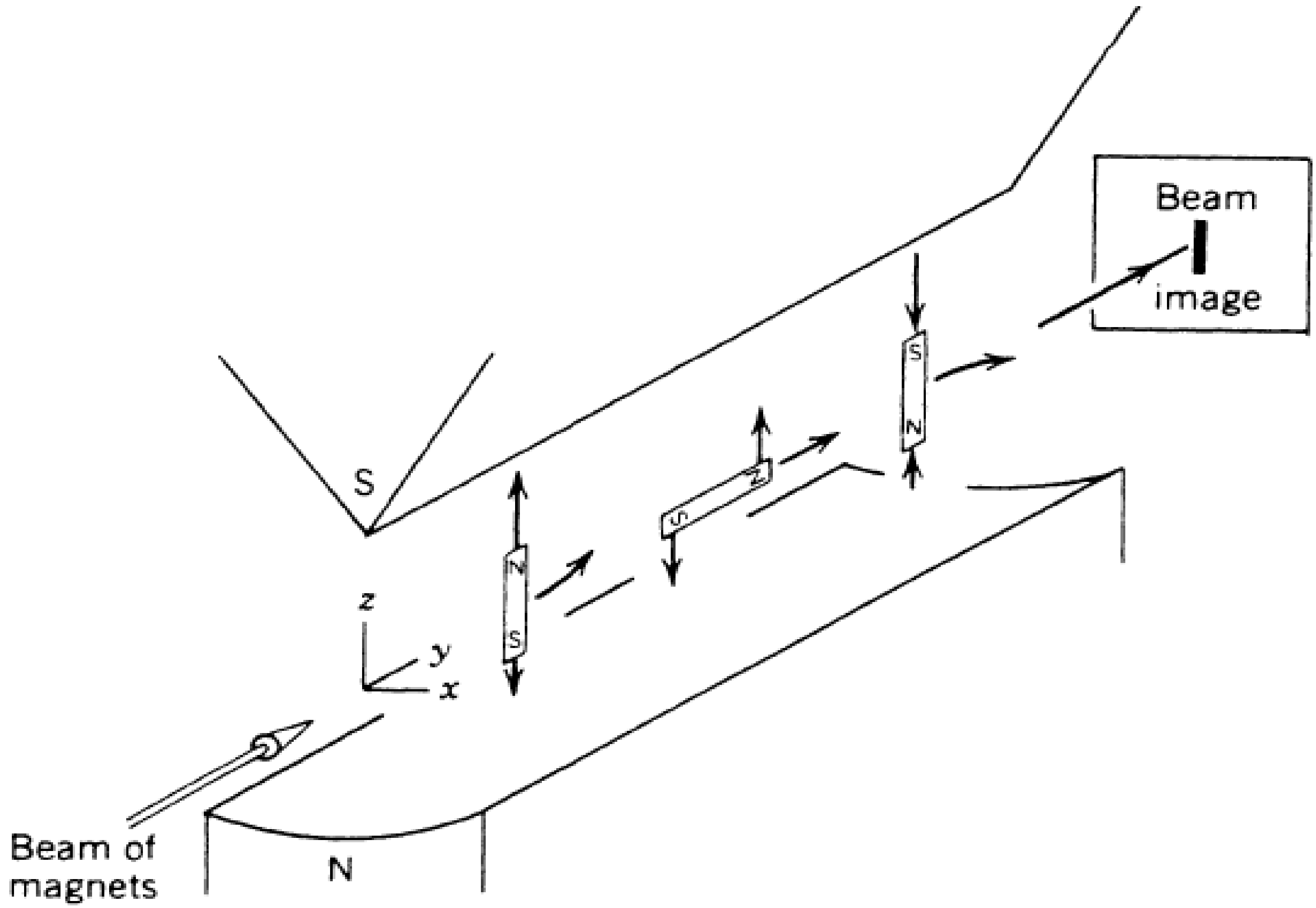


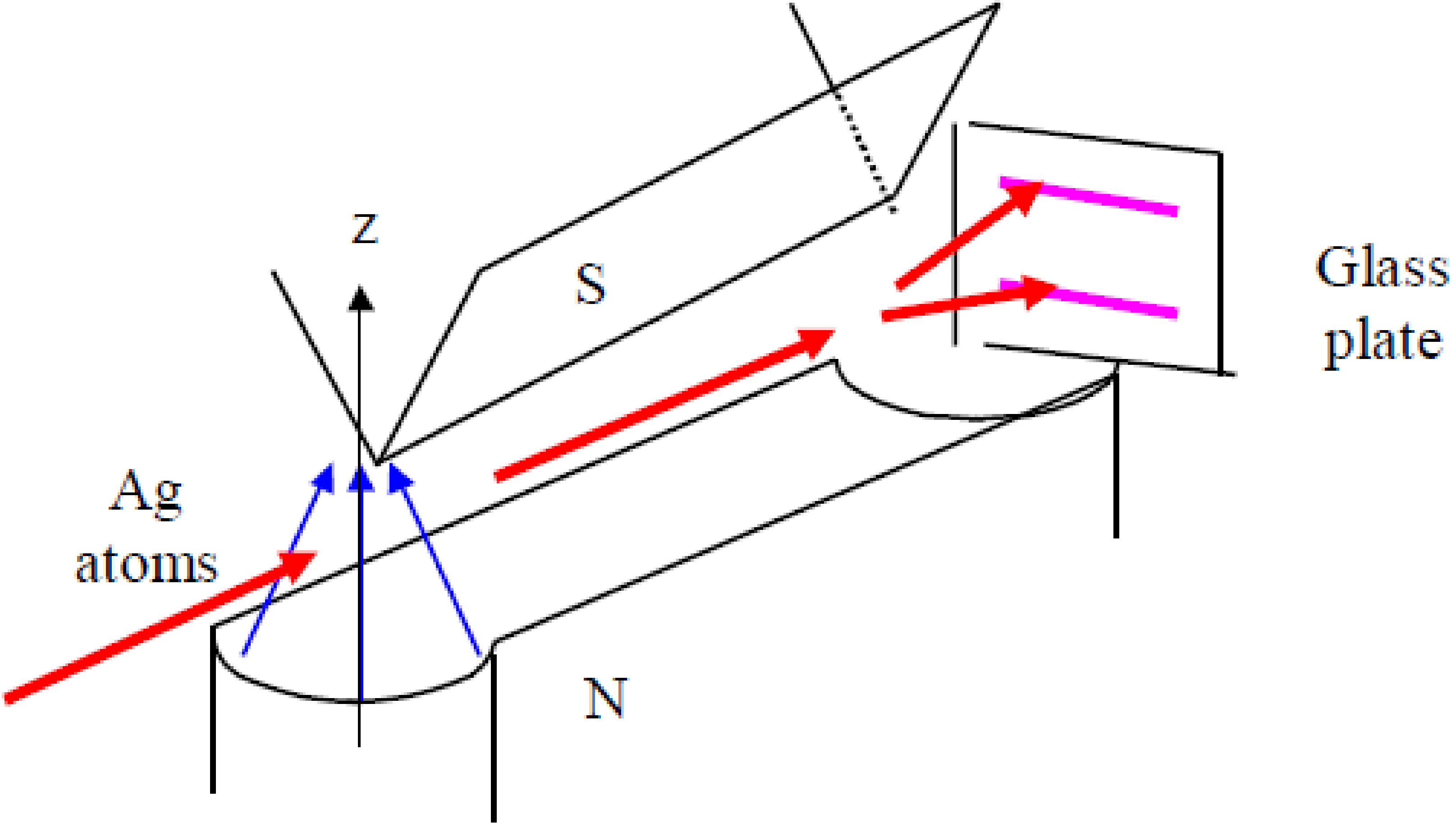
Half go into the screen (+x), half go out of the screen (–x)

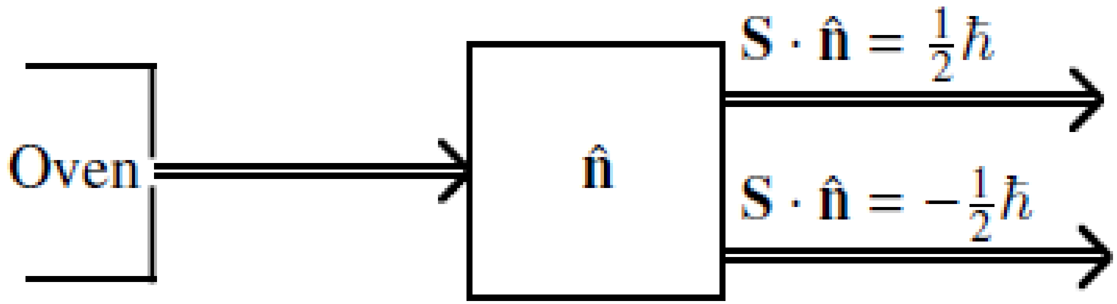
Third Experiment: Take just the atoms that went in +x direction in second experiment, and send them through a third magnetic field, pointed in the z direction?



Half go up (+z), half go down (–z).


Beam
image
S
z
y
x
N
S
S
N
S
N
N
Beam of
magnets
N

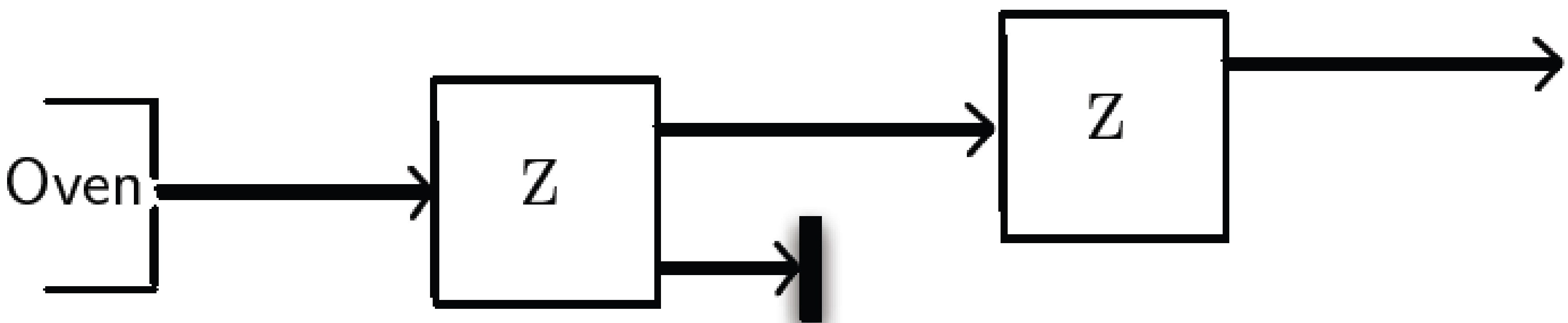

z
S
Glass
plate
Ag
atoms
N

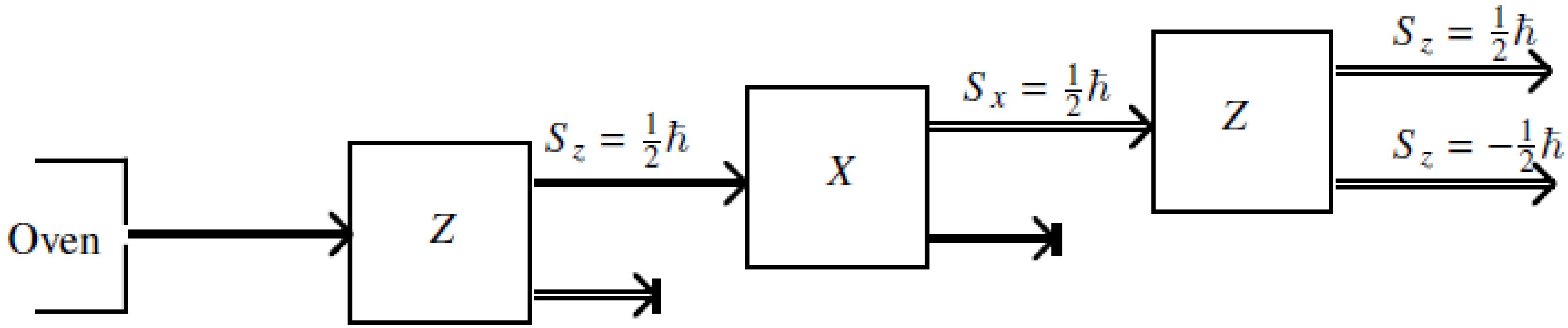


$$+\frac{1}{2}\hbar; \quad -\frac{1}{2}\hbar$$

Two state quantum system

Spin +z, Spin – z





Analogy: Polarized Light
(Classical)

Two dimensional abstract vector space with complex coefficients

P.A.M. Dirac's „bra" and „ket" Notation

Information we can know about a state

In quantum physics a ***physical state*** is represented by a ***state vector i***n a complex vector space, called ***Hilbert space***.

We call the state vector a ***„ket",*** and denote it by $\left|\alpha\right\rangle$

(This state ket is postulated to contain complete information about the physical state. Everything we are allowed to ask about the state is contained in the ket.)

Two kets can be added, and can be multiplied by a complex number, and the result is also a ket

$$\left|\alpha\right\rangle + \left|\beta\right\rangle = \left|\gamma\right\rangle \qquad \lambda\left|\alpha\right\rangle = \left|\alpha\right\rangle\lambda$$

Null ket $\lambda\left|\alpha\right\rangle$ if $\lambda = 0$

$|\alpha\rangle$ and $\lambda|\alpha\rangle$, with $\lambda \neq 0$, represent the same physical state.

(Only the „direction" in vector space is of significance. We are dealing with rays rather than vectors .)

The state space of quantum physics is the Hilbert space

$$|a\rangle, |b\rangle \in \mathscr{H} \quad |a\rangle + |b\rangle = |c\rangle \in \mathscr{H}; \quad \lambda|a\rangle \in \mathscr{H} \quad \lambda \text{ complex number}$$

The dimension of the vector space depends on the physical system (Spin : 2; Finite dim.: *n*; Bounded: countable infinite; Free: continuously infinite)

Observable is represented by a linear operator

The operator acts on the ket from left, and maps a ket on a ket.

$$\hat{\mathbf{A}} \cdot \left(|a\rangle\right) = \hat{\mathbf{A}}|a\rangle \in \mathscr{H}$$

In general $\hat{\mathbf{A}}\left|a\right\rangle \neq c \cdot \left|a\right\rangle$, but there are such kets

$$\hat{\mathbf{A}}\left|a^{(n)}\right\rangle = a^{(n)} \cdot \left|a^{(n)}\right\rangle$$

$$\left|a^{(1)}\right\rangle, \left|a^{(2)}\right\rangle, \ldots, \left|a^{(\mathrm{n})}\right\rangle, \ldots \text{"eigen-kets"}$$

$$a^{(1)}, a^{(2)}, \ldots, a^{(\mathrm{n})}, \ldots \text{eigenvalues of operaot } \hat{\mathbf{A}}$$

In an N-dimensional vector space every ket can be expressed as

$$\left|a\right\rangle = \sum_{n} c_n \left|a^{(n)}\right\rangle$$

Dirac's „bra"-space and „ket"-space

$$\text{Ket} \quad |a\rangle \qquad \text{Bra} \quad \langle a| \qquad\qquad \forall |a\rangle \Leftrightarrow \langle a|$$

The „bra"-space is the „dual vector space" of the ket-space

Rules of duality $|a\rangle \Leftrightarrow \langle a|; \quad |a\rangle + |b\rangle \Leftrightarrow \langle a| + \langle b|;$

$$c_a |a\rangle + c_b |b\rangle \Leftrightarrow c_a^* \langle a| + c_b^* \langle b|$$

Eigen-kets and their dual eigen-bras

$$\left\{ \left| a^{(\mathrm{n})} \right\rangle \right\} \Leftrightarrow \left\{ \left\langle a^{(\mathrm{n})} \right| \right\}$$

The Hilbert space is a linear vector space over the complex numbers, in which the scalar product of the elements exist.

Definition of the scalar product of a bra and a ket

$$\langle b|a\rangle = \text{number (in general complex), for which } \langle b|a\rangle = \langle a|b\rangle^{*}$$

Scalar product is a „**bra**c**ket**"

$$\langle a|a\rangle = \text{real number};\quad \langle a|a\rangle \geq 0;\quad \text{If } \langle a|a\rangle = 0 \rightarrow \langle a| \text{ null ket}$$

To kets are orthogonal

$$|a\rangle \perp |b\rangle \quad \text{if} \quad \langle a|b\rangle = 0$$

Normalized ket:

$$|\bar{a}\rangle = \frac{1}{\sqrt{\langle a|a\rangle}}|a\rangle \quad \rightarrow \langle \bar{a}|\bar{a}\rangle = 1$$

Bra	Ket	Bra-ket	Operator
$\langle b\vert$	$\vert a\rangle$	$\langle b\vert a\rangle$	$\hat{\text{A}}$

Operators $\hat{\mathbf{X}}, \hat{\mathbf{Y}}, \hat{\mathbf{Z}}, \ldots \qquad \hat{\mathbf{A}}, \hat{\mathbf{B}}, \hat{\mathbf{C}}, \ldots$

$$\hat{\mathbf{X}} = \hat{\mathbf{Y}} \quad \text{if} \quad \hat{\mathbf{X}}|a\rangle = \hat{\mathbf{Y}}|a\rangle \quad \text{for} \ \forall|a\rangle$$

$$\text{null operator if} \ \hat{\mathbf{X}}|a\rangle = 0 \quad \text{for} \ \forall|a\rangle$$

$$\hat{\mathbf{X}} + \hat{\mathbf{Y}} = \hat{\mathbf{Y}} + \hat{\mathbf{X}}; \quad \hat{\mathbf{X}} + \left(\hat{\mathbf{Y}} + \hat{\mathbf{Z}}\right) = \left(\hat{\mathbf{X}} + \hat{\mathbf{Y}}\right) + \hat{\mathbf{Z}}$$

Linear Operators

$$\hat{\mathbf{X}}\left(c_a|a\rangle + c_b|b\rangle\right) = c_a\hat{\mathbf{X}}|a\rangle + c_b\hat{\mathbf{X}}|b\rangle$$

An operator acts on a bra from right, and maps a bra on a bra. $\langle a|\hat{\mathbf{X}}$

$\hat{\mathbf{X}}|a\rangle$ és $\langle a|\hat{\mathbf{X}}$ in general are not dual

$\hat{\mathbf{X}}^\dagger$ is the adjoint of $\hat{\mathrm{X}}$ if $\hat{\mathbf{X}}|a\rangle$ and $\langle a|\hat{\mathbf{X}}^\dagger$ are dual

If $\hat{\mathbf{X}} = \hat{\mathbf{X}}^\dagger$ then they are self-adjoint (Hermitian)

Products of Operators In general $\hat{\mathbf{X}}\hat{\mathbf{Y}} \neq \hat{\mathbf{Y}}\hat{\mathbf{X}}$;

$$\left(\hat{\mathbf{X}}\hat{\mathbf{Y}}\right)^\dagger = \hat{\mathbf{Y}}^\dagger\hat{\mathbf{X}}^\dagger; \qquad \hat{\mathbf{X}}\left(\hat{\mathbf{Y}}\hat{\mathbf{Z}}\right) = \left(\hat{\mathbf{X}}\hat{\mathbf{Y}}\right)\hat{\mathbf{Z}} = \hat{\mathbf{X}}\hat{\mathbf{Y}}\hat{\mathbf{Z}}$$

$$\hat{\mathbf{X}}\left(\hat{\mathbf{Y}}|a\rangle\right) = \left(\hat{\mathbf{X}}\hat{\mathbf{Y}}\right)|a\rangle = \hat{\mathbf{X}}\hat{\mathbf{Y}}|a\rangle; \quad \langle b|\hat{\mathbf{X}}\hat{\mathbf{Y}} = \langle b|\hat{\mathbf{X}}\left(\hat{\mathbf{Y}}\right) = \left(\langle b|\hat{\mathbf{X}}\right)\hat{\mathbf{Y}}$$

‚Outer' product $|a\rangle\langle b|$

Associative rules of products

Legal and illegal products between kets, bras and operators

$$\big(|a\rangle\langle b|\big)|c\rangle = |a\rangle\big(\langle b|c\rangle\big); \quad \langle b|c\rangle \ \text{complex number} \rightarrow |a\rangle\langle b|c\rangle \ \text{ket}$$

$$\text{But} \quad \big(\langle b|c\rangle\big)\cdot|a\rangle \ \text{would be illegal} \quad \langle b|\big(|c\rangle|a\rangle\big)$$

$$\hat{\mathbf{X}} = |a\rangle\langle b| \rightarrow \hat{\mathbf{X}}^{\dagger} = |b\rangle\langle a|$$

$$\langle a|\cdot\big(\hat{\mathbf{X}}|b\rangle\big) = \big(\langle a|\hat{\mathbf{X}}\big)\cdot|b\rangle \qquad \langle a|\mathbf{X}|b\rangle$$

$$bra \times ket \qquad\qquad bra \times ket$$

Two sides are equal, thus we can introduce a more concise notation

$$\langle a|\cdot\big(\hat{\mathbf{X}}|b\rangle\big) = \big(\langle a|\hat{\mathbf{X}}\big)\cdot|b\rangle = \langle a|\hat{\mathbf{X}}|b\rangle$$

For a self-adjoint (Hermitian) operator

$$\langle b | \hat{\mathbf{X}} | a \rangle = \langle a | \hat{\mathbf{X}} | b \rangle^*$$

$$\langle b | \mathbf{X} | a \rangle = \langle b | \cdot \left(\mathbf{X} | a \rangle \right) = \left[\left(\langle a | \mathbf{X}^\dagger \right) \cdot | b \rangle \right]^* = \langle a | \mathbf{X}^\dagger | b \rangle^*$$

Matrix representation of kets bras and operators

In quantum physics the mathematical representation of observables are linear self-adjoint operators

Lemma 1. Eigenvalues of self-adjoint operators are real numbers. The eigen-kets belonging to different eigenvalues are orthogonal.

$$\hat{\mathbf{A}}\left|a^{(n)}\right\rangle = a^{(n)} \cdot \left|a^{(n)}\right\rangle \qquad a^{(1)}, a^{(2)}, ..., a^{(\mathrm{n})}, ...\text{eigenvalues of } \hat{\mathbf{A}}$$

$$\left|a^{(1)}\right\rangle, \left|a^{(2)}\right\rangle, ..., \left|a^{(\mathrm{n})}\right\rangle, ...\text{"eigen} - \text{kets"}$$

$$\left\langle a^{(i)} \middle| a^{(j)} \right\rangle = \delta_{ij}$$

Lemma 2. Eigen-kets constitute a complete orthonormal basis.

$$\left|a\right\rangle = \sum_n c^{(n)} \left|a^{(n)}\right\rangle \qquad c^{(n)} = \left\langle a^{(n)} \middle| a\right\rangle$$

$$\left|a\right\rangle = \sum_n \left|a^{(n)}\right\rangle\left\langle a^{(n)} \middle| a\right\rangle \qquad \sum_n \left|a^{(n)}\right\rangle\left\langle a^{(n)}\right| = \mathbf{1}$$

$$\left\langle a \middle| a\right\rangle = \left\langle a \middle| \sum_n \left|a^{(n)}\right\rangle\left\langle a^{(n)}\right| \right\rangle \left|a\right\rangle = \sum_n \left|\left\langle a^{(n)} \middle| a\right\rangle\right|^2$$

If $\left|a\right\rangle$ is normalized, then $\sum_n \left|c_n\right|^2 = \sum_n \left|\left\langle a^{(n)} \middle| a\right\rangle\right|^2 = 1$

Projection operator $\hat{\Lambda}_{a^{(n)}} = \left| a^{(n)} \right\rangle \left\langle a^{(n)} \right|$

$$\hat{\Lambda}_{a^{(n)}} \left| a \right\rangle = \left| a^{(n)} \right\rangle \left\langle a^{(n)} \middle| a \right\rangle = c_{a^{(n)}} \left| a^{(n)} \right\rangle \qquad \sum_n \hat{\Lambda}_{a^{(n)}} = \hat{1} \quad \text{(Completeness)}$$

If N is the dimension of the space of kets, the representation of operator **X**

$$\hat{\mathbf{X}} = \hat{\mathbf{X}} \rightarrow \hat{\mathbf{X}} = \left(\sum_{n=1}^{N} \left| a^{(n)} \right\rangle \left\langle a^{(n)} \right| \right) \hat{\mathbf{X}} \left(\sum_{m=1}^{N} \left| a^{(m)} \right\rangle \left\langle a^{(m)} \right| \right) =$$

$$= \sum_{m=1}^{N} \sum_{n=1}^{N} \left| a^{(m)} \right\rangle \left\langle a^{(m)} \right| \mathbf{X} \left| a^{(n)} \right\rangle \left\langle a^{(n)} \right|$$

$\left\langle a^{(m)} \right| \mathbf{X} \left| a^{(n)} \right\rangle$ N^2 number; $\left\langle a^{(m)} \right|$ is a row vector;

$\left| a^{(n)} \right\rangle$ is a column vector

$$\hat{\mathbf{X}} = \begin{bmatrix} \langle a^{(1)} | \hat{\mathbf{X}} | a^{(1)} \rangle & \langle a^{(1)} | \hat{\mathbf{X}} | a^{(2)} \rangle & \ldots & \langle a^{(1)} | \hat{\mathbf{X}} | a^{(N)} \rangle \\ \langle a^{(2)} | \hat{\mathbf{X}} | a^{(1)} \rangle & \langle a^{(2)} | \hat{\mathbf{X}} | a^{(2)} \rangle & \ldots & \langle a^{(2)} | \hat{\mathbf{X}} | a^{(N)} \rangle \\ \ldots & \ldots & & \ldots \\ \langle a^{(N)} | \hat{\mathbf{X}} | a^{(1)} \rangle & \langle a^{(N)} | \hat{\mathbf{X}} | a^{(2)} \rangle & \ldots & \langle a^{(N)} | \hat{\mathbf{X}} | a^{(N)} \rangle \end{bmatrix}$$

$$|b\rangle = \hat{\mathbf{X}} |a\rangle$$

$$|a\rangle = \sum_n |a^{(n)}\rangle \langle a^{(n)} | a \rangle$$

$$|b\rangle = \sum_n |a^{(n)}\rangle \langle a^{(n)} | b \rangle$$

$$|a\rangle = \begin{bmatrix} \langle a^{(1)} | a \rangle \\ \langle a^{(2)} | a \rangle \\ \ldots \\ \langle a^{(N)} | a \rangle \end{bmatrix}; \quad |b\rangle = \begin{bmatrix} \langle a^{(1)} | b \rangle \\ \langle a^{(2)} | b \rangle \\ \ldots \\ \langle a^{(N)} | b \rangle \end{bmatrix};$$

Observables – physical quantities which can be measured

A „strong" measurement always causes the system to jump into an eigen-state of the dynamical variable that is being measured.

Before the measurement $\left|a\right\rangle = \sum_n \left|a^{(n)}\right\rangle\left\langle a^{(n)}\middle|a\right\rangle$

After the measurement $\left|a\right\rangle \Longrightarrow \left|a^{(n)}\right\rangle$

For example, a silver atom spin orientation will change into either $\left|S_z +\right\rangle$ or $\left|S_z -\right\rangle$ when subjected to a Stern-Gerlach apparatus of type SGz

Measurement, in general, changes the state. The only exception is when the state is already in one of the eigen-states of the observable being measured.

$$\left|a^{(n)}\right\rangle \Longrightarrow \left|a^{(n)}\right\rangle$$

Probability that $\left|a\right\rangle$ goes into state $\left|a^{(n)}\right\rangle$

$$\left|c_n\right|^2 = \left|\left\langle a^{(n)} \middle| a\right\rangle\right|^2$$

Expectation value of a measurement

$$\left\langle \hat{\mathbf{A}} \right\rangle = \left\langle a \middle| \hat{\mathbf{A}} \middle| a \right\rangle$$

Position $\mathbf{x}\left|x'\right\rangle = x'\cdot\left|x'\right\rangle$ $\left|a\right\rangle = \int_{-\infty}^{\infty}\left|x'\right\rangle\left\langle x'\middle|a\right\rangle \mathrm{d}x'$

Measurement of the position

The detector clicks if the object is at the position, thus its state is $\left|x'\right\rangle$ $\left|a\right\rangle \to \left|x'\right\rangle$

$$\left|a\right\rangle = \int_{-\infty}^{\infty}\left|x'\right\rangle\left\langle x'\middle|a\right\rangle \mathrm{d}x' \to \text{measurement} \to$$

$$\to \int_{x'-\Delta/2}^{x'+\Delta/2}\left|x'\right\rangle\left\langle x'\middle|a\right\rangle \mathrm{d}x' \approx \left|\left\langle x'\middle|a\right\rangle\right|^2 (\mathrm{d}x')_\Delta$$

$$\left\langle a\middle|a\right\rangle = \int_{-\infty}^{\infty}\left\langle a\middle|x'\right\rangle\left\langle x'\middle|a\right\rangle \mathrm{d}x' = 1$$

The wave-function of physical state $\left|a\right\rangle$ is $\left\langle x'\middle|a\right\rangle = \psi_a\left(x'\right)$

Momentum The operator of momentum is $\mathbf{p}_{\mathbf{x}'} = -\mathrm{j}\hbar\dfrac{\partial}{\partial x'}$